Electronic Supplementary Material (ESI) for Catalysis Science & Technology.
This journal is © The Royal Society of Chemistry 2021

Electronic Supplementary Material: Exploring the Adsorption Site Coordination as a Strategy to Tune Copper Catalysts for CO_2 Electro-reduction.

Lucas G. Verga,* Paulo C. D. Mendes,* Vivianne K. Ocampo-Restrepo,* and Juarez L. F. Da Silva*

São Carlos Institute of Chemistry, University of São Paulo, P.O. Box 780, 13560-970, *São Carlos, SP, Brazil*

E-mail: lucas.gverga@gmail.com; paulaocdm@gmail.com; vivianne.o.restrepo@gmail.com; juarez_dasilva@iqsc.usp.br

Contents

1 Generalized Coordination Number **S-3**

2 Theoretical Approach Details **S-4**

2.1 Employed Surface Models S-4

2.2 Computational Hydrogen Electrode S-5

2.3 Energetic Analyses: Additional Details S-6

2.4 Selection of Potential-Determining Steps S-7

3 Isolated Cu surfaces and nanoparticles **S-8**

4 CO_2 Adsorption on Cu Surfaces **S-11**

5 Adsorption of CO_2 Reduction Intermediates S-14

5.1 COOH Adsorption S-15

5.2 HCOO Adsorption S-17

5.3 CO Adsorption S-19

5.4 COH Adsorption S-21

5.5 CHO Adsorption S-23

5.6 OH Adsorption S-27

5.7 H Adsorption S-28

6 Adsorption of CO_2 reduction intermediates used for validation S-30

6.1 COOH Adsorption S-30

6.2 HCOO Adsorption S-31

6.3 CO Adsorption S-32

6.4 COH Adsorption S-36

6.5 CHO Adsorption S-37

6.6 OH Adsorption S-38

6.7 H Adsorption S-41

7 Vibrational and solvation corrections S-42

8 Binding energies versus generalized coordination number S-43

9 Impact of solvation models S-47

10 Analysis of other Cu nanoparticle models S-49

11 Atomic coordinates for the adsorption of CO_2 reduction intermediates S-51

11.1 *COOH Adsorption S-51

11.2 *HCOO Adsorption S-94

11.3 *CO Adsorption S-116

11.4 *COH Adsorption S-211

11.5 *CHO Adsorption S-248

11.6 *OH Adsorption S-305
11.7 *H Adsorption S-388
11.8 *CO_2 Adsorption S-412

References **S-457**

1 Generalized Coordination Number

Figure S1 illustrates the procedure to calculate the generalized coordination number, $GCN(i)$,[1,2] for a given adsorption site i.

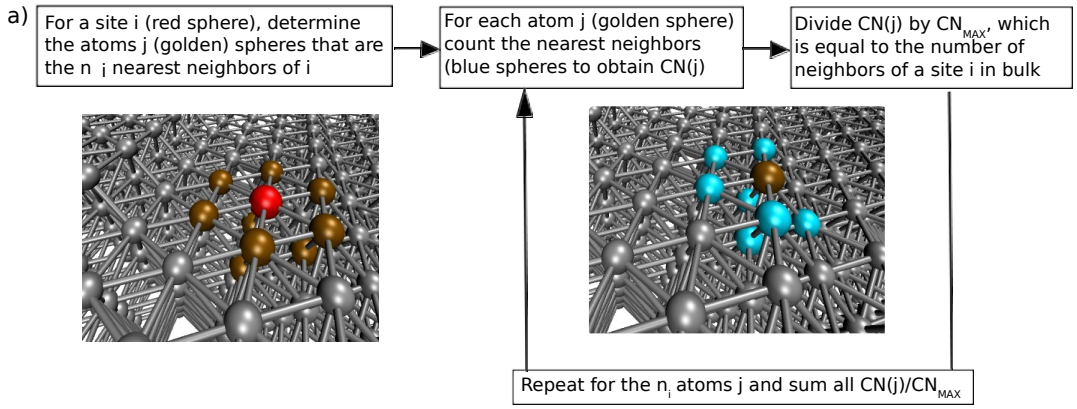


Figure S1: Illustrative scheme on the procedure to calculate the GCN for a given adsorption site.

As discussed in the main manuscript, we set a cutoff value to determine first neighbors of $1.2d_{av}(i)$, where $d_{av}(i)$ is the average weighted bond length for a particular atom calculated. The value $1.2d_{av}$ was selected to ensure that we would be able to identify first-neighbors even for systems with elongated bonds. Table S1 shows how the *GCN* values of top sites from a Cu(533) surface changes as a function of the employed cutoff, showing that the results should not change provided that the applied cutoff is not too small to exclude first-neighbors or to large to include second-neighbors. More discussions about the topic can be also be found in the literature.[3]

Table S1: Calculated *GCN* values for top sites from a Cu(533) surface, where $T1$ ($T4$) is the site with lowest (highest) *GCN*. The data for this table was obtained using different cutoff values for determining an adsorption site first-neighbors from $1.05d_{av}$ to $1.40d_{av}$.

	$1.05d_{av}$	$1.10d_{av}$	$1.20d_{av}$	$1.30d_{av}$	$1.40d_{av}$
$T1$	5.50	5.50	5.50	5.50	6.75
$T2$	7.17	7.17	7.17	7.17	7.33
$T3$	7.67	7.67	7.67	7.67	7.75
$T4$	8.75	8.75	8.75	8.75	9.00

2 Theoretical Approach Details

2.1 Employed Surface Models

The calculations were performed using as substrates a 20-layer, (3×1) surface unit cell for Cu(533) and two modifications of the same surface, which correspond to an added vacancy in the surface step, and the addition of triangular Cu_3 on top of the Cu(533) surface as shown in the main article. For these surfaces, we explored several adsorption sites to construct the correlations of binding energies, E_{bind}, versus *GCN* that are used in the main article. To validate the obtained correlations, we have also performed calculations on icosahedral Cu_n nanoparticles with ($n = 13$, 55, 147, and 309) and on Cu(111), Cu(100), and Cu(211) surfaces constructed with (3×3), (3×3), and (3×1) surface unit cells and 5, 5, and 15 layers, respectively. For all cases, we added the molecules only to one side of the surface, and fixed the bottom two layers for Cu(111) and Cu(100), six layers for Cu(211), and eight layers for Cu(533). The remaining atoms were fully optimized using a $0.025\,\mathrm{eV/\AA}$ convergence criteria for the atomic forces. For nanoparticles, we employed the same thresholds for atomic forces allowing all atoms to relax.

The addition of Cu_3 cluster on the stepped Cu(533) surface was made using FCC adsorption sites on the Cu(533) terrace region, following the results of a previous study from our group.[4] The Cu surfaces used in this study were chosen in order to yield adsorption sites with a wide range of *GCN* varying from 3.09 to 8.75. For each coordination region, we positioned the adsorbates on the top, bridge, and hollow (FCC and HCP) sites with different orientations for the molecules with respect to the surface. For the surfaces used for validate the obtained correlations, we positioned the molecules on all distinct adsorption sites using insights from the most stable

configurations obtained with the Cu(533), defected-Cu(533), and Cu_3/Cu(533) surfaces. Given the high computational cost for running DFT calculations on large metallic nanoparticles, for the icosahedral Cu_n models, we only assessed CO and OH adsorbates as a way to understand how transferable are the correlations obtained on surfaces to nanoparticle models.

2.2 Computational Hydrogen Electrode

We have computed free energy changes, ΔG, for the proton-coupled electron (PCET) reaction steps discussed in the main manuscript using the computational hydrogen electrode model.[5,6] In this model, the reversible hydrogen electrode (RHE) is used as a reference for the applied electrical potential (U). Thus, we consider that at zero electrode potential, ($U = 0\,\mathrm{V}$ vs RHE), for all pH and temperature values, the reaction $\frac{1}{2}\mathrm{H_2} \rightleftharpoons \mathrm{H^+ + e^-}$ is in equilibrium:

$$\frac{1}{2}G_{\mathrm{H_2}} = G_{\mathrm{H^+ + e^-}} \,. \tag{1}$$

Consequently, we can apply the model to compute the free energy change of a PCET reaction step and account for variations in the applied electrode potential by adding a $-eU$ correction to the free energy of hydrogen gas, i.e., $G_{\mathrm{H^+ + e^-}} = \frac{1}{2}G_{\mathrm{H_2}} - eU$. As discussed in the main manuscript, the free energies considered in the model are obtained as:

$$G = E_{tot} + ZPE + \int C_p dT - TS + E_{sol} \,, \tag{2}$$

where, E_{tot} is the total electronic energy, ZPE the zero point energy, $\int C_p dT$ the enthalpic temperature, $-TS$ the entropy contributions, and E_{sol} the solvation correction. The terms, ($ZPE + \int C_p dT - TS$), were obtained using the thermochemistry module from the atomic simulation environment package,[7] while for the solvation corrections we applied values from the literature.[6,8]

For adsorbed systems the quantities ($ZPE + \int C_p dT - TS$) were obtained under the harmonic limit for 298.15 K. For non-adsorbed species, the same quantities were obtained in the ideal-gas limit, following the approach detailed by Peterson *et al.*[6] including a -0.51 eV correction for gas-phase CO due to inconsistencies between experimental thermochemical data and the ones

calculated with the PBE functional. Both adsorbed and non-adsorbed quantities were obtained in one of our previous studies.[4] The reaction energies were calculated at $U = 0$ and the onset potential U_{onset} associated to the potential determining step (PDS) of a given reaction pathway was determined based on the largest positive free energy value ΔG_{MAX} between the different reaction steps:

$$U_{onset} = -\Delta G_{MAX} / \mathrm{e}^{-} \ . \tag{3}$$

2.3 Energetic Analyses: Additional Details

The binding energies, E_{bind}, were used to generate our *GCN*-dependent free energy change analysis. For example, for the reaction step $^{*}\mathrm{CO} + \mathrm{H}^{+} + \mathrm{e}^{-} \longrightarrow {}^{*}\mathrm{CHO}$, the free energy change can be described as:

$$\Delta G(^{*}\mathrm{CO} + \mathrm{H}^{+} + \mathrm{e}^{-} \longrightarrow {}^{*}\mathrm{CHO}) = G(^{*}\mathrm{CHO}) - G(^{*}\mathrm{CO}) - 0.5G(\mathrm{H_2}) \ , \tag{4}$$

where the free energy of a state can be rewritten from equation 2 as:

$$G(^{*}\mathrm{CHO}) = E_{tot}^{^{*}\mathrm{CHO}} + (ZPE + \int C_p dT - TS)^{^{*}\mathrm{CHO}} + E_{sol}^{^{*}\mathrm{CHO}} = E_{tot}^{^{*}\mathrm{CHO}} + E_{extra}^{^{*}\mathrm{CHO}} \ . \tag{5}$$

Applying the definition of E_{bind} and the free energy notation for each state from equation 5 on the free energy change equation 4, we obtain the following equation:

$$\Delta G(^{*}\mathrm{CO} + \mathrm{H}^{+} + \mathrm{e}^{-} \longrightarrow {}^{*}\mathrm{CHO}) = (E_{bind}^{^{*}\mathrm{CHO}} - E_{bind}^{^{*}\mathrm{CO}}) + (E_{extra}^{^{*}\mathrm{CHO}} - E_{extra}^{^{*}\mathrm{CO}} - 0.5E_{extra}^{\mathrm{H_2}}) \ . \tag{6}$$

As discussed in the manuscript,the sum of the terms $(ZPE + \int C_p dT - TS)$ for adsorbed systems is almost constant with respect to variations on the adsorption site coordination[4] and we also consider that the solvation energies should be similar on distinct adsorption sites. As all the terms of E_{extra} are considered to be constant with respect to *GCN*, the variations of ΔG as a function of *GCN* can be obtained from the variations of E_{bind} as a function of *GCN*.

For all the adsorbed systems, we also calculated the adsorption, E_{ad}, and interaction energies,

E_{int}, using the following equations:

$$E_{ad} = E_{tot}^{\text{Mol/sub}} - E_{tot}^{\text{Mol}} - E_{tot}^{\text{Sub}} \,, \tag{7}$$

$$E_{int} = E_{tot}^{\text{Mol/sub}} - E_{tot}^{\text{Mol } Frozen} - E_{tot}^{\text{Sub } Frozen} \,, \tag{8}$$

where $E_{tot}^{\text{Mol/sub}}$ is the total energy of the system composed by adsorbate and substrate, while $E_{tot}^{\text{CO}_2}$ and E_{tot}^{Sub} are the total energies of the isolated molecule and substrate optimized separately. For the calculation of the interaction energies, the only change is that the energies of molecule, $E_{tot}^{\text{Mol } Frozen}$, and substrate, $E_{tot}^{\text{Sub } Frozen}$, are obtained by freezing the molecule and substrate on the structures obtained after the optimization with the systems interacting.

2.4 Selection of Potential-Determining Steps

As discussed in the main manuscript, the possible potential-determining steps for the reduction of CO_2 towards CO, HCOOH on Cu catalysts can be narrowed, according to the literature,[4,6,8–18] to the following eight proton-coupled electron transfers (PCET) steps:

$$CO_2 + H^+ + e^- \longrightarrow {}^*COOH \,, \tag{9}$$

$$CO_2 + H^+ + e^- \longrightarrow {}^*HCOO \,, \tag{10}$$

$${}^*COOH + H^+ + e^- \longrightarrow {}^*CO + H_2O \,, \tag{11}$$

$${}^*COOH + H^+ + e^- \longrightarrow HCOOH \,, \tag{12}$$

$${}^*HCOO + H^+ + e^- \longrightarrow HCOOH \,, \tag{13}$$

$${}^*OH + H^+ + e^- \longrightarrow H_2O \,, \tag{14}$$

$${}^*CO + H^+ + e^- \longrightarrow {}^*CHO \,, \tag{15}$$

$${}^*CO + H^+ + e^- \longrightarrow {}^*COH \,. \tag{16}$$

For CO_2 reduction to CO, we considered as possible PDS the reaction steps described in

equation 9 and 11, while *CO desorption was included to augment the discussion but was not considered as a possible PDS. For CO_2 reduction to HCOOH, we considered as possible PDS the reaction steps described in equation 9 and 12 for the reaction pathway through the *COOH intermediate, while the pathway through the *HCOO intermediate was modeled with equations 10 and 13. For CH_4 production, we considered the reaction steps described in equations 9, 11, 15, and 14 for the pathway passing through *CHO, and the reaction from equations 9, 11, 16, and 14 for the pathway passing through *COH. For each value of *GCN*, we compared the different pathways toward a given product considering only the selected reaction steps and picked the one with the lowest U_{onset}. Within the reactions of the chosen pathway, the least favorable step was assigned as the PDS.

3 Isolated Cu surfaces and nanoparticles

As previously explained, our calculations were performed for: i) surfaces used to generate the E_{bind} vs *GCN* correlations, namely Cu(533), defected-Cu(533), and Cu_3/Cu(533), that are show in Figure S2; ii) surfaces used to validate the E_{bind} vs *GCN* correlations, namely Cu(111), Cu(100), and Cu(211), that are show in Figure S3; and iii) Icosahedral Cu_n nanoparticles with ($n = 13$, 55, 147, and 309) used to validate the E_{bind} vs *GCN* correlations, that are show in Figure S4.

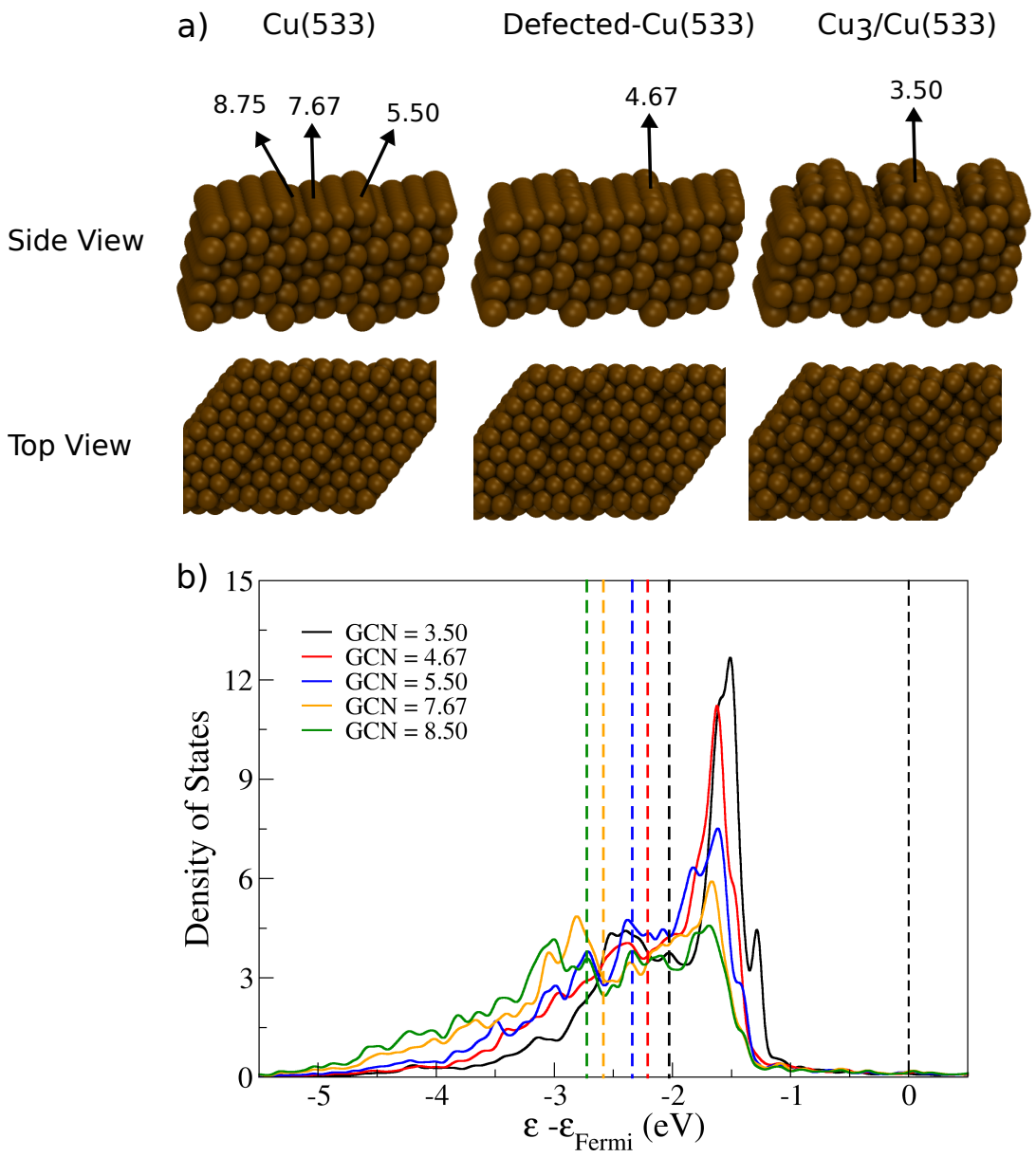


Figure S2: Cu surfaces used to analyze the correlation of E_{bind} on the adsorption site *GCN*, namely Cu(533), defected-Cu(533), and Cu_3/Cu(533). a) shows side and top views of the surfaces and indicates adsorption regions with different *GCN* values, b) shows the *d*-projected density of states for each region of different *GCN* values, averaged by the number of atoms in the region and accompanied of their d-band centers that are represented as dashed lines.

Figures S2 to S4 show the employed structures together with examples of *GCN* values for each structure and their d-band projected density of states, which was averaged for the number of atoms used to construct each plot, and the computed d-band centers. For all the cases, we observe that a decrease in the adsorption site coordination, or *GCN* value, leads to upshifts of the d-band centers, which should reflect as stronger adsorption (binding) energies. For the Cu nanoparticles, we observe that both the density of states profile and the d-band centers change

as we increase the nanoparticle size. However, these changes become less significant as the nanoparticle increases, with the results from Cu_{147} and Cu_{309} being similar both in the density of states profile and d-band centers.

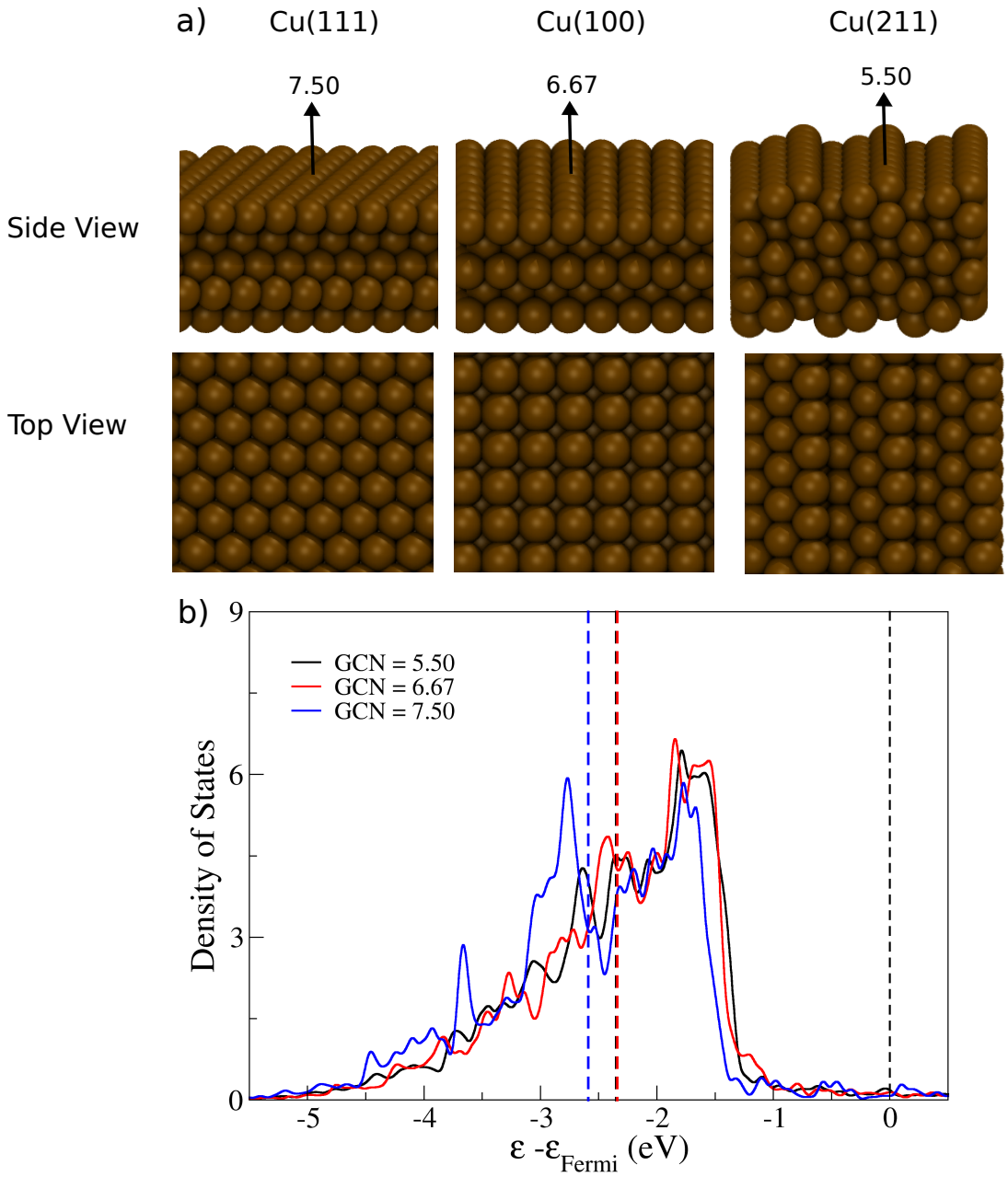


Figure S3: Cu surfaces used to validate the obtained correlation between E_{bind} and the adsorption site *GCN*, namely Cu(111), Cu(100), and Cu(211). a) shows side and top views of the surfaces and indicates adsorption regions with different *GCN* values, b) shows the *d*-projected density of states for each region of different *GCN* values, averaged by the number of atoms in the region and accompanied of their d-band centers that are represented as dashed lines.

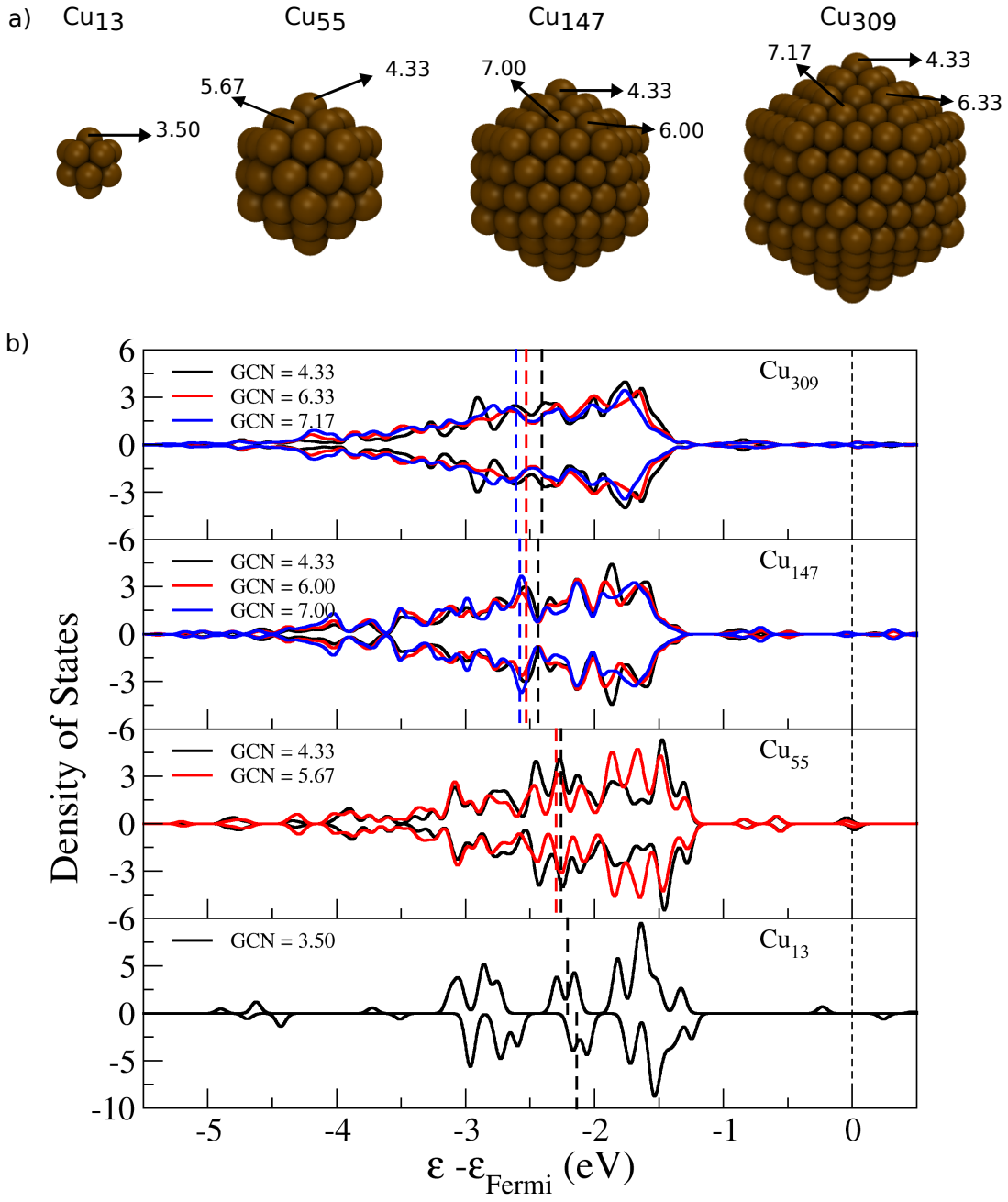


Figure S4: Icosahedral Cu clusters used to validate the dependence of E_{bind} on the adsorption site *GCN*, namely Cu_{13}, Cu_{55}, Cu_{147}, and Cu_{309}. a) shows clusters and indicates adsorption regions with different *GCN* values, b) shows the *d*-projected density of states for each region of different *GCN* values and Np sizes, averaged by the number of atoms in the region and accompanied of their d-band centers that are represented as dashed lines.

4 CO_2 Adsorption on Cu Surfaces

As a starting point, we have simulated the CO_2 adsorption on sites with different coordination levels. We have placed CO_2 on different sites using a linear and a bent CO_2 structure and

considered different orientations in relation to the surface. Figure S5 shows the distinct structures that we have obtained together with the calculated adsorption energies.

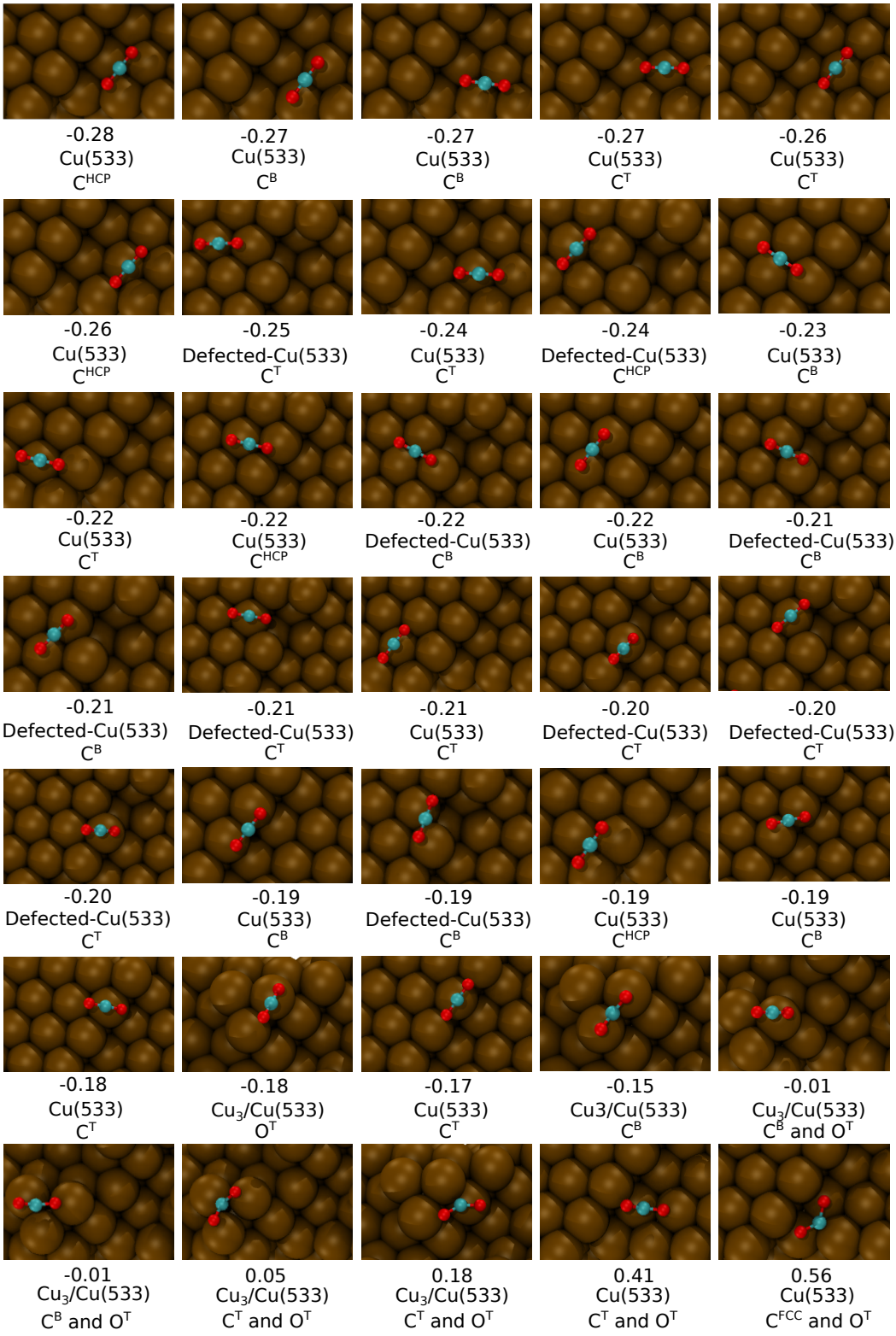


Figure S5: CO_2 interacting with different Cu sites and their respective adsorption energies.

Additionally to the structures provided on Figure S5, we summarize on table S2 the

geometrical and energetic data for all the computed structures. We show adsorption, binding, interaction and deformation energies, as well as, the interatomic distances between Cu and C atoms, Cu and the closest O, the C−O distances, and the O−C−O angles for all cases. We observed the CO_2 molecule binding in three distinct adsorption modes: i) bent CO_2, ${CO_2}^{B}$, and ii) linear CO_2 adopting a parallel, ${CO_2}^{L-P}$, or iii) tilted, ${CO_2}^{L-T}$, configuration with respect to the surface atoms. In general, as already observed in the literature[19,20] and by our own group,[21,22] the chemisorption and activation of CO_2 on Cu is energetically unfavorable as compared to the physisorption of CO_2. In our calculations, most of the low energy structures presented C−Cu distances ranging from 3.02 Å to 3.02 Å with similar values of adsorption energies between adsorption sites ranging from 3.02 eV to 3.02 eV.

The bent CO_2 structures were only observed for few adsorption sites, which can be divided into two groups. The first group happens for C atoms near highly coordinated sites located under the steps of Cu(533) surfaces in which one or both O atoms are close to the Cu atoms in the step. The second group happens for CO_2 adsorbed on highly undercoordinated sites on Cu_3/Cu(533), which mimics, to a certain extent, the sites near vertices of smaller nanoparticles. Interestingly, in a recent contribution from our group, we have observed physisorbed CO_2 as the most stable case for Cu clusters and we were unable to find a case of stable bent configuration for Cu(111) surfaces or Cu_{147} nanoparticles.[22] However, bent CO_2 appeared as high energy structures for smaller cluster near highly undercoodinated sites.[22] These results show that our approach can reproduce effects observed in other Cu systems that are attributed to the existence of adsorption sites with low-coordination.

Table S2: CO_2 configuration together with their adsorption, binding, interaction, and deformation energies in (eV), shortest distance between the substrate and C and O atoms, maximum C–O bond length, and OCO angle for CO_2 molecules interacting with different adsorption sites.

Configuration	E_{ad} (eV)	E_{bind} (eV)	E_{int} (eV)	ΔE^{Mol} (eV)	ΔE^{Sub} (eV)	C–Cu (Å)	O–Cu (Å)	C–O^{MAX} (Å)	OCO (deg)
$CO_2^{\mathrm{L-P}}$	−0.28	−0.28	−0.28	0.00	0.00	3.59	3.37	1.17	179.44
$CO_2^{\mathrm{L-P}}$	−0.27	−0.27	−0.27	0.00	0.00	3.53	3.30	1.17	179.54
$CO_2^{\mathrm{L-P}}$	−0.27	−0.27	−0.27	0.00	0.00	3.54	3.33	1.17	179.52
$CO_2^{\mathrm{L-P}}$	−0.27	−0.27	−0.27	0.00	0.00	3.43	3.41	1.17	179.55
$CO_2^{\mathrm{L-P}}$	−0.26	−0.26	−0.26	0.00	0.00	3.37	3.56	1.17	179.49
$CO_2^{\mathrm{L-P}}$	−0.26	−0.26	−0.26	0.00	0.00	3.47	3.34	1.17	179.55
$CO_2^{\mathrm{L-P}}$	−0.25	−0.25	−0.25	0.00	0.00	3.53	3.35	1.17	179.47
$CO_2^{\mathrm{L-P}}$	−0.24	−0.24	−0.24	0.00	0.00	3.52	3.43	1.17	179.57
$CO_2^{\mathrm{L-P}}$	−0.24	−0.24	−0.24	0.00	0.00	3.54	3.34	1.17	179.48
$CO_2^{\mathrm{L-P}}$	−0.23	−0.23	−0.23	0.00	0.00	3.54	3.21	1.17	179.49
$CO_2^{\mathrm{L-P}}$	−0.22	−0.22	−0.22	0.00	0.00	3.36	3.33	1.17	179.50
$CO_2^{\mathrm{L-P}}$	−0.22	−0.22	−0.22	0.00	0.00	3.49	3.13	1.18	179.52
$CO_2^{\mathrm{L-P}}$	−0.22	−0.22	−0.22	0.00	0.00	3.53	2.85	1.18	179.47
$CO_2^{\mathrm{L-P}}$	−0.22	−0.22	−0.22	0.00	0.00	3.47	3.25	1.17	179.60
$CO_2^{\mathrm{L-T}}$	−0.21	−0.21	−0.21	0.00	0.00	3.14	2.64	1.18	179.54
$CO_2^{\mathrm{L-P}}$	−0.21	−0.21	−0.21	0.00	0.00	3.53	3.22	1.17	179.51
$CO_2^{\mathrm{L-P}}$	−0.21	−0.21	−0.21	0.00	0.00	3.23	3.36	1.17	179.38
$CO_2^{\mathrm{L-P}}$	−0.21	−0.21	−0.21	0.00	0.00	3.37	3.55	1.17	179.55
$CO_2^{\mathrm{L-T}}$	−0.20	−0.20	−0.20	0.00	0.00	3.11	2.48	1.18	179.77
$CO_2^{\mathrm{L-T}}$	−0.20	−0.20	−0.20	0.00	0.00	3.32	3.41	1.17	179.50
$CO_2^{\mathrm{L-T}}$	−0.20	−0.20	−0.20	0.00	0.00	3.02	2.45	1.18	179.90
$CO_2^{\mathrm{L-P}}$	−0.19	−0.19	−0.19	0.00	0.00	3.23	2.95	1.17	179.89
$CO_2^{\mathrm{L-T}}$	−0.19	−0.19	−0.19	0.00	0.00	3.37	3.26	1.17	179.62
$CO_2^{\mathrm{L-P}}$	−0.19	−0.19	−0.19	0.00	0.00	3.48	3.27	1.17	179.59
$CO_2^{\mathrm{L-T}}$	−0.19	−0.19	−0.19	0.00	0.00	3.33	2.87	1.18	179.84
$CO_2^{\mathrm{L-T}}$	−0.18	−0.18	−0.18	0.00	0.00	3.28	3.03	1.18	179.86
$CO_2^{\mathrm{L-T}}$	−0.18	−0.18	−0.18	0.00	0.00	3.02	2.42	1.18	179.85
$CO_2^{\mathrm{L-P}}$	−0.17	−0.17	−0.17	0.00	0.00	3.22	3.43	1.17	179.64
$CO_2^{\mathrm{L-P}}$	−0.15	−0.15	−0.16	0.00	0.01	3.15	2.75	1.18	179.60
CO_2^{B}	−0.01	−0.01	−0.97	0.94	0.02	2.14	2.15	1.22	146.20
CO_2^{B}	−0.01	−0.01	−1.96	1.82	0.14	2.07	1.99	1.28	134.45
CO_2^{B}	0.05	0.05	−2.09	1.98	0.16	2.04	2.07	1.26	132.70
CO_2^{B}	0.18	0.18	−1.45	1.59	0.05	2.07	2.07	1.27	136.99
CO_2^{B}	0.41	0.41	−1.87	2.20	0.08	2.12	2.06	1.26	128.98
CO_2^{B}	0.56	0.56	−2.45	2.82	0.18	2.04	2.08	1.29	123.86

5 Adsorption of CO_2 Reduction Intermediates

As discussed in the main text, we have considered in this work only the adsorbates involved in the most important reaction steps towards $C1$ products. For all the cases, we tested the molecules interacting with top, bridge, FCC and HCP adsorption sites with different levels of coordination,

which are indicated in the following figures as A^S, where A is the nearest atom from an adsorbate to the surface and S the adsorption site. For each system, we also tested different orientations of the adsorbates with respect to the surface. While certain adsorbates favored a single adsorption configuration and adsorption site type, molecules such as COOH stabilized on several adsorption sites and showed a wider variety of possible configurations. As a result, the obtained number of distinct configurations after geometry optimizations varied for each case. For completeness, we show in the next sections all the distinct structures obtained on different Cu surfaces and nanoparticles, together with energetic and structural data for each system.

5.1 COOH Adsorption

For COOH adsorption, we have observed 3 different configurations of the adsorbate with respect to the substrate: i) bound via the C atom with the O and OH groups pointing away from the surface, ii) bound via the C and O atoms, and i) bound via the C atom and OH group. For a same site, the configuration with C and O binding to the surface was the one with stronger adsorption energies.

For completeness, Table S3 shows all the energetic and structural data. For some cases, we have observed surface reconstruction or even C-OH bond breaking during the geometry optimization. These effects can be easily noticed due to the negative deformation energies for the substrate, ΔE^{Sub}, or high deformation energies for the molecules, ΔE^{Mol}. These cases were not considered for the free energy change or E_{bind} vs GCN analysis because the surface reconstructions would change the energy of the reference system and the optimizations that lead to C-OH bond breaking do not represent the state of adsorbed COOH. If we analyze a same adsorption configuration, for example, the one bound via the C and O atoms, we see that the increase of the site coordination weakens the adsorption energies, with the strongest value being -2.53 eV for the Cu_3/Cu(533) system and the weakest -1.69 eV for the top site below the step on Cu(533).

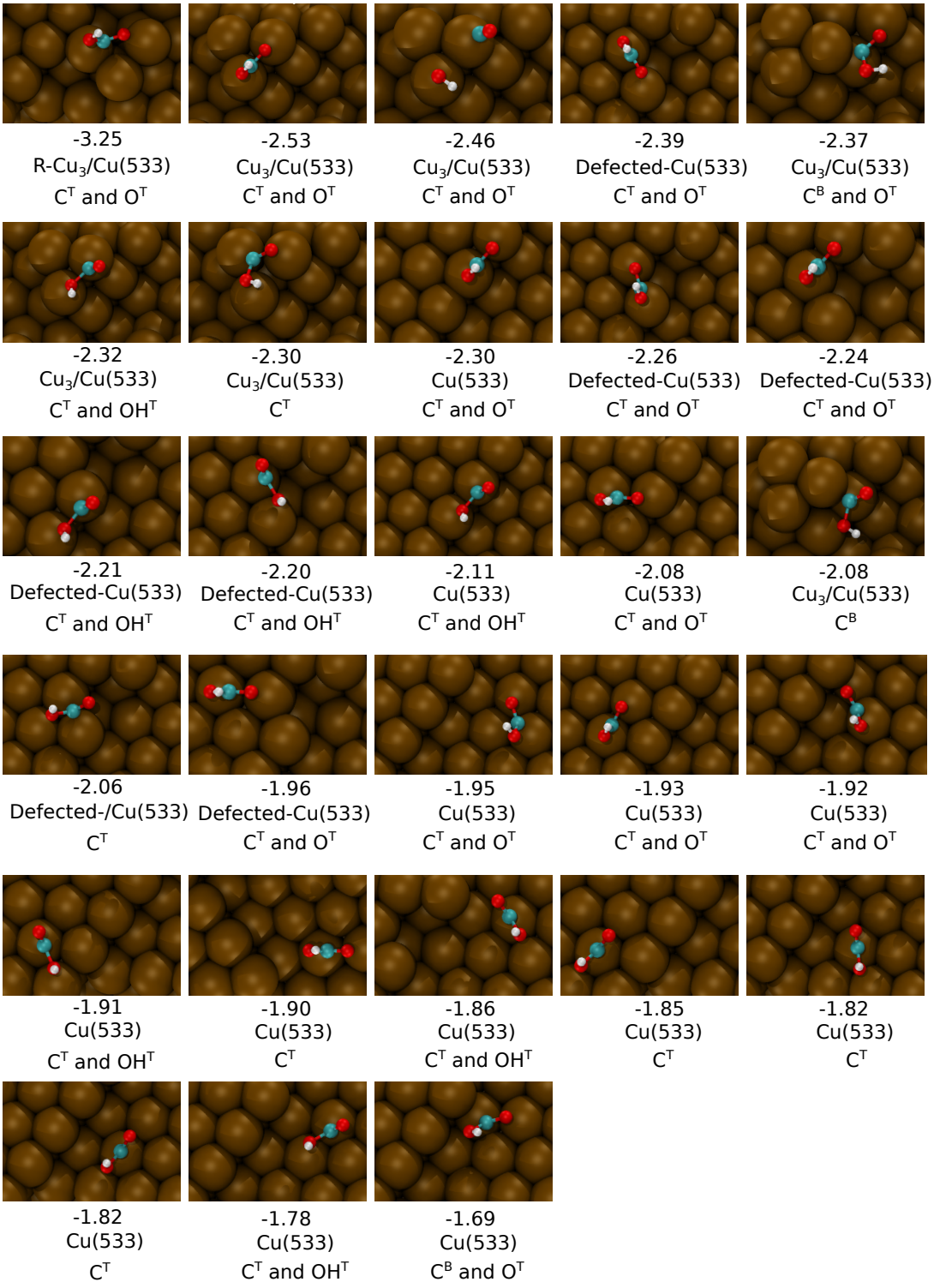


Figure S6: COOH interacting with different Cu sites and their respective adsorption energies. We also indicate the Cu surface for each case and describe the adsorption site as A^S, where A is the nearest atom from an adsorbate to the surface and S the adsorption site.

Table S3: Adsorption, binding, interaction, and deformation energies in (eV), together with the shortest distance between the substrate and C and O atoms, C−O, C−OH, and O−H bond lengths, for COOH molecules interacting with different adsorption sites.

E_{ad} (eV)	E_{bind} (eV)	E_{int} (eV)	ΔE^{Mol} (eV)	ΔE^{Sub} (eV)	C−Cu (Å)	O−Cu (Å)	C−O (Å)	C−OH (Å)	O−H (Å)
−3.25	−1.21	−3.20	0.43	−0.47	1.96	1.98	1.27	1.35	0.99
−2.53	−0.49	−3.03	0.40	0.11	1.93	2.00	1.27	1.34	0.99
−2.46	−0.43	−4.31	1.80	0.05	1.84	1.82	1.14	NA	0.98
−2.39	−0.35	−2.79	0.33	0.07	1.94	2.03	1.26	1.34	0.99
−2.37	−0.34	−2.88	0.36	0.15	1.99	2.05	1.26	1.35	0.99
−2.32	−0.28	−2.87	0.47	0.08	1.94	2.03	1.20	1.48	0.99
−2.30	−0.27	−3.01	0.48	0.23	1.94	2.05	1.26	1.42	0.99
−2.30	−0.26	−2.69	0.32	0.07	1.92	2.05	1.26	1.34	0.99
−2.26	−0.23	−2.68	0.34	0.08	1.93	2.06	1.26	1.34	0.99
−2.24	−0.20	−2.61	0.31	0.06	1.93	2.11	1.26	1.35	0.99
−2.21	−0.18	−2.67	0.38	0.07	1.93	2.06	1.20	1.46	0.99
−2.20	−0.16	−2.61	0.37	0.05	1.96	2.08	1.20	1.45	0.99
−2.11	−0.08	−2.48	0.32	0.05	1.94	2.11	1.20	1.44	0.99
−2.08	−0.05	−2.54	0.36	0.09	1.98	2.08	1.27	1.34	0.99
−2.08	−0.04	−2.37	0.20	0.09	1.98	2.64	1.22	1.40	0.99
−2.06	−0.03	−2.26	0.17	0.04	2.03	NA	1.22	1.38	0.99
−1.96	0.08	−2.38	0.33	0.10	1.96	2.11	1.26	1.35	0.99
−1.95	0.09	−2.28	0.27	0.07	1.95	2.22	1.25	1.35	0.99
−1.93	0.10	−2.30	0.29	0.07	1.95	2.17	1.25	1.35	0.99
−1.92	0.11	−2.43	0.34	0.16	1.99	2.20	1.25	1.35	0.99
−1.91	0.12	−2.30	0.32	0.07	1.98	2.19	1.20	1.44	0.99
−1.90	0.14	−2.27	0.30	0.07	1.96	2.17	1.25	1.35	0.99
−1.86	0.17	−2.09	0.18	0.05	1.97	NA	1.22	1.38	0.99
−1.85	0.19	−2.04	0.16	0.03	1.97	NA	1.22	1.37	0.99
−1.82	0.21	−2.05	0.18	0.05	1.98	2.56	1.21	1.39	0.99
−1.82	0.22	−2.00	0.15	0.03	1.97	NA	1.22	1.37	0.99
−1.78	0.25	−2.04	0.20	0.05	1.99	2.45	1.21	1.40	0.99
−1.69	0.34	−2.08	0.31	0.08	2.02	2.24	1.25	1.38	0.99

5.2 HCOO Adsorption

For HCOO adsorption, we have observed only one orientation of the adsorbate with respect to the substrate. The molecule adsorbs on all sites via the two O atom, with the CH group pointing away from the surface. As a consequence, we end up with fewer distinct configurations for HCOO as compared with COOH. For completeness, Table S4 shows all the energetic and structural data. Differently from COOH, for HCOO no significant change happens for substrate and molecule

deformation energies due to a variation in the adsorption site coordination. Similarly to the other molecules, the increase of site coordination weakens the adsorption and interaction energies. The strongest value for adsorption energies was -3.78 eV for the Cu_3/Cu(533) system and the weakest -2.85 eV for the top site below the step on Cu(533).

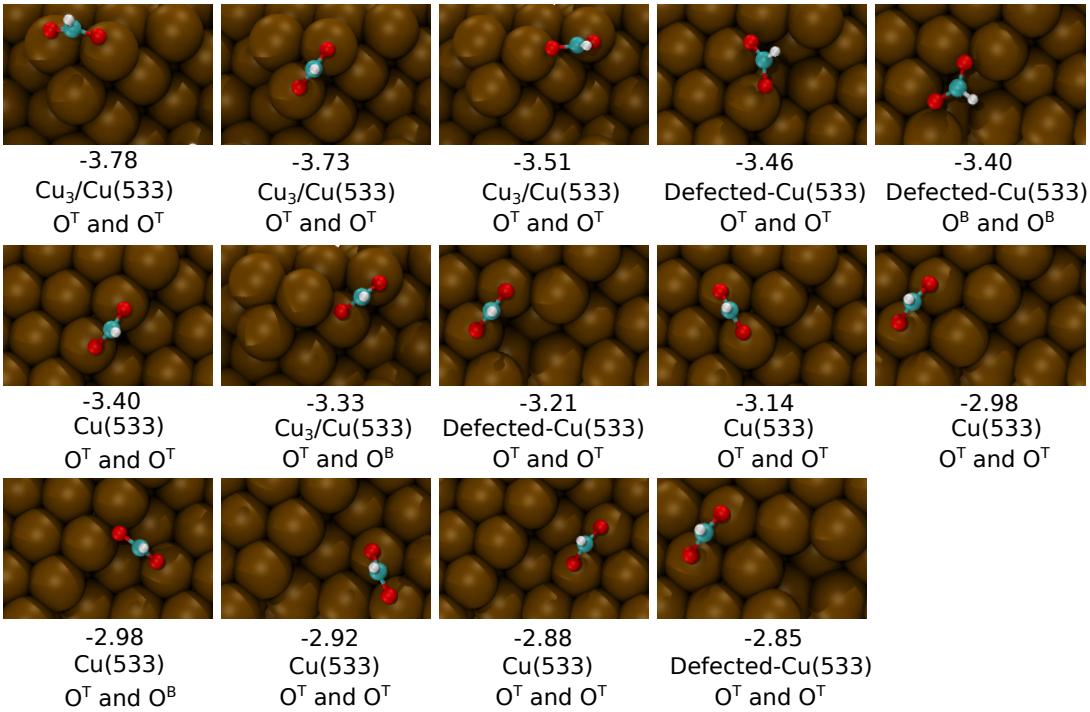


Figure S7: HCOO interacting with different Cu sites and their respective adsorption energies. We also indicate the Cu surface for each case and describe the adsorption site as A^S, where A is the nearest atom from an adsorbate to the surface and S the adsorption site.

Table S4: Adsorption, binding, interaction, and deformation energies in (eV), together with the shortest distance between the substrate and O atoms, C−O, and C−H bond lengths, for HCOO molecules interacting with different adsorption sites.

E_{ad} (eV)	E_{bind} (eV)	E_{int} (eV)	ΔE^{Mol} (eV)	ΔE^{Sub} (eV)	O−Cu$_{MIN}$ (Å)	C−O$_{MIN}$ (Å)	C−H (Å)
−3.78	−1.53	−4.15	0.32	0.05	1.94	1.27	1.11
−3.73	−1.48	−4.11	0.32	0.06	1.94	1.27	1.11
−3.51	−1.26	−3.85	0.27	0.07	1.92	1.26	1.11
−3.46	−1.20	−3.87	0.36	0.06	1.97	1.26	1.11
−3.40	−1.15	−3.75	0.30	0.05	2.10	1.27	1.11
−3.40	−1.14	−3.77	0.32	0.05	1.96	1.27	1.11
−3.33	−1.07	−3.81	0.36	0.13	2.00	1.25	1.11
−3.21	−0.96	−3.60	0.33	0.05	2.00	1.27	1.11
−3.14	−0.88	−3.54	0.32	0.08	1.98	1.27	1.11
−2.98	−0.73	−3.40	0.30	0.12	2.10	1.25	1.11
−2.98	−0.73	−3.39	0.32	0.09	2.10	1.25	1.11
−2.92	−0.67	−3.33	0.32	0.09	2.03	1.27	1.11
−2.88	−0.62	−3.28	0.31	0.09	2.03	1.27	1.11
−2.85	−0.60	−3.25	0.31	0.09	2.03	1.27	1.11

5.3 CO Adsorption

For CO adsorption, the molecule adsorbs on all sites via the C atom, also leading to fewer distinct configurations for CO as compared with COOH. However, we see more distinct configurations for CO as compared with HCOO. For CO molecules, the geometry optimizations yielded CO on several adsorption site types. The preferred adsorption site changed with the surface coordination, with top sites being favored on low-coordinated regions, such as the ones found on Cu_3/Cu(533), and hollow sites being favored on more coordinated regions. Table S5 shows all the energetic and structural data for the systems, showing that the increase of site coordination weakens the adsorption and interaction energies.

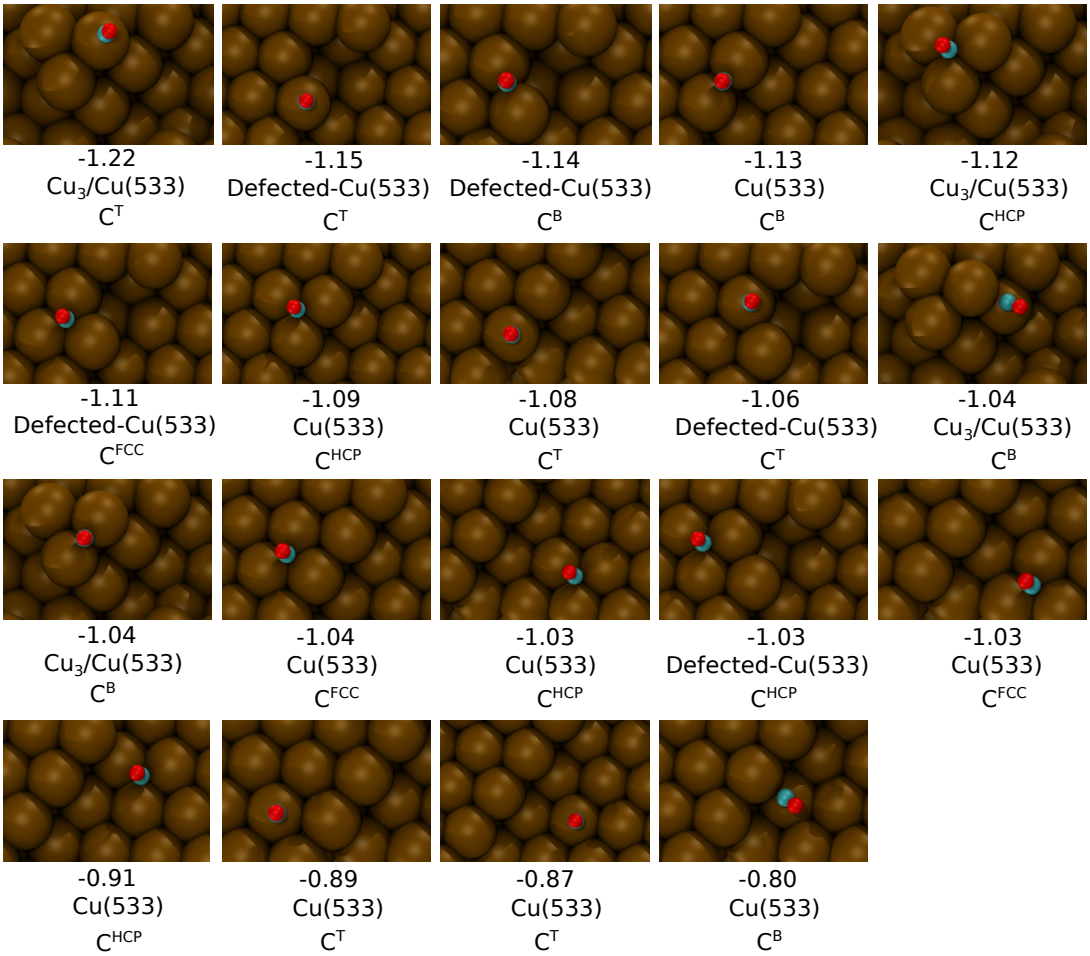


Figure S8: CO interacting with different Cu sites and their respective adsorption energies. We also indicate the Cu surface for each case and describe the adsorption site as A^S, where A is the nearest atom from an adsorbate to the surface and S the adsorption site.

Table S5: Adsorption, binding, interaction, and deformation energies in (eV), shortest distance between the substrate and C atoms and C−O bond lengths for CO molecules interacting with different adsorption sites.

E_{ad} (eV)	E_{bind} (eV)	E_{int} (eV)	ΔE^{Mol} (eV)	ΔE^{Sub} (eV)	C−Cu (Å)	C−O (Å)
−1.22	−0.46	−1.25	0.01	0.02	1.82	1.15
−1.15	−0.40	−1.18	0.01	0.02	1.83	1.15
−1.14	−0.39	−1.23	0.05	0.04	1.95	1.17
−1.13	−0.37	−1.21	0.04	0.05	1.97	1.17
−1.12	−0.36	−1.26	0.11	0.04	2.02	1.18
−1.11	−0.36	−1.23	0.09	0.03	2.01	1.18
−1.09	−0.33	−1.21	0.09	0.04	2.02	1.18
−1.08	−0.32	−1.11	0.01	0.03	1.84	1.15
−1.06	−0.31	−1.10	0.01	0.02	1.84	1.15
−1.04	−0.29	−1.18	0.05	0.08	1.93	1.17
−1.04	−0.29	−1.14	0.05	0.04	1.96	1.17
−1.04	−0.28	−1.16	0.08	0.03	2.04	1.18
−1.03	−0.28	−1.16	0.08	0.04	2.03	1.18
−1.03	−0.27	−1.09	0.01	0.04	2.03	1.18
−1.03	−0.27	−1.15	0.08	0.04	2.03	1.18
−0.91	−0.16	−1.04	0.09	0.04	2.01	1.18
−0.89	−0.13	−0.94	0.01	0.04	1.85	1.15
−0.87	−0.11	−0.91	0.01	0.03	1.85	1.15
−0.80	−0.05	−0.92	0.05	0.07	1.95	1.17

5.4 COH Adsorption

For COH adsorption, the molecule adsorbs on all sites via the C atom. As compared with CO adsorption, the orientation of the O−H group with respect to the surface creates more distinct configurations for this molecule. The orientation of the O−H bond with respect to the surface had almost no impact on adsorption or interaction energies. HCP and FCC adsorption sites were generally preferred and the only exceptions happened for a few cases of higher energy configurations with adsorption on bridge sites. Table S6 shows all the energetic and structural data for the systems, showing that the increase of site coordination also weakens the adsorption and interaction energies.

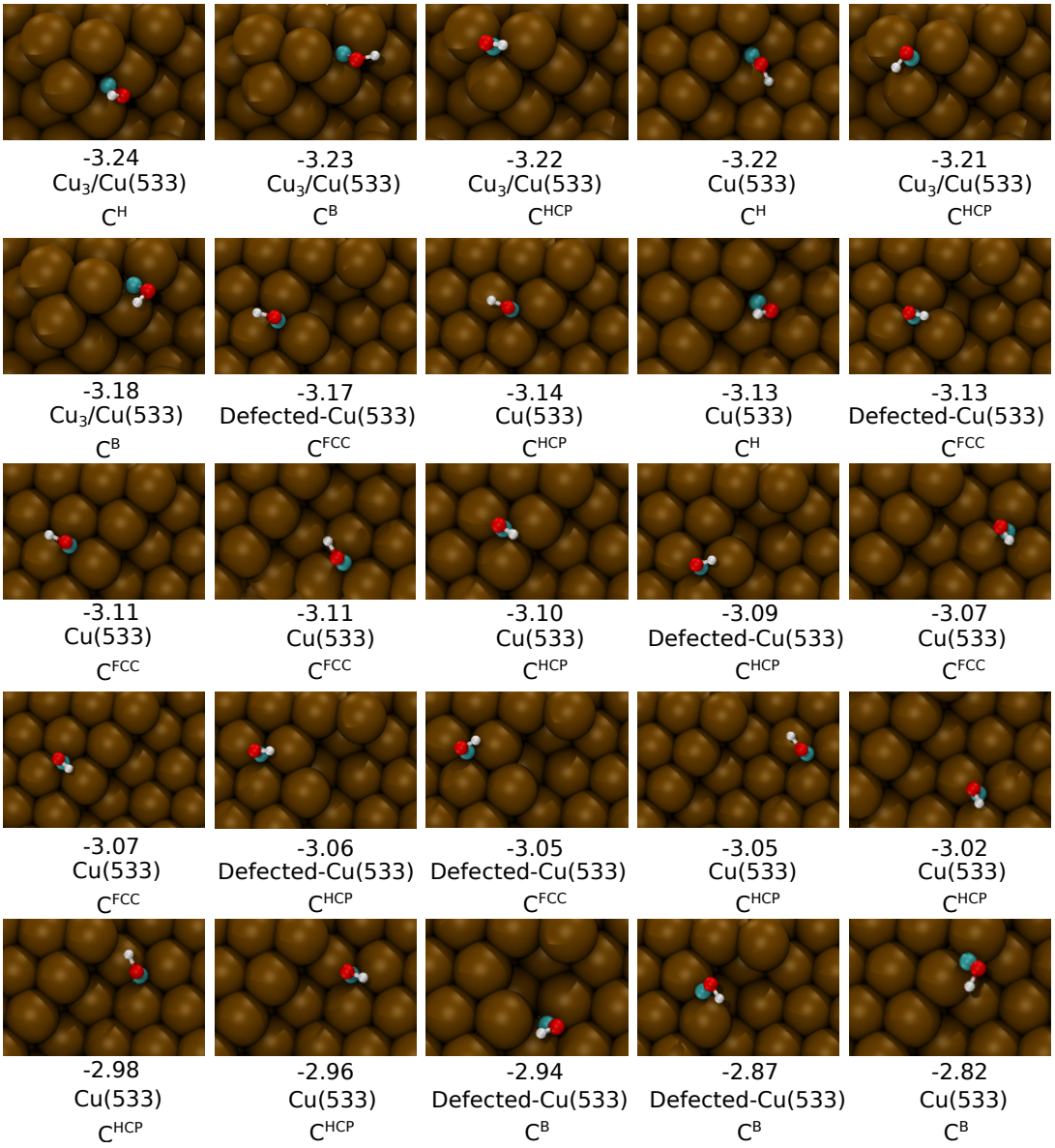


Figure S9: COH interacting with different Cu sites and their respective adsorption energies. We also indicate the Cu surface for each case and describe the adsorption site as A^S, where A is the nearest atom from an adsorbate to the surface and S the adsorption site.

Table S6: Adsorption, binding, interaction, and deformation energies in (eV), shortest distance between the substrate and C atoms, C−OH, and O−H bond lengths for COH molecules interacting with different adsorption sites.

E_{ad} (eV)	E_{bind} (eV)	E_{int} (eV)	ΔE^{Mol} (eV)	ΔE^{Sub} (eV)	C−Cu (Å)	C−OH (Å)	O−H (Å)
−3.24	0.52	−3.53	0.18	0.11	2.00	1.37	0.98
−3.23	0.52	−3.46	0.10	0.12	1.94	1.34	0.98
−3.22	0.53	−3.43	0.11	0.10	1.92	1.35	0.98
−3.22	0.54	−3.44	0.15	0.08	1.99	1.36	0.99
−3.21	0.55	−3.43	0.11	0.11	1.91	1.35	0.98
−3.18	0.58	−3.40	0.11	0.12	1.93	1.35	0.98
−3.17	0.58	−3.33	0.08	0.08	1.91	1.34	0.98
−3.14	0.62	−3.30	0.08	0.08	1.92	1.34	0.98
−3.13	0.62	−3.40	0.20	0.07	2.00	1.38	0.98
−3.13	0.63	−3.30	0.09	0.08	1.91	1.34	0.98
−3.11	0.64	−3.27	0.08	0.07	1.90	1.34	0.98
−3.11	0.64	−3.25	0.07	0.07	1.90	1.33	0.98
−3.10	0.65	−3.28	0.09	0.09	1.92	1.34	0.98
−3.09	0.67	−3.31	0.09	0.12	1.90	1.34	0.98
−3.07	0.68	−3.22	0.08	0.08	1.91	1.33	0.98
−3.07	0.69	−3.24	0.09	0.09	1.90	1.34	0.98
−3.06	0.70	−3.23	0.08	0.09	1.91	1.33	0.98
−3.05	0.71	−3.21	0.08	0.08	1.91	1.33	0.98
−3.05	0.71	−3.21	0.07	0.09	1.91	1.33	0.98
−3.02	0.74	−3.18	0.08	0.08	1.91	1.33	0.98
−2.98	0.77	−3.13	0.06	0.08	1.90	1.33	0.99
−2.96	0.79	−3.12	0.09	0.07	1.92	1.34	0.98
−2.94	0.82	−3.16	0.13	0.10	1.96	1.35	0.98
−2.87	0.89	−2.98	0.04	0.07	1.86	1.31	0.98
−2.82	0.94	−2.92	0.03	0.07	1.87	1.31	0.98

5.5 CHO Adsorption

For CHO adsorption, we have observed 2 different configurations of the adsorbate with respect to the substrate: i) bound only via the C atom, and ii) bound via the C and O atom. For a same site, the configuration with both C and O binding to the surface was usually the one with stronger adsorption energies. Table S7 shows all the energetic and structural data for the distinct configurations. As commented for the COOH adsorption, we have observed, for some cases, surface reconstruction during the geometry optimization and such configurations were not considered for the free energy change or E_{bind} vs *GCN* analysis. As compared with the previous

adsorbates, the CHO molecule adsorbs on different configurations and can be stabilized on several adsorption site types, leading to more distinct configurations than the previous adsorbates. Again, the increase of the site coordination weakened the adsorption energies.

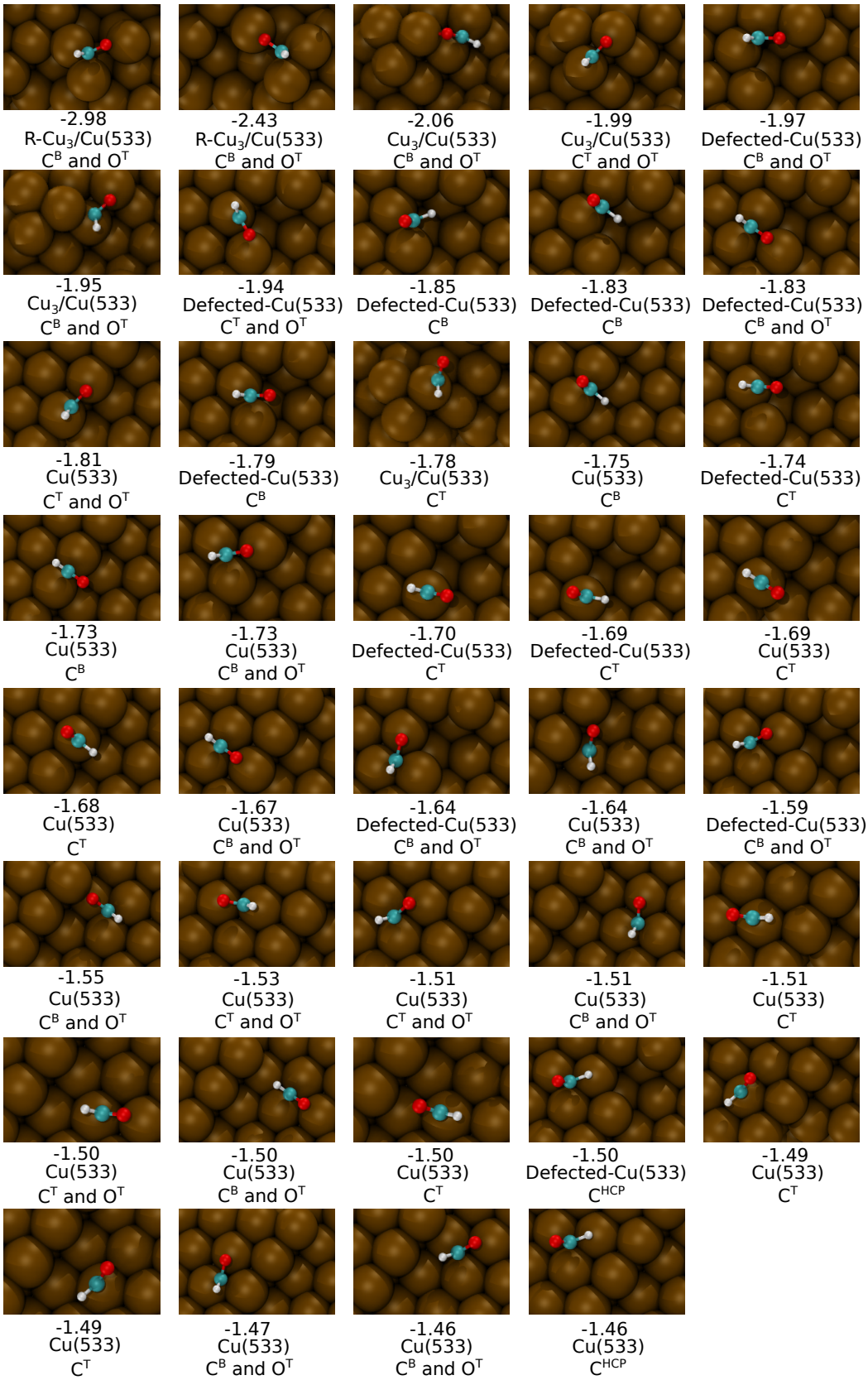


Figure S10: CHO interacting with different Cu sites and their respective adsorption energies. We also indicate the Cu surface for each case and describe the adsorption site as A^S, where A is the nearest atom from an adsorbate to the surface and S the adsorption site.

Table S7: Adsorption, binding, interaction, and deformation energies in (eV), shortest distance between the substrate and C and O atoms, C−O, and C−H bond lengths for CHO molecules interacting with different adsorption sites.

E_{ad} (eV)	E_{bind} (eV)	E_{int} (eV)	ΔE^{Mol} (eV)	ΔE^{Sub} (eV)	C−Cu (Å)	O−Cu (Å)	C−O (Å)	C−H_{MIN} (Å)
−2.98	−1.11	−3.00	0.35	−0.32	2.04	1.95	1.27	1.12
−2.43	−0.56	−2.88	0.34	0.11	2.04	1.95	1.27	1.12
−2.06	−0.19	−2.49	0.33	0.10	1.99	1.97	1.27	1.12
−1.99	−0.12	−2.34	0.25	0.11	1.92	2.02	1.26	1.12
−1.97	−0.10	−2.41	0.30	0.13	2.05	2.05	1.27	1.12
−1.95	−0.09	−2.36	0.28	0.12	2.01	2.05	1.26	1.12
−1.94	−0.07	−2.21	0.20	0.07	1.92	2.04	1.25	1.12
−1.85	0.02	−1.92	0.05	0.03	2.08	NA	1.22	1.14
−1.83	0.03	−1.92	0.05	0.03	2.08	NA	1.22	1.13
−1.83	0.04	−2.29	0.32	0.14	2.02	2.02	1.27	1.11
−1.81	0.05	−2.06	0.19	0.06	1.92	2.07	1.25	1.12
−1.79	0.07	−1.92	0.09	0.03	2.05	2.61	1.23	1.12
−1.78	0.09	−1.84	0.04	0.02	1.92	NA	1.21	1.13
−1.75	0.12	−1.83	0.05	0.03	2.06	NA	1.22	1.13
−1.74	0.12	−1.82	0.06	0.02	1.96	NA	1.22	1.12
−1.73	0.13	−1.84	0.07	0.04	2.08	NA	1.22	1.12
−1.73	0.14	−2.16	0.31	0.12	2.05	2.05	1.27	1.11
−1.70	0.17	−1.75	0.03	0.02	1.96	NA	1.22	1.12
−1.69	0.18	−1.73	0.02	0.01	1.93	NA	1.21	1.12
−1.69	0.18	−1.74	0.03	0.02	1.95	NA	1.21	1.12
−1.68	0.19	−1.72	0.02	0.01	1.94	NA	1.20	1.13
−1.67	0.20	−2.10	0.31	0.13	2.05	2.06	1.27	1.11
−1.64	0.23	−2.03	0.29	0.10	1.93	NA	1.20	1.13
−1.64	0.23	−2.12	0.37	0.11	2.05	2.06	1.28	1.11
−1.59	0.28	−1.94	0.26	0.09	2.06	2.08	1.27	1.11
−1.55	0.31	−1.99	0.28	0.16	2.12	2.09	1.26	1.12
−1.53	0.34	−1.72	0.13	0.05	1.95	2.26	1.24	1.12
−1.51	0.36	−1.74	0.18	0.05	1.98	2.24	1.25	1.12
−1.51	0.36	−1.79	0.21	0.08	2.05	2.19	1.25	1.12
−1.51	0.36	−1.59	0.03	0.05	1.98	NA	1.21	1.12
−1.50	0.36	−1.68	0.13	0.05	1.94	2.25	1.24	1.12
−1.50	0.36	−1.79	0.21	0.08	2.05	2.18	1.25	1.12
−1.50	0.37	−1.60	0.05	0.06	1.98	NA	1.21	1.12
−1.50	0.37	−1.76	0.22	0.04	2.03	2.12	1.26	1.11
−1.49	0.37	−1.58	0.03	0.05	1.98	NA	1.21	1.12
−1.49	0.38	−1.56	0.03	0.04	1.98	NA	1.21	1.12
−1.47	0.40	−1.78	0.23	0.08	2.00	2.17	1.26	1.11
−1.46	0.41	−1.73	0.20	0.06	2.05	2.21	1.25	1.12
−1.46	0.41	−1.64	0.15	0.04	2.10	NA	1.22	1.20

5.6 OH Adsorption

For OH adsorption, the molecule adsorbed on all sites via the O atom, also leading to fewer distinct configurations as compared with COOH, COH, or CHO. Table S8 shows all the energetic and structural data for the systems. Again, the geometry optimizations lead to some surface reconstruction cases that were not considered for the free energy change or E_{bind} vs *GCN* analysis. In terms of adsorption site preference, OH adsorbed preferentially on hollow sites, with the exceptions being molecules adsorbed on bridge sites for some low-coordinated regions.

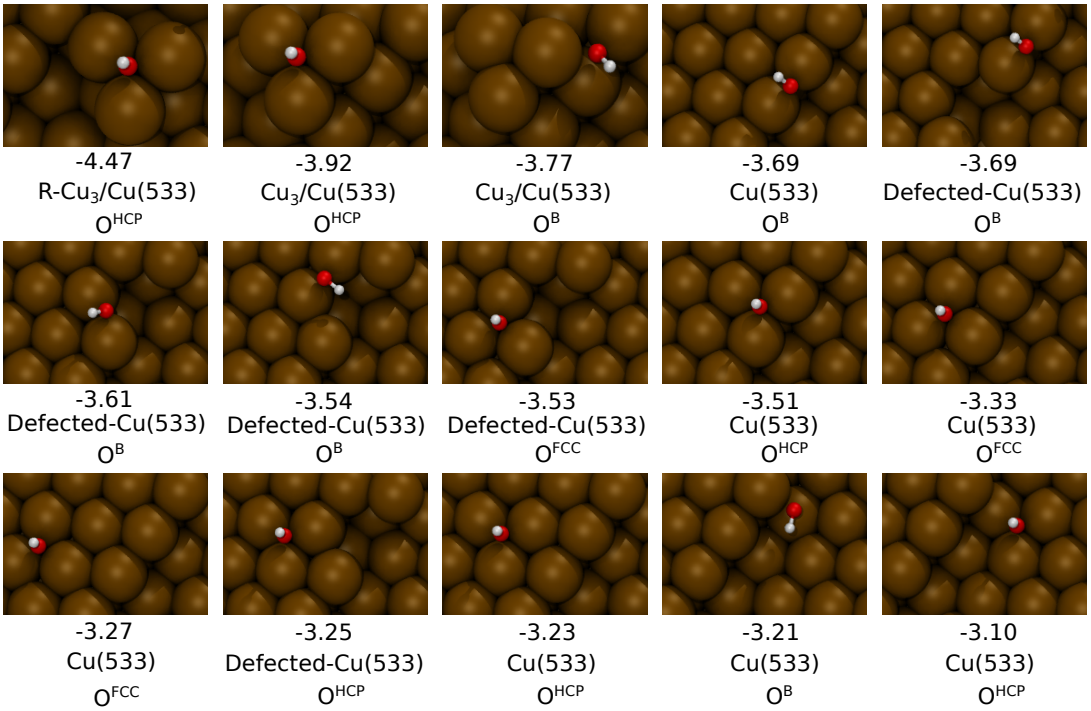


Figure S11: OH interacting with different Cu sites and their respective adsorption energies. We also indicate the Cu surface for each case and describe the adsorption site as A^S, where A is the nearest atom from an adsorbate to the surface and S the adsorption site.

Table S8: Adsorption, binding, interaction, and deformation energies in (eV), shortest distance between the substrate and O atoms and O−H bond lengths for OH molecules interacting with different adsorption sites.

E_{ad} (eV)	E_{bind} (eV)	E_{int} (eV)	ΔE^{Mol} (eV)	ΔE^{Sub} (eV)	O−Cu (Å)	O−H (Å)
−4.47	−1.15	−4.12	0.00	−0.35	2.02	0.97
−3.92	−0.60	−4.01	0.00	0.09	2.02	0.97
−3.77	−0.45	−3.88	0.00	0.11	2.02	0.97
−3.69	−0.37	−3.77	0.00	0.08	1.95	0.97
−3.69	−0.37	−3.74	0.00	0.05	1.96	0.97
−3.61	−0.29	−3.67	0.00	0.06	1.94	0.97
−3.54	−0.23	−3.62	0.00	0.08	1.96	0.97
−3.53	−0.21	−3.69	0.00	0.16	1.99	0.97
−3.51	−0.19	−3.62	0.00	0.11	1.98	0.97
−3.33	−0.01	−3.47	0.00	0.14	2.02	0.97
−3.27	0.05	−3.40	0.00	0.13	2.02	0.97
−3.25	0.07	−3.36	0.00	0.11	2.03	0.97
−3.23	0.09	−3.34	0.01	0.10	2.03	0.97
−3.21	0.11	−3.27	0.00	0.06	1.95	0.98
−3.10	0.22	−3.20	0.01	0.09	2.02	0.97

5.7 H Adsorption

We have also calculate the adsorption of H that can be used to study the hydrogen evolution reaction (HER) as a function of *GCN* to understand how we could expect this reaction to compete with the CO_2 reduction reaction. Figure S12 shows the configurations for H adsorption while Table S9 shows all the energetic and structural data for the systems. For H adsorption, most initial structures lead to H being adsorbed on hollow sites. Differently from the other cases, the adsorption energies of H was less affected by the adsorption site coordination with a range of only 0.11 eV of difference for sites varying from 7.67 to 3.50 of GCN. The only exceptions happened for highly coordinated adsorption sites below the Cu(533) step that weakened the adsorption energies by almost 0.20 eV. These results indicate that the dependence of the HER as a function of *GCN* should be smaller than the one for CO_2 reduction reaction, and that we could expect the HER U_{onset} to not linearly vary with the adsorption site coordination.

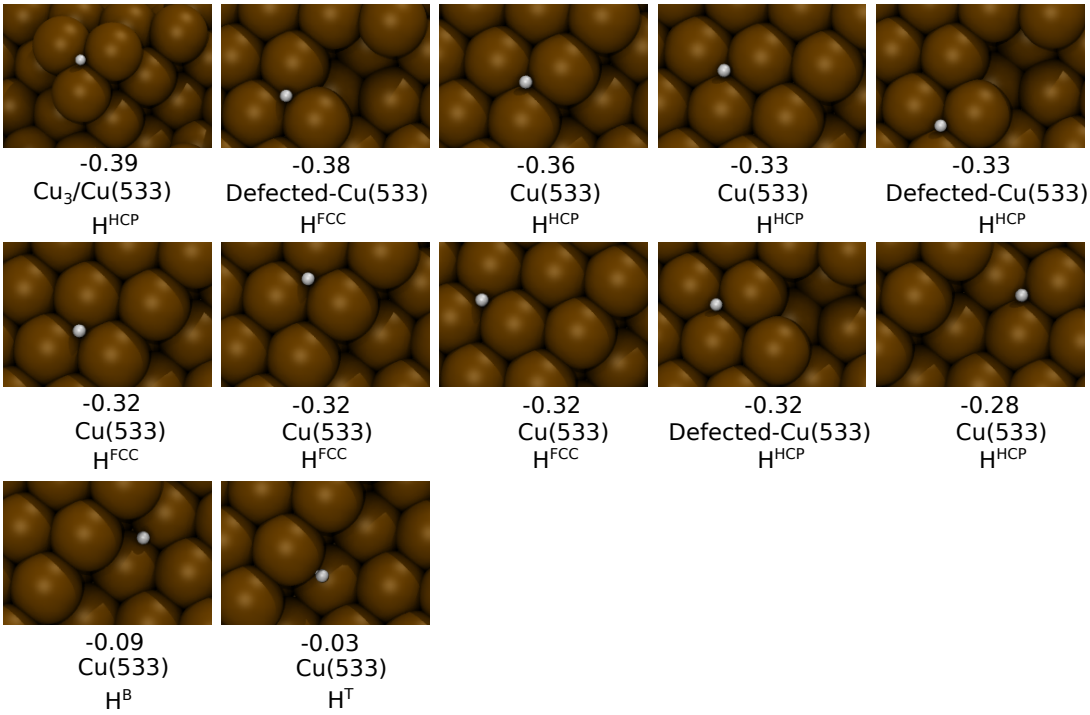


Figure S12: H interacting with different Cu sites and their respective adsorption energies. We also indicate the Cu surface for each case and describe the adsorption site as A^S, where A is the nearest atom from an adsorbate to the surface and S the adsorption site.

Table S9: Adsorption, binding, interaction, and deformation energies in (eV), together with the shortest distance between the substrate and H atoms for H interacting with different adsorption sites.

E_{ad} (eV)	E_{bind} (eV)	E_{int} (eV)	ΔE^{Sub} (eV)	H−Cu (Å)
−0.39	−0.39	−0.42	0.03	1.75
−0.38	−0.38	−0.40	0.02	1.72
−0.36	−0.36	−0.38	0.02	1.73
−0.33	−0.33	−0.36	0.03	1.73
−0.33	−0.33	−0.35	0.02	1.74
−0.32	−0.32	−0.35	0.03	1.74
−0.32	−0.32	−0.34	0.02	1.74
−0.32	−0.32	−0.34	0.02	1.72
−0.32	−0.32	−0.34	0.02	1.73
−0.28	−0.28	−0.31	0.03	1.72
−0.09	−0.09	−0.11	0.02	1.73
−0.03	−0.03	−0.05	0.02	1.63

6 Adsorption of CO_2 reduction intermediates used for validation

As discussed before, we also performed calculations to validate the correlations between *GCN* and E_{bind} obtained for each molecule. For these calculations, we analyzed the adsorption of the molecules on Cu(111), Cu(100), and Cu(211) surfaces. For all the adsorbates, we initialized the calculations by positioning the molecules on top, bridge, and hollow (FCC and HCP) sites mimicking the lowest energy configurations from the calculations used to obtain the correlations. We also calculated CO and OH interaction with icosahedral Cu_n nanoparticles with ($n = 13$, 55, 147, and 309), where we studied adsorption sites near the vertices and close to the center of the particle facets. In the following sections, we show the distinct configurations obtained for each surface and adsorbate as well as their main energetic and structural results.

6.1 COOH Adsorption

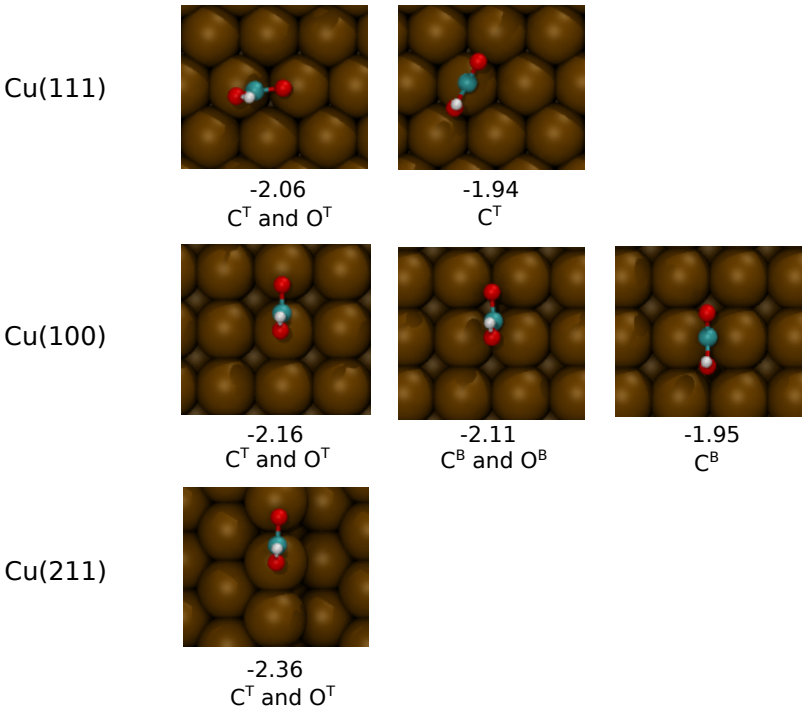


Figure S13: COOH interacting with different Cu sites and their respective adsorption energies. We also the adsorption site as A^S, where A is the nearest atom from an adsorbate to the surface and S the adsorption site.

Table S10: Adsorption, binding, interaction, and deformation energies in (eV), together with the shortest distance between the substrate and C and O atoms, C−O, C−OH, and O−H bond lengths, for COOH molecules interacting with different adsorption sites.

E_{ad} (eV)	E_{bind} (eV)	E_{int} (eV)	ΔE^{Mol} (eV)	ΔE^{Sub} (eV)	C−Cu (Å)	O−Cu (Å)	C−O (Å)	C−OH (Å)	O−H (Å)
				Cu(111)					
−2.06	−0.03	−2.42	0.30	0.06	1.95	2.15	1.26	1.34	0.99
−1.94	0.09	−2.11	0.15	0.03	1.96	3.09	1.22	1.37	0.99
				Cu(100)					
−2.16	−0.12	−2.56	0.33	0.07	1.94	2.07	1.26	1.34	0.99
−2.11	−0.07	−2.68	0.49	0.08	2.04	2.21	1.29	1.35	0.99
−1.95	0.09	−2.21	0.21	0.05	2.09	3.12	1.23	1.39	0.99
				Cu(211)					
−2.38	−0.34	−2.80	0.34	0.08	1.93	2.03	1.26	1.34	0.99

6.2 HCOO Adsorption

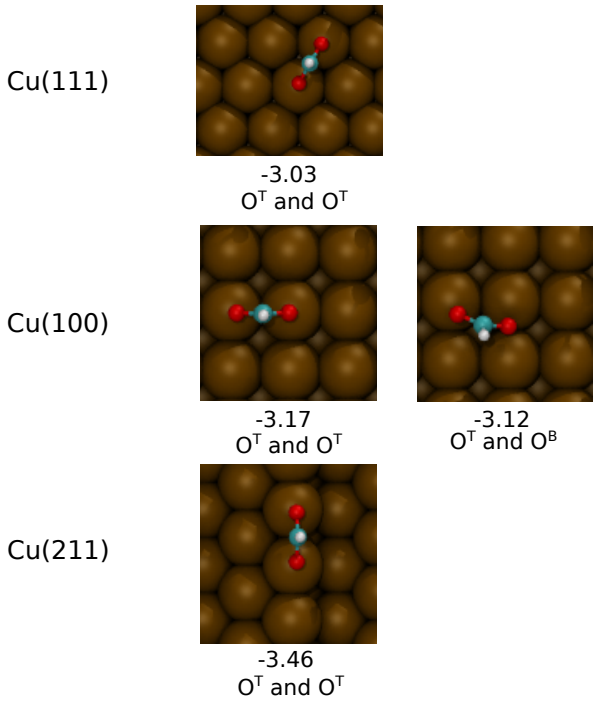


Figure S14: HCOO interacting with different Cu sites and their respective adsorption energies. We also the adsorption site as A^S, where A is the nearest atom from an adsorbate to the surface and S the adsorption site.

Table S11: Adsorption, binding, interaction, and deformation energies in (eV), together with the shortest distance between the substrate and O atoms, C−O, and C−H bond lengths, for HCOO molecules interacting with different adsorption sites.

E_{ad} (eV)	E_{bind} (eV)	E_{int} (eV)	ΔE^{Mol} (eV)	ΔE^{Sub} (eV)	O−Cu$_{MIN}$ (Å)	C−O$_{MIN}$ (Å)	C−H (Å)
Cu(111)							
−3.03	−0.78	−3.42	0.32	0.07	2.01	1.27	1.11
Cu(100)							
−3.17	−0.92	−3.56	0.32	0.07	1.99	1.27	1.11
−3.12	−0.87	−3.56	0.32	0.08	2.04	1.26	1.11
Cu(211)							
−3.46	−1.20	−3.84	0.32	0.06	1.96	1.27	1.11

6.3 CO Adsorption

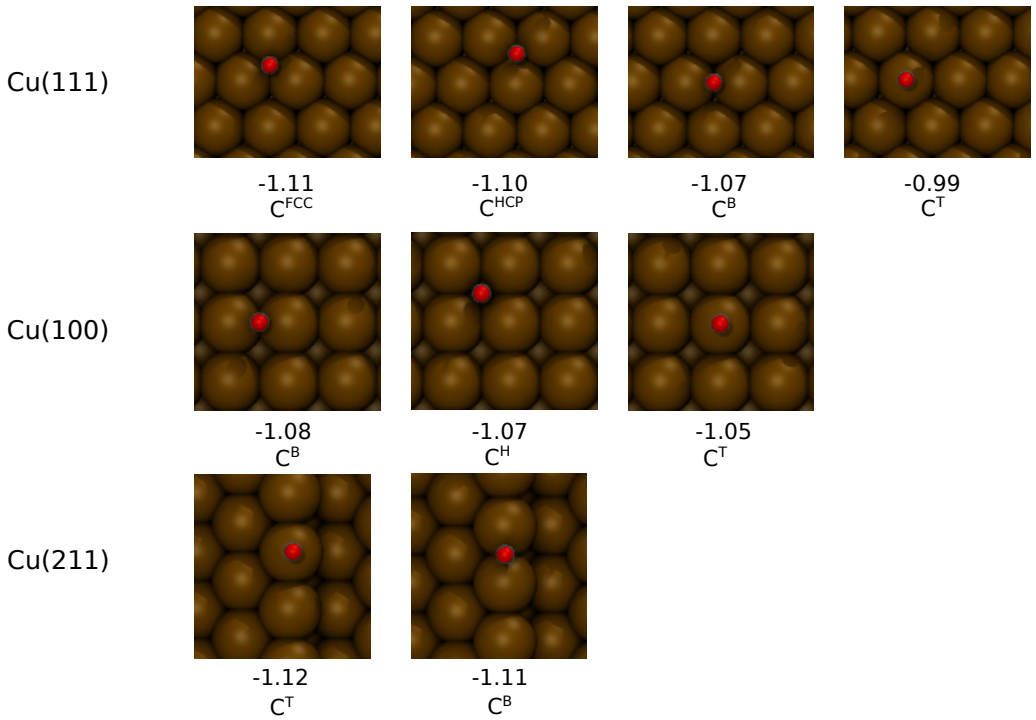


Figure S15: CO interacting with different Cu sites and their respective adsorption energies. We also the adsorption site as A^S, where A is the nearest atom from an adsorbate to the surface and S the adsorption site.

Table S12: Adsorption, binding, interaction, and deformation energies in (eV), shortest distance between the substrate and C atoms and C−O bond lengths for CO molecules interacting with different adsorption sites.

E_{ad} (eV)	E_{bind} (eV)	E_{int} (eV)	ΔE^{Mol} (eV)	ΔE^{Sub} (eV)	C−Cu (Å)	C−O (Å)
			Cu(111)			
−1.11	−0.36	−1.22	0.08	0.03	2.05	1.18
−1.10	−0.35	−1.22	0.08	0.04	2.05	1.18
−1.07	−0.32	−1.15	0.06	0.03	1.98	1.17
−0.99	−0.24	−1.03	0.01	0.03	1.85	1.15
			Cu(100)			
−1.08	−0.33	−1.17	0.05	0.05	1.98	1.17
−1.07	−0.32	−1.27	0.15	0.06	2.14	1.19
−1.05	−0.30	−1.10	0.01	0.03	1.84	1.15
			Cu(211)			
−1.12	−0.36	−1.15	0.01	0.03	1.84	1.15
−1.11	−0.35	−1.20	0.04	0.05	1.97	1.17

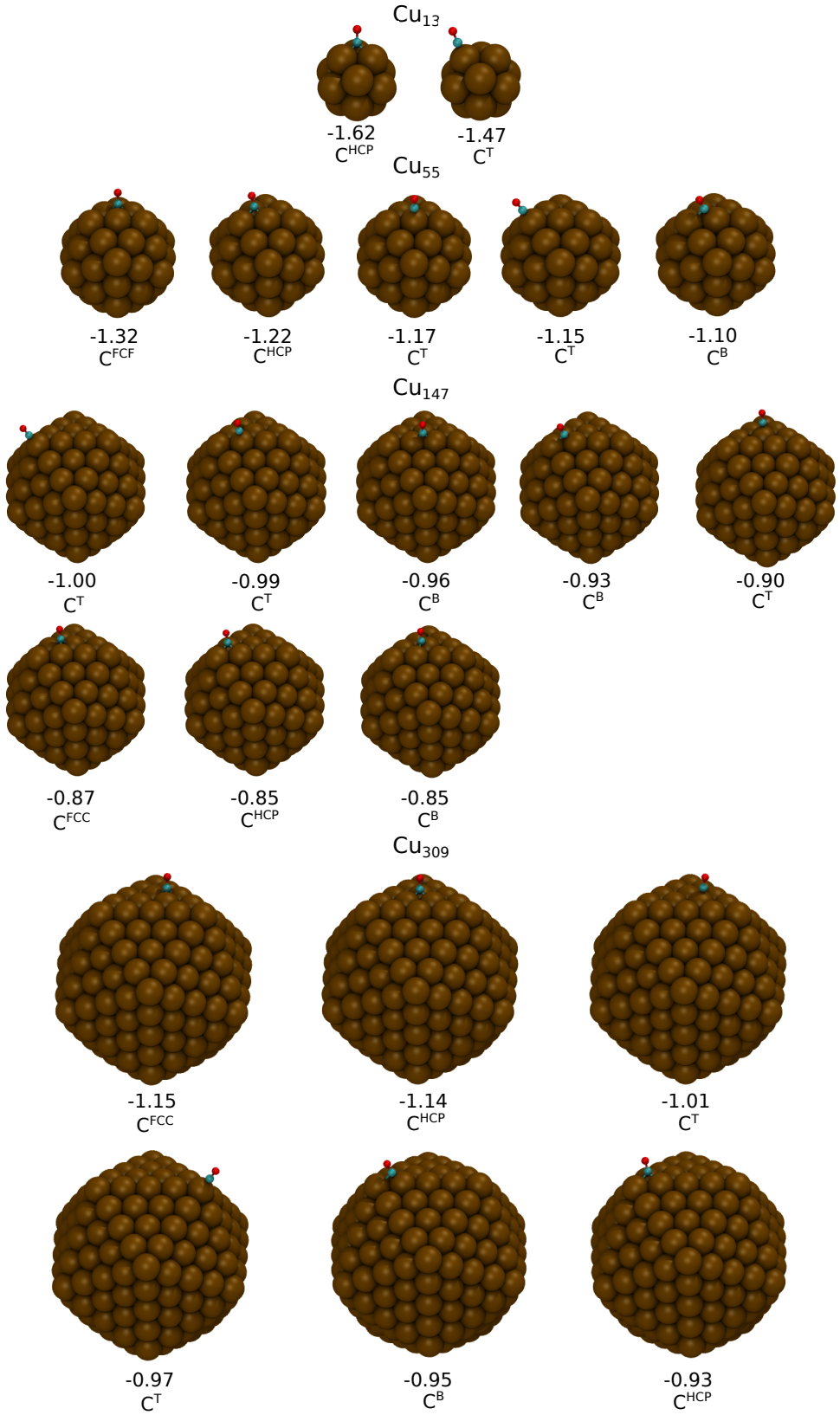


Figure S16: CO interacting with different Cu sites and their respective adsorption energies. We also the adsorption site as A^S, where A is the nearest atom from an adsorbate to the surface and S the adsorption site.

Table S13: Adsorption, binding, interaction, and deformation energies in (eV), shortest distance between the substrate and C atoms and C−O bond lengths for CO molecules interacting with different adsorption sites.

E_{ad} (eV)	E_{bind} (eV)	E_{int} (eV)	ΔE^{Mol} (eV)	ΔE^{Sub} (eV)	C−Cu (Å)	C−O (Å)
			Cu_{13}			
−1.62	−0.86	−1.79	0.14	0.04	2.02	1.19
−1.47	−0.71	−1.51	0.01	0.03	1.79	1.15
			Cu_{55}			
−1.32	−0.56	−1.49	0.11	0.06	2.04	1.19
−1.22	−0.47	−1.42	0.12	0.07	2.00	1.19
−1.17	−0.41	−1.22	0.01	0.04	1.83	1.15
−1.15	−0.39	−1.18	0.01	0.03	1.83	1.15
−1.10	−0.35	−1.21	0.05	0.06	1.87	1.17
			Cu_{147}			
−1.00	−0.25	−1.03	0.01	0.02	1.84	1.15
−0.99	−0.23	−1.05	0.01	0.05	1.85	1.15
−0.96	−0.20	−1.08	0.05	0.08	1.97	1.17
−0.93	−0.17	−1.04	0.04	0.07	1.89	1.17
−0.90	−0.15	−0.98	0.01	0.06	1.86	1.15
−0.87	−0.12	−1.02	0.09	0.06	2.05	1.18
−0.85	−0.10	−1.02	0.10	0.08	2.02	1.18
−0.85	−0.10	−0.97	0.06	0.06	1.97	1.17
			Cu_{309}			
−1.15	−0.39	−1.29	0.10	0.04	2.03	1.18
−1.14	−0.38	−1.28	0.09	0.05	2.04	1.18
−1.01	−0.25	−1.05	0.01	0.03	1.85	1.15
−0.97	−0.22	−1.00	0.01	0.02	1.85	1.15
−0.95	−0.19	−1.02	0.04	0.04	1.85	1.16
−0.93	−0.17	−1.08	0.10	0.05	2.01	1.18

6.4 COH Adsorption

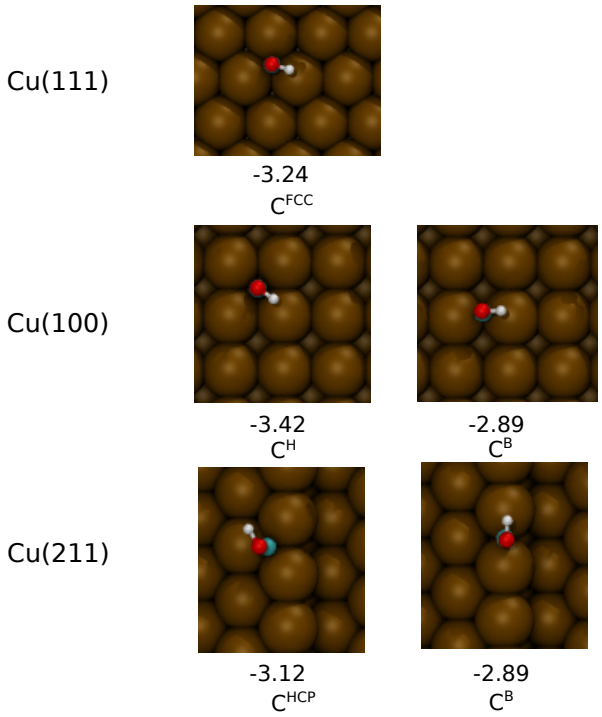


Figure S17: COH interacting with different Cu sites and their respective adsorption energies. We also the adsorption site as A^S, where A is the nearest atom from an adsorbate to the surface and S the adsorption site.

Table S14: Adsorption, binding, interaction, and deformation energies in (eV), shortest distance between the substrate and C atoms, C−OH, and O−H bond lengths for COH molecules interacting with different adsorption sites.

E_{ad} (eV)	E_{bind} (eV)	E_{int} (eV)	ΔE^{Mol} (eV)	ΔE^{Sub} (eV)	C−Cu (Å)	C−OH (Å)	O−H (Å)
			Cu(111)				
−3.24	0.52	−3.39	0.08	0.06	1.91	1.34	0.98
			Cu(100)				
−3.42	0.34	−3.68	0.17	0.09	2.02	1.37	0.98
−2.89	0.87	−3.03	0.05	0.09	1.87	1.32	0.98
			Cu(211)				
−3.12	0.64	−3.28	0.08	0.08	1.90	1.34	0.98
−2.89	0.87	−3.00	0.04	0.07	1.87	1.31	0.98

6.5 CHO Adsorption

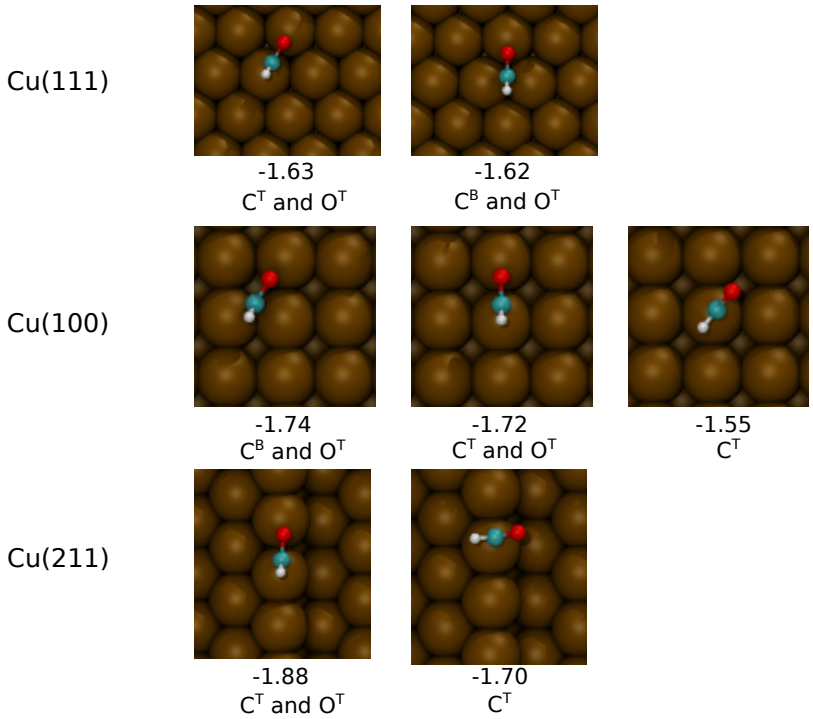


Figure S18: CHO interacting with different Cu sites and their respective adsorption energies. We also the adsorption site as A^S, where A is the nearest atom from an adsorbate to the surface and S the adsorption site.

Table S15: Adsorption, binding, interaction, and deformation energies in (eV), shortest distance between the substrate and C and O atoms, C−O, and C−H bond lengths for CHO molecules interacting with different adsorption sites.

E_{ad} (eV)	E_{bind} (eV)	E_{int} (eV)	ΔE^{Mol} (eV)	ΔE^{Sub} (eV)	C−Cu (Å)	O−Cu (Å)	C−O (Å)	C−H_{MIN} (Å)
				Cu(111)				
−1.63	0.24	−1.85	0.17	0.05	1.95	2.16	1.24	1.12
−1.62	0.25	−1.96	0.26	0.08	2.06	2.12	1.26	1.11
				Cu(100)				
−1.74	0.13	−2.16	0.34	0.09	1.99	2.08	1.27	1.12
−1.72	0.15	−1.96	0.17	0.07	1.92	2.12	1.24	1.12
−1.55	0.32	−1.62	0.04	0.02	1.96	3.21	1.21	1.13
				Cu(211)				
−1.88	−0.02	−2.14	0.19	0.06	1.92	2.06	1.25	1.12
−1.70	0.17	−1.75	0.04	0.02	1.95	2.80	1.21	1.12

6.6 OH Adsorption

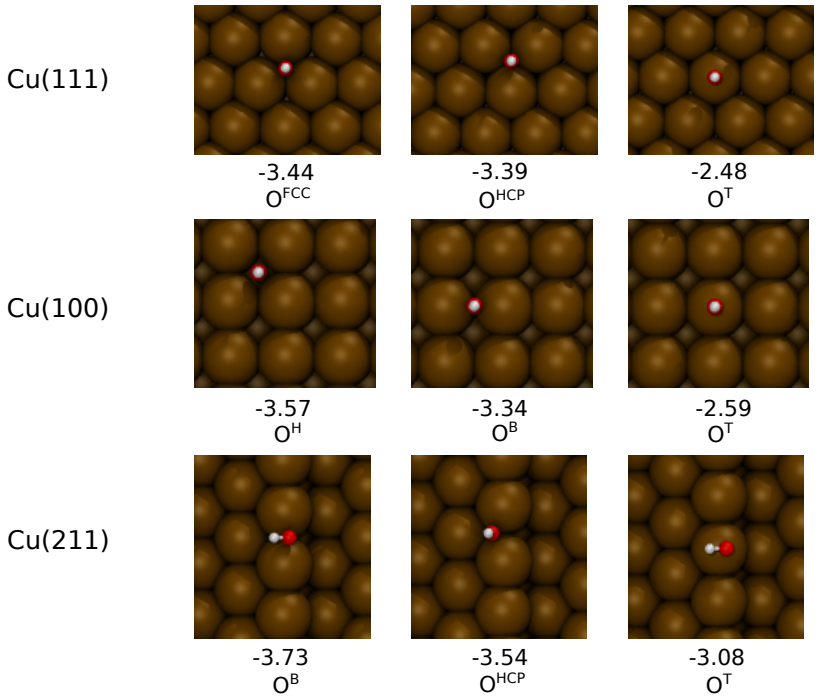


Figure S19: OH interacting with different Cu sites and their respective adsorption energies. We also the adsorption site as A^S, where A is the nearest atom from an adsorbate to the surface and S the adsorption site.

Table S16: Adsorption, binding, interaction, and deformation energies in (eV), shortest distance between the substrate and O atoms and O−H bond lengths for OH molecules interacting with different adsorption sites.

E_{ad} (eV)	E_{bind} (eV)	E_{int} (eV)	ΔE^{Mol} (eV)	ΔE^{Sub} (eV)	O−Cu (Å)	O−H (Å)
			Cu(111)			
−3.44	−0.12	−3.57	0.00	0.13	2.02	0.97
−3.39	−0.07	−3.49	0.00	0.09	2.04	0.97
−2.48	0.84	−2.51	0.01	0.01	1.84	0.96
			Cu(100)			
−3.57	−0.25	−3.64	0.00	0.07	2.17	0.98
−3.34	−0.02	−3.47	0.01	0.13	1.94	0.97
−2.59	0.73	−2.62	0.01	0.02	1.82	0.96
			Cu(211)			
−3.73	−0.41	−3.81	0.00	0.08	1.95	0.97
−3.54	−0.22	−3.64	0.01	0.10	1.95	0.97
−3.08	0.24	−2.62	0.01	0.02	1.83	0.97

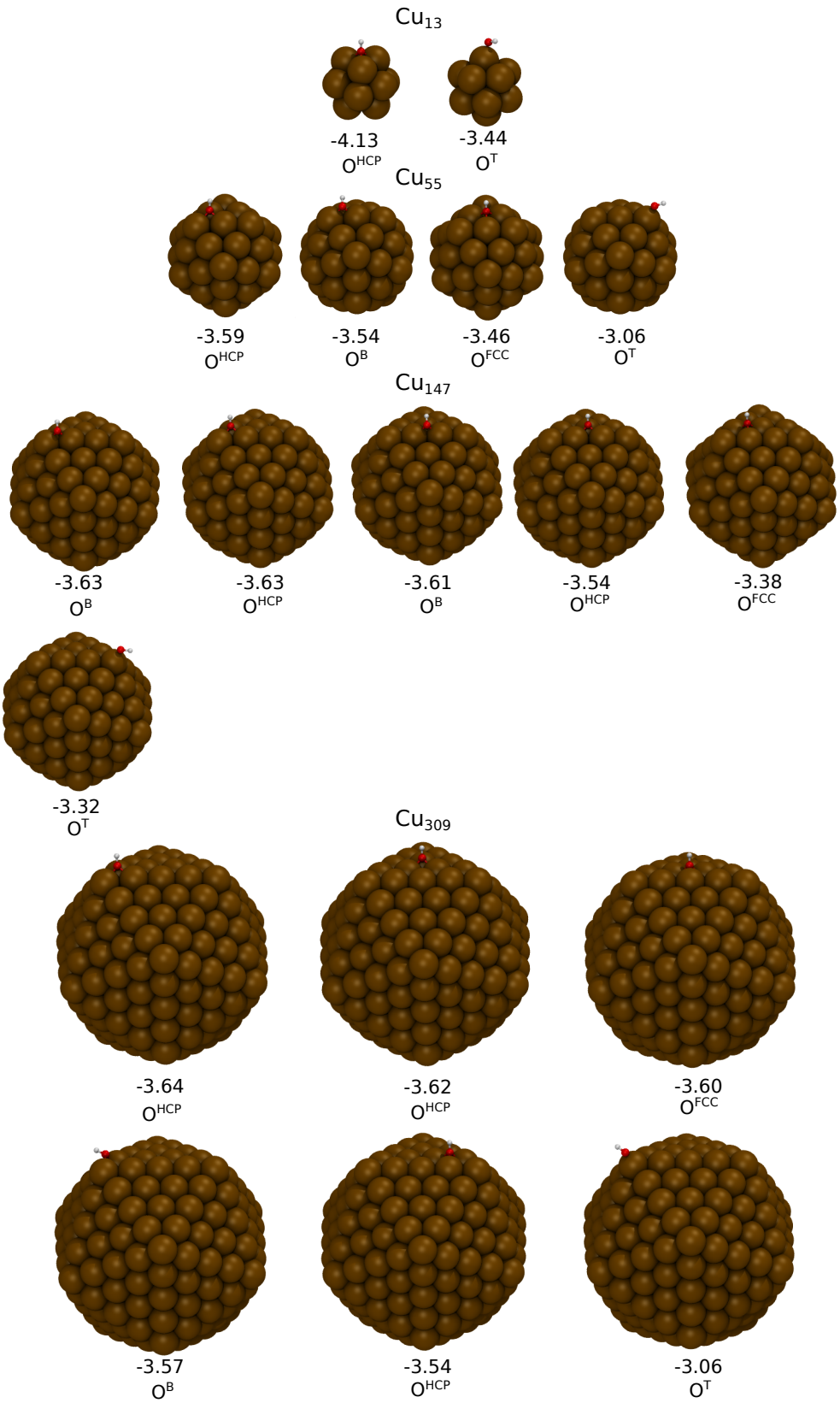


Figure S20: OH interacting with different Cu sites and their respective adsorption energies. We also the adsorption site as A^S, where A is the nearest atom from an adsorbate to the surface and S the adsorption site.

Table S17: Adsorption, binding, interaction, and deformation energies in (eV), shortest distance between the substrate and O atoms and O−H bond lengths for OH molecules interacting with different adsorption sites.

E_{ad} (eV)	E_{bind} (eV)	E_{int} (eV)	ΔE^{Mol} (eV)	ΔE^{Sub} (eV)	O−Cu (Å)	O−H (Å)
			Cu_{13}			
−4.13	−1.81	−4.57	0.00	0.44	2.03	0.97
−3.44	−0.12	−3.46	0.00	0.02	1.80	0.97
			Cu_{55}			
−3.59	−0.27	−3.74	0.00	0.15	2.04	0.97
−3.54	−0.22	−3.66	0.00	0.11	1.96	0.97
−3.46	−0.14	−3.63	0.00	0.17	2.06	0.97
−3.06	0.26	−3.13	0.00	0.06	1.81	0.97
			Cu_{147}			
−3.63	−0.32	−3.73	0.00	0.09	1.94	0.97
−3.63	−0.32	−3.76	0.00	0.12	1.99	0.97
−3.61	−0.29	−3.72	0.01	0.11	1.96	0.97
−3.54	−0.22	−3.70	0.00	0.16	2.00	0.97
−3.38	−0.66	−3.55	0.00	0.17	2.05	0.97
−3.32	0.00	−3.73	0.00	0.03	1.80	0.97
			Cu_{309}			
−3.64	−0.32	−3.77	0.00	0.13	2.01	0.97
−3.62	−0.30	−3.74	0.01	0.12	2.04	0.97
−3.60	−0.28	−3.77	0.00	0.17	2.03	0.97
−3.57	−0.25	−3.66	0.00	0.08	1.96	0.97
−3.54	−0.22	−3.72	0.00	0.17	2.03	0.97
−3.06	0.25	−3.10	0.00	0.03	1.81	0.97

6.7 H Adsorption

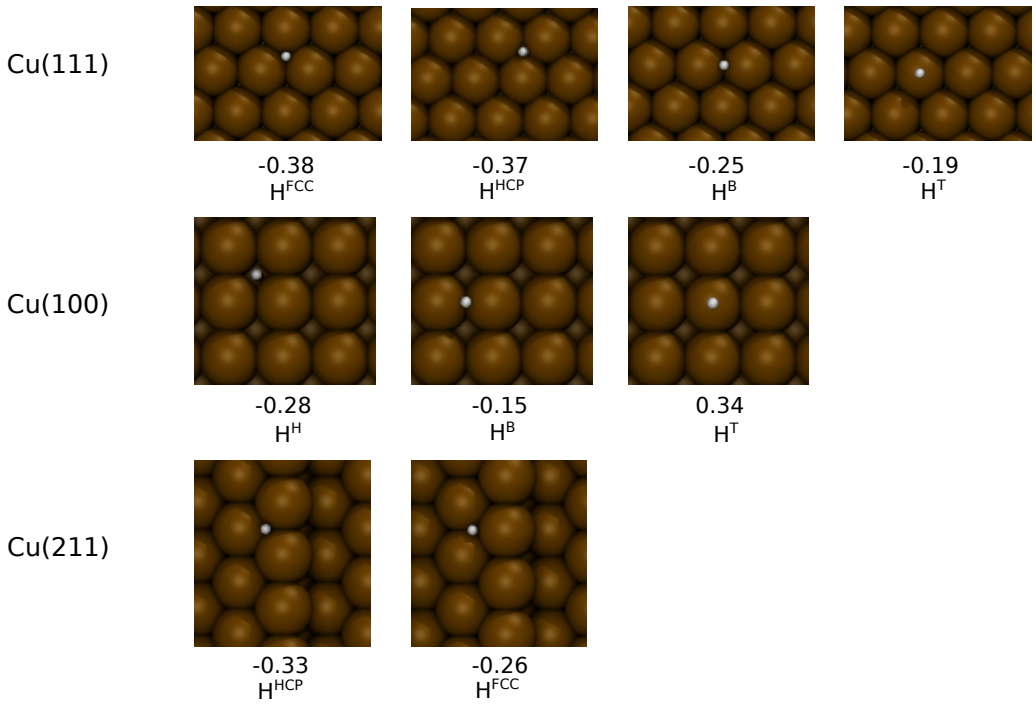


Figure S21: H interacting with different Cu sites and their respective adsorption energies. We also the adsorption site as A^S, where A is the nearest atom from an adsorbate to the surface and S the adsorption site.

Table S18: Adsorption, binding, interaction, and deformation energies in (eV), together with the shortest distance between the substrate and H atoms for H interacting with different adsorption sites.

E_{ad} (eV)	E_{bind} (eV)	E_{int} (eV)	ΔE^{Sub} (eV)	H−Cu (Å)
		Cu(111)		
−0.38	−0.38	−0.39	0.02	1.74
−0.37	−0.37	−0.39	0.02	1.74
−0.25	−0.25	−0.26	0.01	1.66
0.19	0.19	0.19	0.00	1.51
		Cu(100)		
−0.28	−0.28	−0.30	0.02	1.87
−0.15	−0.15	−0.18	0.03	1.64
0.34	0.34	0.33	0.01	1.52
		Cu(211)		
−0.33	−0.33	−0.35	0.02	1.72
−0.26	−0.26	−0.29	0.03	1.72

7 Vibrational and solvation corrections

The free energy energy changes of the reaction steps as a function of the adsorption site *GCN* were studied considering all the terms described in equation 2, including the ZPE, $\int C_p dT$, and TS terms and solvation energies, E_{sol}. The ZPE, $\int C_p dT$, and TS were obtained in a previous contribution from our group that studied in more details the reaction mechanisms for CO_2 electroreduction on Cu surfaces.[4]

In our previous work, we observed that ZPE, $\int C_p dT$, and TS values obtained for adsorption sites with different levels of coordination are similar, with the deviations among the different sites being no higher than 0.03 eV.[4] Thus, we considered acceptable to use the average value obtained for these three adsorption sites for all the other adsorption sites. For the solvation energies, we employed the values obtained from two different papers from the literature,[6,8] and compared in section 9 how the different solvation energies impacted our insights. In the work of Peterson et al.[6], the authors only describe the solvation energies applied to a set of intermediates that do not include *HCOO, and hence, we assumed that no solvation energy was applied for such intermediate. Table S19 shows the values for ZPE, $\int C_p dT$, and TS together with the sum of those quantities and the used E_{sol}.

Table S19: Values of ZPE, $\int C_p dT$, TS, and the sum of the three quantities obtained averaging the results from Cu surfaces with three different coordination regions.[4] E_{sol} obtained from the literature, $SC1$[6] and $SC2$.[8] The solvation energy for *HCOO intermediate was assumed as zero. All energetic quantities are given in eV.

	ZPE	$\int C_p dT$	TS	$Total$	E_{sol}^{SC1}	E_{sol}^{SC2}
COOH	0.61	0.11	0.21	0.50	−0.25	−0.28
HCOO	0.63	0.10	0.19	0.53	0.00*	0.00*
CO	0.19	0.08	0.17	0.10	−0.10	0.00
COH	0.47	0.08	0.14	0.41	−0.25	−0.45
CHO	0.46	0.08	0.15	0.39	−0.10	0.00
OH	0.35	0.05	0.08	0.31	−0.50	−0.58
H	0.16	0.01	0.01	0.16	0.00	0.00

For the non-adsorbed species, we have considered the same values of fugacities and assumptions that are widely employed in the literature.[6,10,18,23] To account for the inconsistency

of thermochemical data calculated with the PBE functional, an additional −0.51 eV was added as a gas-phase correction (GPC) to the energy of CO as calculated by Peterson *et al.*.[6]

Table S20: Averages and standard deviations of $ZPE + \int C_p dT - TS$ and gas-phase correction values for all non-adsorbed species, together with the assumed fugacities obtained by Peterson *et al.*.[6]

	Fugacity (Pa)	ZPE (eV)	$\int C_p dT$ (eV)	TS (eV)	GPC (eV)
CO_2	101325	0.31	0.10	0.66	
CO	5562	0.13	0.10	0.67	−0.51
HCOOH	2	0.89	0.11	1.04	
H_2	30296	0.27	0.09	0.43	
CH_4	20467	1.19	0.10	0.62	
H_2O	3534	0.56	0.10	0.67	

8 Binding energies versus generalized coordination number

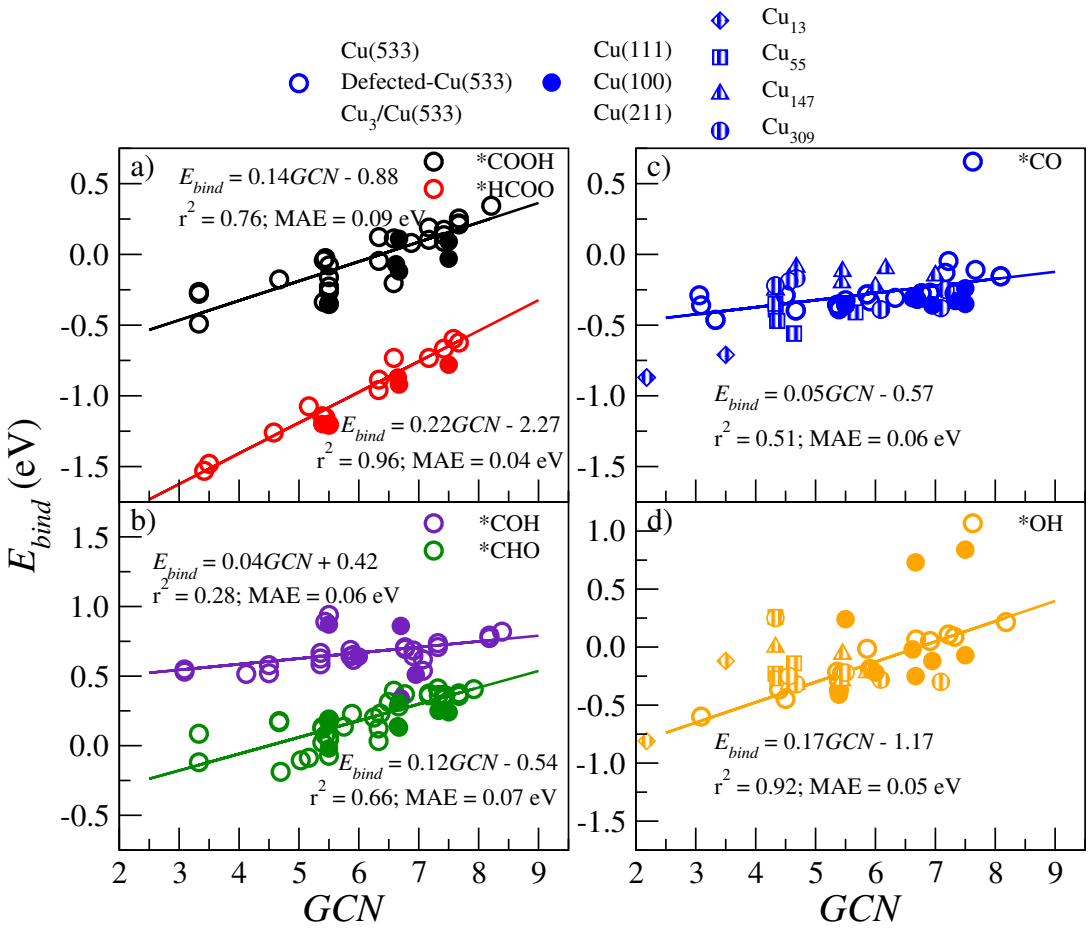


Figure S22: Binding energies versus *GCN* values of the respective adsorption sites considering all the distinct configurations obtained for each adsorbate.

Figure S22 shows the dependency of binding energies and *GCN* for the six adsorbates using all obtained data. To assess how the inclusion of all the adsorbate configurations in the E_{bind} vs *GCN* equations impacts our main insights, we show on Figure S23 the diagrams of the negative of the free energy variation for the most important reaction steps vs the values of *GCN* for the formation of CO, HCOOH, and CH_4 using the equations from Figure S22. As compared with the results from the main manuscript, the overall trends are almost unaltered.

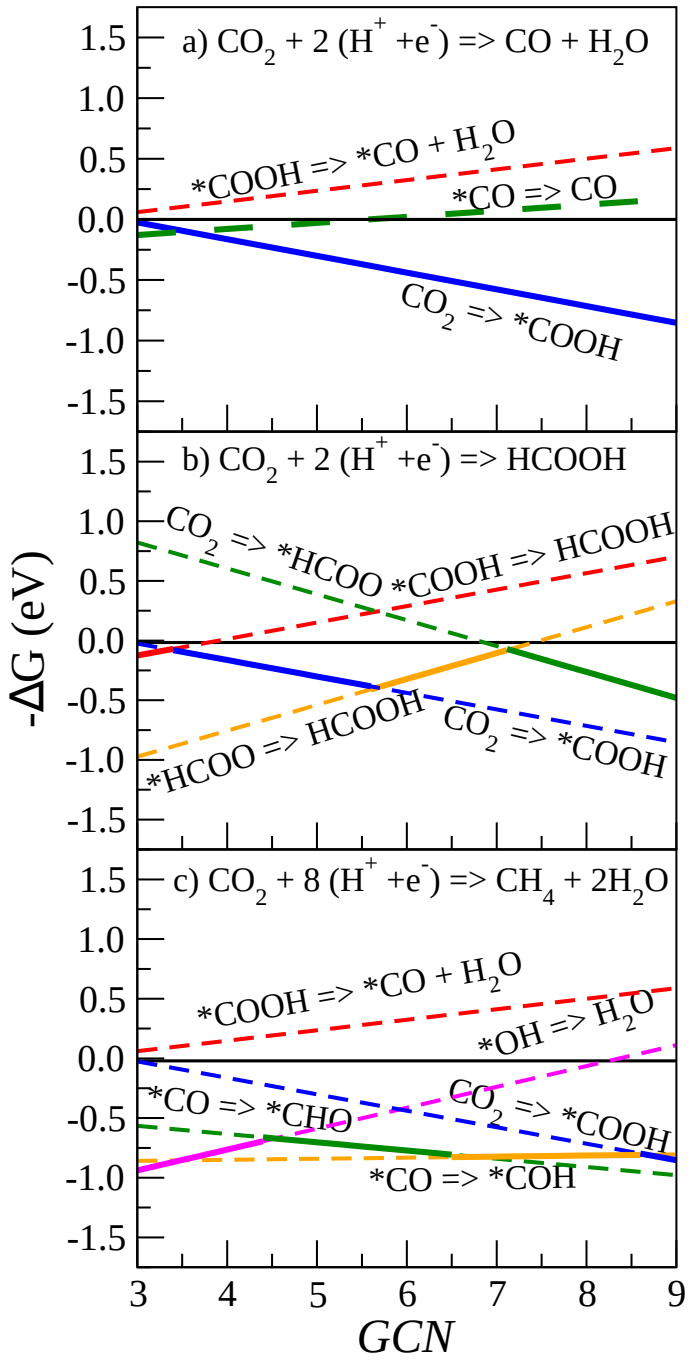


Figure S23: Negative of free energy change, $-\Delta G$, for each reaction step considered as a possible PDS for the reduction of CO_2 toward a) CO, b) HCOOH, c) CH_4 as a function of *GCN* for Cu surfaces. Solid lines mark the reaction step that acts as PDS for each product and *GCN* value.

The main changes from Figure S23 and the main manuscript are some slight shifts in the *GCN* values where the change of PDS for each reaction happens. Using the HCOOH formation as an example, we observe the existence of a reaction pathway bifurcation between the *COOH and *HCOO routes regardless of the fitting strategy. In both cases, the pathway

through *COOH is favorable for more undercoordinated sites, represented by lower values of *GCN*. The difference between the two fitting strategies is that the bifurcation is predicted for *GCN* $\geq$ than 5.7 or 5.9, if the fitting is performed with all the data or only energetically preferred configurations, respectively. All the other changes can be observed by comparing the results from Table S21 with the ones listed in the main manuscript.

Table S21: List of potential determining steps (PDS) for each range of *GCN* values for the CO_2 reduction towards CO, HCOOH, and CH_4. The data for this table was obtained with using the results from Figure S23

Product	PDS	GCN Range
CO	$CO_2 \longrightarrow$ *COOH	$3.0 \leq GCN \leq 9.0$
HCOOH	*COOH $\longrightarrow$ HCOOH	$3.0 \leq GCN \leq 3.5$
	$CO_2 \longrightarrow$ *COOH	$3.5 \leq GCN \leq 5.7$
	*HCOO $\longrightarrow$ HCOOH	$5.7 \leq GCN \leq 7.1$
	$CO_2 \longrightarrow$ *HCOO	$7.1 \leq GCN \leq 9.0$
CH_4	*OH $\longrightarrow H_2O$	$3.0 \leq GCN \leq 4.3$
	*CO $\longrightarrow$ *CHO	$4.3 \leq GCN \leq 6.6$
	*CO $\longrightarrow$ *COH	$6.6 \leq GCN \leq 8.6$
	$CO_2 \longrightarrow$ *COOH	$8.6 \leq GCN \leq 9.0$

9 Impact of solvation models

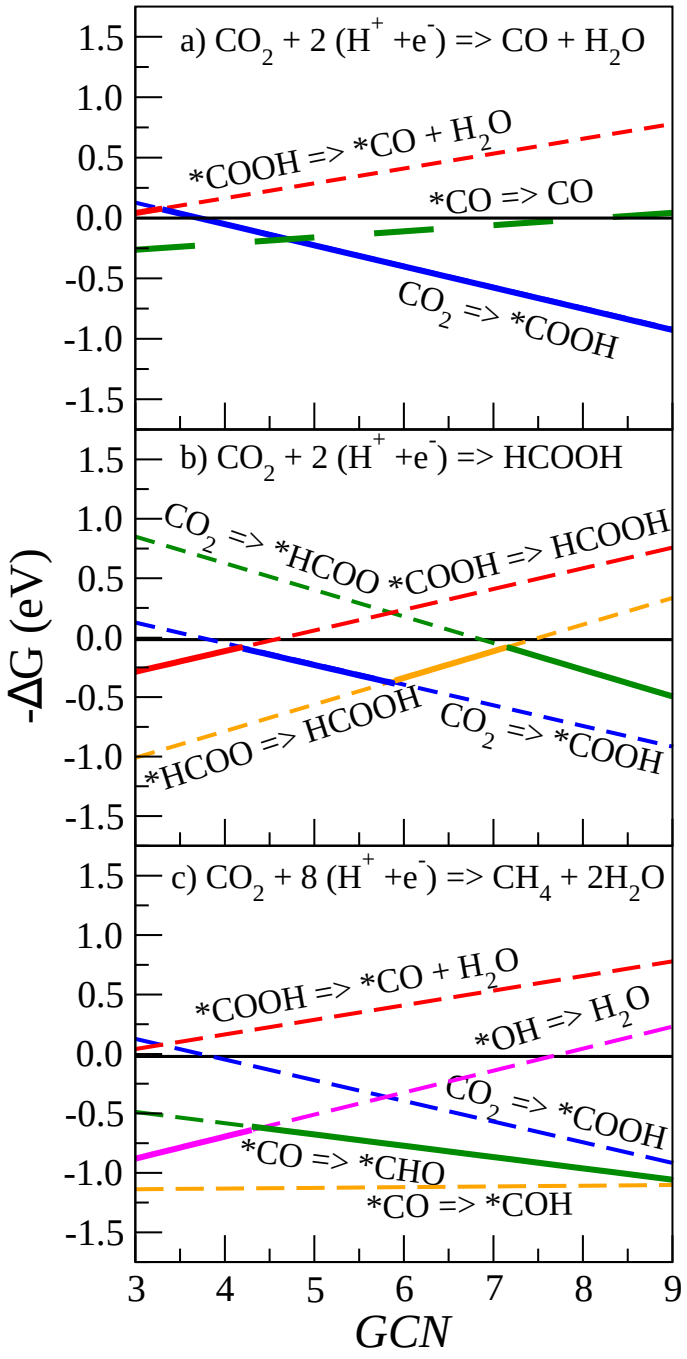


Figure S24: Negative of free energy change, $-\Delta G$, for each reaction step considered as a possible PDS for the reduction of CO_2 toward a) CO, b) HCOOH, c) CH_4 as a function of *GCN* for Cu surfaces. Solid lines mark the reaction step that acts as PDS for each product and *GCN* value. Here, we consider the equations for E_{bind} vs *GCN* from the main manuscript and the solvation energies from Peterson *et al.*.[6]

As discussed before, we employed as solvation energies the values obtained from two different papers from the literature.[6,8] While all the discussions in the main manuscript were performed using the solvation energies from the recent work from Rendón–Calle et al.,[8] here we show how the main results from our paper would change by using the the solvation energies from the work of Peterson et al..[6] Figure S24 shows the diagrams of the negative of the free energy variation for the most important reaction steps vs the values of *GCN* for the formation of CO, HCOOH, and CH_4 using the equations for E_{bind} vs *GCN* from the main manuscript and the solvation energies from Peterson et al..[6]

The main differences between the results obtained with both solvation schemes happen for the diagram towards CH_4. The solvation scheme from Peterson et al..[6] favors the *CHO path for all values of *GCN*. The reaction path through *CHO, when analyzed solely based on thermodynamic arguments, leads to CH_2O as an intermediate, which disagrees with experimental data.[9] Meanwhile the solvation scheme from Rendón–Calle et al.[8] shows a change between the *COH and *CHO path depending on the value of the adsorption site *GCN*. The favoring of the *COH path could make the experimental and theoretical data more comparable; however, the fact that this path is only favored for some *GCN* values could indicate that further analysis, such as kinetic data, might be needed when searching for the preferred reaction mechanisms. Apart from that, we see that most of the discussion from the paper remains the same with respect to this change in the employed solvation energies as illustrated by the list of PDS for different products and *GCN* values on Table S22 and the parity plot and selectivity analysis from Figure S25.

Table S22: List of potential determining steps (PDS) for each range of *GCN* values for the CO_2 reduction towards CO, HCOOH, and CH_4.

Product	PDS	GCN Range
CO	*COOH $\longrightarrow$ *CO + H_2O	$3.0 \leq$ GCN ≤ 3.3
	$CO_2 \longrightarrow$ *COOH	$3.3 \leq$ GCN ≤ 9.0
HCOOH	*COOH $\longrightarrow$ HCOOH	$3.0 \leq$ GCN ≤ 4.2
	$CO_2 \longrightarrow$ *COOH	$4.2 \leq$ GCN ≤ 5.9
	*HCOO $\longrightarrow$ HCOOH	$5.9 \leq$ GCN ≤ 7.1
	$CO_2 \longrightarrow$ *HCOO	$7.1 \leq$ GCN ≤ 9.0
CH_4	*OH $\longrightarrow$ H_2O	$3.0 \leq$ GCN ≤ 4.2
	*CO $\longrightarrow$ *CHO	$4.2 \leq$ GCN ≤ 9.0

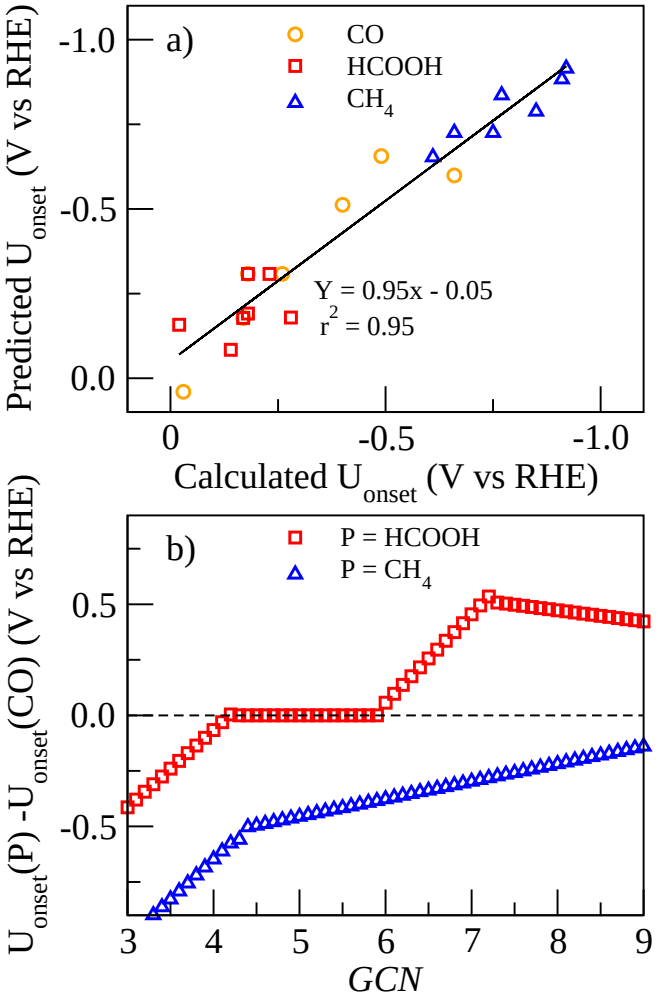


Figure S25: a) Parity plot between U_{onset} computed with the predicted binding energies with the correlation to *GCN* versus the ones obtained with the calculated values. b) selectivity analysis as a function of *GCN* using U_{onset} of CO as reference. c) evolution of *GCN* as a function of Cu nanoparticle size for spherical Cu nanoparticle models.

10 Analysis of other Cu nanoparticle models

In the main manuscript, we have used icosahedral Cu nanoparticles as our models to investigate size effects through the *GCN* descriptor. Here, we show the same discussions from the main manuscript considering different nanoparticle models. Figure S26 shows the fraction of the adsorption site population on different *GCN* range for Cu nanoparticles as a function of their size considering a) spherical, b) cuboctahedral, and c) structures obtained from Basin-Hopping Monte Carlo (BHMC) simulations.[24] The icosahedral and cuboctahedral models were obtained

using the cluster module from the atomic simulation environment package.[7] The spherical nanoparticle models were constructed by simply constructing a Cu bulk supercell and removing all atoms that were contained on spheres of user specified diameters, which was varied from 1 to 7 nm using 0.1 nm steps. Meanwhile, the BHMC nanoparticles were obtained with the methodology of a previous work[24] using a embedded atom method.[25,26]

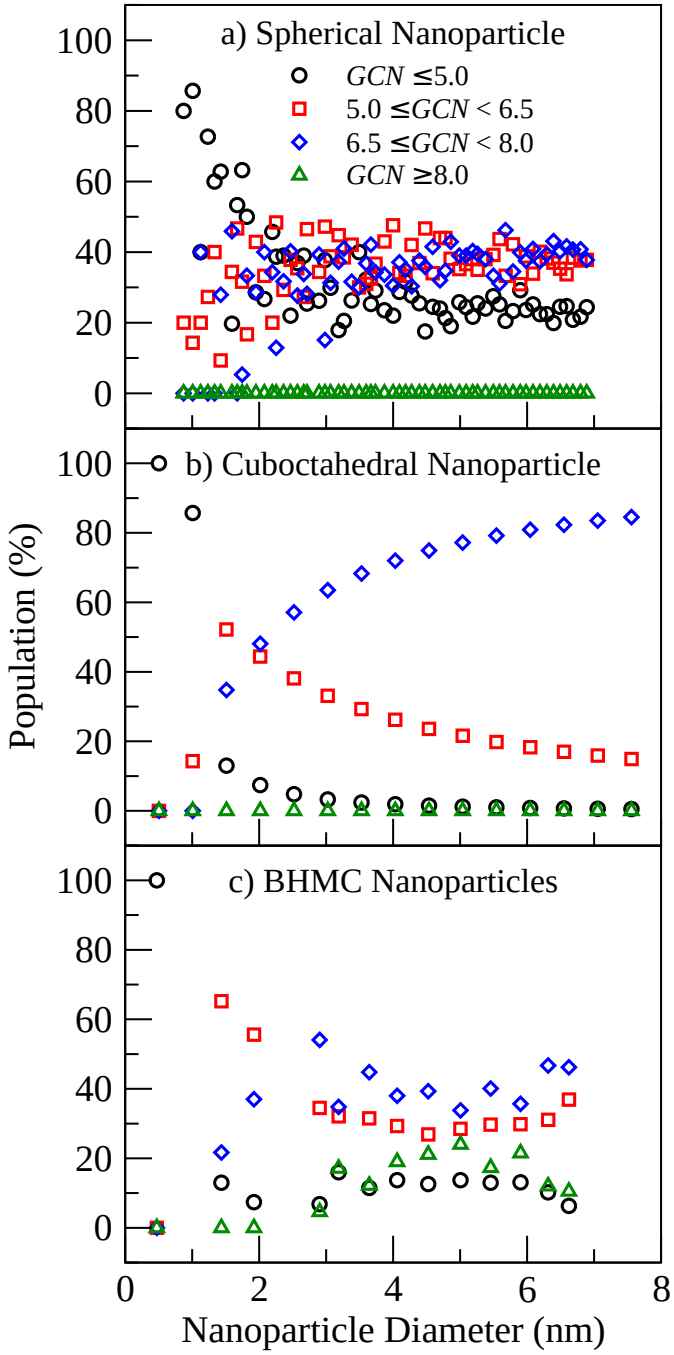


Figure S26: Evolution of the population of sites for different ranges of *GCN* values as a function of the Cu nanoparticle size for different nanoparticle models: a) spherical Cu, b) cuboctahedral, and c) Cu nanoparticles found via a Basin-Hopping Monte Carlo approach.

The behavior observed for cuboctahedral nanoparticles is very similar to the behavior describe in the manuscript for icosahedral models. Again, we see that a decrease in nanoparticle size increases the low coordinated adsorption sites in detriment of sites with intermediate or high coordination. For the spherical and BHMC Cu nanoparticle models, we also observe a similar behavior of increasing number of sites with low-coordination as we decrease the nanoparticle size; however, the trends are not as well-behaved as for the more symmetrical models. In both cases, we see that the number of sites with extremely low coordination $GCN \leq 5.0$ rapidly decreases with the nanoparticle size, but sites with $5.0 \leq GCN \leq 6.5$ and $6.5 \leq GCN \leq 8.0$ tend to coexist for several sizes on these systems. However, in all the cases, the nanoparticle models below 2 nm have a majority of low-coordinated exposed sites, which according to our analysis would translate to a increase in activity towards CO and CH_4, and selectivity for the former, which qualitatively agrees to the results observed experimentally.[27]

11 Atomic coordinates for the adsorption of CO_2 reduction intermediates

11.1 *COOH Adsorption

COOH/R-Cu_3/Cu(533)	E_{ads} = −3.25 eV				
1.00000000000000					
10.3878408006999994	0.0000000000000000	0.0000000000000000			
4.5828709415000004	6.0103788927000004	0.0000000000000000			
0.0000000000000000	0.0000000000000000	26.5000000000000000			
Cu C O H					
63 1 2 1					
Selective dynamics					
Direct					
0.0032853599999996	0.9972806999999975	0.3042624500000031	F	F	F
0.0028217400000017	0.3308767700000033	0.3042691500000032	F	F	F
0.0026800899999984	0.6645640400000019	0.3042978000000005	F	F	F
0.2572489900000008	0.6186597399999982	0.3218759499999990	F	F	F
0.2571973700000001	0.2857762699999995	0.3217927099999969	F	F	F
0.2571614599999990	0.9524293899999989	0.3219123699999997	F	F	F
0.5099116399999986	0.5747781399999994	0.3415763200000015	F	F	F
0.5095861200000016	0.2417833900000019	0.3416938299999970	F	F	F
0.5096986000000001	0.9088501900000026	0.3416314700000029	F	F	F
0.7627858999999972	0.5310134699999978	0.3609394899999998	F	F	F
0.7629538699999969	0.1970798500000015	0.3608490599999996	F	F	F
0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F

0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0467182560827695	0.2960940265747496	0.4663302504248321	T	T	T
0.0465651861831873	0.6289780961414664	0.4663428776613543	T	T	T
0.0475151592898087	0.9618578370634694	0.4661617676255503	T	T	T
0.3035249536530671	0.2484558425300136	0.4867864552450456	T	T	T
0.3041375051432453	0.5812064820681186	0.4867108106311164	T	T	T
0.3038754434797895	0.9160502973407390	0.4867369000431196	T	T	T
0.5604478120871690	0.2012596399104183	0.5069526791224632	T	T	T
0.5608868212056706	0.5349293743432000	0.5061928734831582	T	T	T
0.5594857719998458	0.8694459503184930	0.5071352862869958	T	T	T
0.8184724432738051	0.1538547932522718	0.5274646227554385	T	T	T
0.8170176714009543	0.4885493695961287	0.5277736048863488	T	T	T
0.8161829858545104	0.8219883266359957	0.5281062791309523	T	T	T
0.0732758715182342	0.1098263903169823	0.5485030334914285	T	T	T
0.0725436880191168	0.4434693446673066	0.5489964679971493	T	T	T
0.0733673135837378	0.7747541619417504	0.5482486780463560	T	T	T
0.3285867847632247	0.0660269934362461	0.5694460072350225	T	T	T
0.3297046880762764	0.3928989978945339	0.5686441268528100	T	T	T
0.3305435564554671	0.7289032285645405	0.5674979332711843	T	T	T
0.5850684633360999	0.0158094552380064	0.5902558206587827	T	T	T
0.5892173843177559	0.3467905125445583	0.5881667314849324	T	T	T
0.5874785290286013	0.6802559630344263	0.5887389202849533	T	T	T
0.8432394307447950	0.6354972710217481	0.6106498509166656	T	T	T
0.8434033943749100	0.3018799438918762	0.6103982688613456	T	T	T
0.8431115648819016	0.9682188232362208	0.6099318944024859	T	T	T
0.1017142684366803	0.5861183376270276	0.6329046150745157	T	T	T
0.1000203816587160	0.2564299753997972	0.6330967682976620	T	T	T
0.0999652343010169	0.9241611998616506	0.6304335059239534	T	T	T
0.3563557361436267	0.5409454687120743	0.6467755261282306	T	T	T
0.3539658452391166	0.2113556604355935	0.6564581396419271	T	T	T
0.3541326527828588	0.8793138328887125	0.6483775718088651	T	T	T
0.6092798408154465	0.4957498487286998	0.6742569019945108	T	T	T
0.6122531122692081	0.1599883583060873	0.6732656346655261	T	T	T
0.6090252355592227	0.8298520480972300	0.6746787338293885	T	T	T
0.8640481167939811	0.4520029877987284	0.6910917850188483	T	T	T
0.8690342388801611	0.1139241103891919	0.6915890562034406	T	T	T
0.8700666269300115	0.7815353691918219	0.6916445755503915	T	T	T
0.4359630032476147	0.8059896575262400	0.7338709836385533	T	T	T
0.4320480003376375	0.4595232544823062	0.7319720404203878	T	T	T
0.1360627678241286	0.7397304774766766	0.7126006033108396	T	T	T
0.1861890893640847	0.8133300298451616	0.7771238368284727	T	T	T
0.0993612837078430	0.8288550433856869	0.8170659760392311	T	T	T
0.2706466227655966	0.8804260973271596	0.7846689862441778	T	T	T
0.1210893232331927	0.8930838715598384	0.8452083874375589	T	T	T

COOH/Cu_3/Cu(533) E_{ads} = −2.53 eV
1.00000000000000

10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
63 1 2 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F
0.2571614599999990 0.9524293899999989 0.3219123699999997 F F F
0.5099116399999986 0.5747781399999994 0.3415763200000015 F F F
0.5095861200000016 0.2417833900000019 0.3416938299999970 F F F
0.5096986000000001 0.9088501900000026 0.3416314700000029 F F F
0.7627858999999972 0.5310134699999978 0.3609394899999998 F F F
0.7629538699999969 0.1970798500000015 0.3608490599999996 F F F
0.7629705100000024 0.8638077299999978 0.3608832600000014 F F F
0.0188077500000006 0.4844866199999984 0.3845455499999986 F F F
0.0188649600000019 0.1508076399999965 0.3844206699999972 F F F
0.0189457299999987 0.8174492599999965 0.3845321800000008 F F F
0.2777182000000025 0.4350678200000004 0.4051130599999979 F F F
0.2779364200000032 0.1018241299999971 0.4049400600000013 F F F
0.2778532499999997 0.7683188099999967 0.4050370400000034 F F F
0.5346647900000008 0.3873898000000011 0.4243529600000002 F F F
0.5347255300000029 0.0542446099999978 0.4245416400000011 F F F
0.5343893300000033 0.7214487199999979 0.4243017399999971 F F F
0.7896143700000025 0.3418778500000030 0.4451831499999983 F F F
0.7893677400000030 0.0085227100000012 0.4452920299999974 F F F
0.7895473399999986 0.6754118300000016 0.4453449800000016 F F F
0.0467802328121962 0.2946841910134168 0.4662857118922688 T T T
0.0463118300184959 0.6288202693888465 0.4666633421335504 T T T
0.0468470587055236 0.9613722992910354 0.4664436521701631 T T T
0.3030811682039172 0.2477903776476822 0.4871519777956124 T T T
0.3029086555358447 0.5814286811634020 0.4870765828240806 T T T
0.3033679349786027 0.9146408947438047 0.4869547644444978 T T T
0.5581392147851432 0.2022245905089406 0.5067824232663085 T T T
0.5590105613803615 0.5350427896858463 0.5062520633158272 T T T
0.5586873653900639 0.8685963772812784 0.5064745491634213 T T T
0.8158855001247431 0.1537425061291486 0.5273734484125825 T T T
0.8159140862230387 0.4877402756744402 0.5273603865842489 T T T
0.8149759665705005 0.8220573013183383 0.5277009943409894 T T T
0.0722802544739594 0.1071631661229375 0.5488089147293209 T T T
0.0715045809852910 0.4415674405590835 0.5486961015366703 T T T
0.0719122026310259 0.7749767303100938 0.5493614600763479 T T T
0.3272890297165105 0.0617538289950659 0.5692818338960990 T T T
0.3256254393534732 0.3964024820916450 0.5695365178161040 T T T
0.3276889257342006 0.7283437278780269 0.5690121387710789 T T T
0.5828610665787082 0.0154201632170015 0.5886306748916610 T T T
0.5843858897907381 0.3483799303665833 0.5879990308700798 T T T
0.5847088799989919 0.6807017579635684 0.5879290703766387 T T T
0.8417105451236964 0.6343398938363478 0.6096572544826770 T T T
0.8430209667634330 0.2984491005521903 0.6093167854810346 T T T
0.8422282888708850 0.9660175282385524 0.6100951772860128 T T T
0.0941023988298824 0.5892892550862143 0.6343475108834085 T T T
0.0972373558676480 0.2543800850185676 0.6325185657844514 T T T
0.0985041572280281 0.9199495990444575 0.6342741067884532 T T T

0.3496481289528717	0.5397044496497898	0.6508464261168996	T	T	T
0.3493550212349774	0.2105929270026010	0.6521365490342177	T	T	T
0.3501987025818849	0.8806276443730070	0.6511032362326290	T	T	T
0.6072950099682473	0.4960383361624849	0.6704725745112370	T	T	T
0.6032008329720782	0.1634532604610897	0.6708531030778886	T	T	T
0.6029636548857411	0.8350954169705602	0.6713310266639567	T	T	T
0.8632192234178291	0.4510145395139773	0.6898251618419238	T	T	T
0.8603529448452747	0.1161243101036433	0.6908806049627501	T	T	T
0.8530421133518828	0.7909138459518275	0.6924623477004843	T	T	T
0.6336030958791952	0.6541637797240725	0.7491637097174006	T	T	T
0.6224053854986877	0.3030455962817271	0.7502809381700573	T	T	T
0.3730888898575344	0.6905944565487019	0.7266401223698509	T	T	T
0.6139152220168071	0.4161998920617336	0.8164152051487577	T	T	T
0.5971134793760697	0.3395987546576720	0.8596362829173074	T	T	T
0.6268585592806204	0.5721251475716542	0.8202748855098250	T	T	T
0.5977970742624450	0.4257680927577852	0.8875490675551347	T	T	T

COOH/Cu_3/Cu(533) E_{ads} = −2.46 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
63 1 2 1
Selective dynamics
Direct

0.0032853599999996	0.9972806999999975	0.3042624500000031	F	F	F
0.0028217400000017	0.3308767700000033	0.3042691500000032	F	F	F
0.0026800899999984	0.6645640400000019	0.3042978000000005	F	F	F
0.2572489900000008	0.6186597399999982	0.3218759499999990	F	F	F
0.2571973700000001	0.2857762699999995	0.3217927099999969	F	F	F
0.2571614599999990	0.9524293899999989	0.3219123699999997	F	F	F
0.5099116399999986	0.5747781399999994	0.3415763200000015	F	F	F
0.5095861200000016	0.2417833900000019	0.3416938299999970	F	F	F
0.5096986000000001	0.9088501900000026	0.3416314700000029	F	F	F
0.7627858999999972	0.5310134699999978	0.3609394899999998	F	F	F
0.7629538699999969	0.1970798500000015	0.3608490599999996	F	F	F
0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F
0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0465744300407161	0.2947702036916199	0.4663003545652301	T	T	T
0.0460670501679006	0.6287812308942734	0.4665841694333701	T	T	T
0.0467113627995934	0.9614018958542988	0.4664298199599604	T	T	T
0.3028797974368950	0.2478461524040374	0.4871415115883257	T	T	T
0.3029382734988383	0.5812120869958161	0.4870805538188518	T	T	T
0.3030664925805731	0.9146152864358992	0.4869643032558881	T	T	T
0.5580791214273025	0.2020696619003106	0.5068331664045349	T	T	T

0.5587544154883981	0.5349897762594549	0.5062648051938148	T	T	T
0.5586448568001668	0.8682846890142659	0.5065953338009672	T	T	T
0.8156786990685556	0.1536967812348622	0.5273510211318163	T	T	T
0.8155402548370434	0.4878421108186902	0.5274361211243683	T	T	T
0.8146245633805428	0.8222329783277749	0.5278171989576803	T	T	T
0.0719245797885768	0.1071579730998582	0.5488422522485694	T	T	T
0.0710816179098760	0.4417317721018274	0.5486502698156464	T	T	T
0.0717137000089965	0.7748941912487362	0.5491600932366887	T	T	T
0.3273157014042297	0.0613658656354120	0.5691153470757925	T	T	T
0.3258677784236398	0.3959037217111866	0.5694856790861713	T	T	T
0.3276094544126711	0.7279347036356627	0.5691254560368831	T	T	T
0.5827667500796860	0.0151174860227378	0.5889229579270479	T	T	T
0.5841124286583541	0.3481261929752058	0.5881343650203021	T	T	T
0.5844032912829041	0.6801177257000681	0.5882075277034570	T	T	T
0.8413576499867456	0.6339674244868098	0.6097466979928773	T	T	T
0.8424272734349045	0.2984710072392154	0.6093091147217369	T	T	T
0.8421072915739969	0.9663841597337046	0.6100618478001991	T	T	T
0.0953045486520120	0.5878609155934635	0.6338171791102863	T	T	T
0.0976533690215612	0.2537103512566253	0.6322313943093150	T	T	T
0.0985871283330472	0.9194187912133842	0.6342076336038016	T	T	T
0.3494983504003204	0.5392626893279198	0.6510355881716163	T	T	T
0.3499731351200717	0.2093022870252409	0.6521480258361743	T	T	T
0.3502241629844485	0.8803761236377698	0.6511136288011307	T	T	T
0.6060922966272281	0.4954042691212051	0.6709101095703890	T	T	T
0.6034715266274678	0.1625190221605367	0.6711979393384077	T	T	T
0.6039657816661690	0.8324650763539608	0.6718260580614183	T	T	T
0.8643314654084263	0.4491209145481457	0.6897592118419316	T	T	T
0.8615386232708223	0.1160993364598717	0.6908324363045069	T	T	T
0.8562988527898961	0.7881400045551440	0.6914496406512695	T	T	T
0.6330651417577567	0.6341186005458711	0.7507173217145806	T	T	T
0.6280104827408262	0.3031972892856839	0.7499625440377985	T	T	T
0.3702299929745278	0.6949695270460687	0.7270277401589701	T	T	T
0.6686165623415233	0.6987929917908943	0.8137403023579574	T	T	T
0.6218276163951307	0.3325114890618294	0.8184398383056011	T	T	T
0.7054002125704466	0.7240536158561268	0.8522434914595128	T	T	T
0.7299615879513679	0.2449965945050950	0.8330365849614723	T	T	T

COOH/Defected-Cu(533) E_{ads} = −2.39 eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H

59 1 2 1

Selective dynamics

Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F

0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0468672628848594	0.2942039756272834	0.4660626269554271	T	T	T
0.0464387857873660	0.6271691857348287	0.4657878510108020	T	T	T
0.0466673343193236	0.9609523157771207	0.4659239457409896	T	T	T
0.3032835496953012	0.2468789786000158	0.4867545523182244	T	T	T
0.3037415965754136	0.5799878057924772	0.4864537631995489	T	T	T
0.3032620729206599	0.9133779674738420	0.4866862621984183	T	T	T
0.5591565570710131	0.2005269675508004	0.5069823604943267	T	T	T
0.5591828481575121	0.5333589231337044	0.5066242037631383	T	T	T
0.5586411560535964	0.8667547110725593	0.5069729907597988	T	T	T
0.8156110890152135	0.1524932336178040	0.5275226207011130	T	T	T
0.8152145363118137	0.4859848918197116	0.5275825976968491	T	T	T
0.8154334596436570	0.8202696153475699	0.5279094225883085	T	T	T
0.0710397838325250	0.1069126542493777	0.5483678876954627	T	T	T
0.0708641648286701	0.4400965078865440	0.5485867038636485	T	T	T
0.0718803784029589	0.7722612400607218	0.5476333595823704	T	T	T
0.3262894751024561	0.0605621093673179	0.5689367447213982	T	T	T
0.3272579702024814	0.3934477372281506	0.5687145481768994	T	T	T
0.3275001558378179	0.7260172899775768	0.5688024563037573	T	T	T
0.5840304926500082	0.0118485136185740	0.5885338237418338	T	T	T
0.5849959050857692	0.3467417687051366	0.5893342326975670	T	T	T
0.5848607535661259	0.6758354987202324	0.5892835554876399	T	T	T
0.8410846713938369	0.6258086117339303	0.6101414726516978	T	T	T
0.8419087355159931	0.2980704940597079	0.6110333908223566	T	T	T
0.8436632841949461	0.9646133027772876	0.6103181023553645	T	T	T
0.0971254978436917	0.5838033106451590	0.6320242176266575	T	T	T
0.0935862367048443	0.2543912313438170	0.6329886055558731	T	T	T
0.0980181430802034	0.9177450742173363	0.6314343204645638	T	T	T
0.3496794875828044	0.5395755444849328	0.6510670883531304	T	T	T
0.3496735903968400	0.2075781433755566	0.6515072580209136	T	T	T
0.3481801936105313	0.8766578056996508	0.6509800707568800	T	T	T
0.6019608180657343	0.4995954651072907	0.6730397530280499	T	T	T
0.6054355278919417	0.1576647650500291	0.6704343391298835	T	T	T
0.6051809813515874	0.8272071389044910	0.6703080995659718	T	T	T
0.8736282740789179	0.0976874764737161	0.6914177754202839	T	T	T
0.8597426778816626	0.7761083357301288	0.6881405789847435	T	T	T
0.6533657021611674	0.4436085834173866	0.7442295931783605	T	T	T
0.5499305433061679	0.5749194462603242	0.7810727460441029	T	T	T
0.7896289042188798	0.2696130903672724	0.7570571629147835	T	T	T
0.6027693706180770	0.5029448744693497	0.8135531557822020	T	T	T

COOH/Cu_3/Cu(533) E_{ads} = −2.37 eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000

0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
63 1 2 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F
0.2571614599999990 0.9524293899999989 0.3219123699999997 F F F
0.5099116399999986 0.5747781399999994 0.3415763200000015 F F F
0.5095861200000016 0.2417833900000019 0.3416938299999970 F F F
0.5096986000000001 0.9088501900000026 0.3416314700000029 F F F
0.7627858999999972 0.5310134699999978 0.3609394899999998 F F F
0.7629538699999969 0.1970798500000015 0.3608490599999996 F F F
0.7629705100000024 0.8638077299999978 0.3608832600000014 F F F
0.0188077500000006 0.4844866199999984 0.3845455499999986 F F F
0.0188649600000019 0.1508076399999965 0.3844206699999972 F F F
0.0189457299999987 0.8174492599999965 0.3845321800000008 F F F
0.2777182000000025 0.4350678200000004 0.4051130599999979 F F F
0.2779364200000032 0.1018241299999971 0.4049400600000013 F F F
0.2778532499999997 0.7683188099999967 0.4050370400000034 F F F
0.5346647900000008 0.3873898000000011 0.4243529600000002 F F F
0.5347255300000029 0.0542446099999978 0.4245416400000011 F F F
0.5343893300000033 0.7214487199999979 0.4243017399999971 F F F
0.7896143700000025 0.3418778500000030 0.4451831499999983 F F F
0.7893677400000030 0.0085227100000012 0.4452920299999974 F F F
0.7895473399999986 0.6754118300000016 0.4453449800000016 F F F
0.0471108320373466 0.2933934300128136 0.4663119406324758 T T T
0.0458754937165214 0.6287076116722021 0.4664879301630807 T T T
0.0461087300005230 0.9605765813537377 0.4662373065517452 T T T
0.3027944779078150 0.2478265982484100 0.4867472115754614 T T T
0.3028065075872537 0.5796999194208170 0.4875542487857866 T T T
0.3031428541581430 0.9119485520034549 0.4868298141705646 T T T
0.5578252314059780 0.2000598361210607 0.5068034845393319 T T T
0.5589611938532630 0.5327556559694595 0.5062263042802283 T T T
0.5598537551734469 0.8646954011839906 0.5061718168758009 T T T
0.8160048753185487 0.1509631517564969 0.5278659294725733 T T T
0.8169317352169621 0.4848420112437553 0.5274023738320921 T T T
0.8151852159835308 0.8197911912695427 0.5279081917315642 T T T
0.0725292076263098 0.1030003070029504 0.5483713513944096 T T T
0.0710600041396469 0.4417358431068987 0.5482470192953550 T T T
0.0713920221479967 0.7735295104259623 0.5494720073505631 T T T
0.3284109036065446 0.0596928583174398 0.5672073802810116 T T T
0.3265320151657373 0.3936156953191423 0.5709467668878051 T T T
0.3265693329692255 0.7234089427487671 0.5699394478199384 T T T
0.5836939510747153 0.0075884350346629 0.5880637610537085 T T T
0.5835265228312125 0.3437420389360424 0.5875431757398473 T T T
0.5859415041237401 0.6755583079238618 0.5875640136350733 T T T
0.8408425449765595 0.6322187739841263 0.6111035677399661 T T T
0.8438413400833675 0.2939256276740195 0.6094971810873804 T T T
0.8443149359809357 0.9589405927351411 0.6114630311869880 T T T
0.0973365022340558 0.5849080884134630 0.6338452932812423 T T T
0.1013572630747111 0.2501683069178496 0.6291341435264659 T T T
0.0949012380407576 0.9207136406697020 0.6362617051541050 T T T
0.3483839234422748 0.5413740991132567 0.6571707898775637 T T T
0.3496294953870733 0.2070156165415041 0.6528338447843975 T T T

0.3475718860935786 0.8817151221538431 0.6474669335177595 T T T
0.6055627021949462 0.4921903935074096 0.6672473455520023 T T T
0.6064033441758859 0.1453089563560524 0.6677402416894214 T T T
0.6014701969328304 0.8230001617565039 0.6734159282353548 T T T
0.8857703628323371 0.4217857451127738 0.6886626055361340 T T T
0.8486631134844819 0.1242843863577255 0.6930442415504753 T T T
0.8625574784004959 0.7821976854526426 0.6947881027068215 T T T
0.6863723540409543 0.5447630554902274 0.7505689879834537 T T T
0.5735756202192837 0.3375533969706027 0.7420403678869009 T T T
0.3994990202680030 0.7359707771660416 0.7291737264734585 T T T
0.8849888479894333 0.5087256378764162 0.7713530457575475 T T T
0.9805377361386081 0.3385307538846187 0.8039236334934531 T T T
0.9152034367956590 0.6459472423195178 0.7657192054291222 T T T
0.0621444073803201 0.3545466171741084 0.8168096681255378 T T T

COOH/Cu_3/Cu(533) E_{ads} = −2.32 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
63 1 2 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F
0.2571614599999990 0.9524293899999989 0.3219123699999997 F F F
0.5099116399999986 0.5747781399999994 0.3415763200000015 F F F
0.5095861200000016 0.2417833900000019 0.3416938299999970 F F F
0.5096986000000001 0.9088501900000026 0.3416314700000029 F F F
0.7627858999999972 0.5310134699999978 0.3609394899999998 F F F
0.7629538699999969 0.1970798500000015 0.3608490599999996 F F F
0.7629705100000024 0.8638077299999978 0.3608832600000014 F F F
0.0188077500000006 0.4844866199999984 0.3845455499999986 F F F
0.0188649600000019 0.1508076399999965 0.3844206699999972 F F F
0.0189457299999987 0.8174492599999965 0.3845321800000008 F F F
0.2777182000000025 0.4350678200000004 0.4051130599999979 F F F
0.2779364200000032 0.1018241299999971 0.4049400600000013 F F F
0.2778532499999997 0.7683188099999967 0.4050370400000034 F F F
0.5346647900000008 0.3873898000000011 0.4243529600000002 F F F
0.5347255300000029 0.0542446099999978 0.4245416400000011 F F F
0.5343893300000033 0.7214487199999979 0.4243017399999971 F F F
0.7896143700000025 0.3418778500000030 0.4451831499999983 F F F
0.7893677400000030 0.0085227100000012 0.4452920299999974 F F F
0.7895473399999986 0.6754118300000016 0.4453449800000016 F F F
0.0467835221334241 0.2940653295738471 0.4662842079755762 T T T
0.0461765111561974 0.6280098568725236 0.4665920570874320 T T T
0.0470095351558015 0.9604913852897141 0.4663559552870282 T T T
0.3030568562318052 0.2468933307890637 0.4872786471444002 T T T
0.3032421562194187 0.5798403627179169 0.4870549328232627 T T T
0.3032762095742498 0.9134662093579635 0.4869232390150060 T T T
0.5581592333234937 0.2006380074604195 0.5066236205921371 T T T
0.5591658634116143 0.5335067867387622 0.5063033009290763 T T T
0.5587776131045743 0.8668926607637033 0.5066328573942087 T T T

0.8161797171400309 0.1519702303861337 0.5272577832661440 T T T
0.8159312329390076 0.4863023770533914 0.5274751439523158 T T T
0.8149720924558821 0.8200186413960395 0.5277267185036649 T T T
0.0724357272535343 0.1052967195861498 0.5486474908502572 T T T
0.0714957512684862 0.4399218258484225 0.5487837219574061 T T T
0.0724249832294888 0.7723056606044025 0.5490202900133525 T T T
0.3276462779696629 0.0590682001025513 0.5691929481488884 T T T
0.3261817091773906 0.3939348041037647 0.5699104638002197 T T T
0.3282140132404976 0.7251828102540117 0.5690216397827044 T T T
0.5829455001469697 0.0124344969953185 0.5886706885613364 T T T
0.5845562267553817 0.3451104221566794 0.5878233638314398 T T T
0.5849279570542762 0.6774237068543414 0.5882779697027161 T T T
0.8417117920231121 0.6314412714330615 0.6100421134834733 T T T
0.8432864188460130 0.2954036757495686 0.6092160015725199 T T T
0.8428091033206968 0.9624052496289224 0.6096070849158153 T T T
0.0948132742518695 0.5860475721865086 0.6343697086910467 T T T
0.0982885533527735 0.2505029489589603 0.6322677129394307 T T T
0.0996267147521692 0.9158583758788765 0.6333457735053472 T T T
0.3498582878214407 0.5371625683067762 0.6517348010624957 T T T
0.3497046785071731 0.2066945850369990 0.6522814203556919 T T T
0.3507027111040912 0.8764377269812016 0.6511427135221126 T T T
0.6090510096827444 0.4896126150904934 0.6704646856378957 T T T
0.6035970489400668 0.1580390001575012 0.6703088373481663 T T T
0.6031824613855079 0.8292115313338897 0.6722205019484804 T T T
0.8654688058931796 0.4455966642373355 0.6898923237195405 T T T
0.8650306425742897 0.1082806930734108 0.6900175078406505 T T T
0.8536707300111956 0.7871966618322404 0.6923456265339212 T T T
0.6380966397762506 0.6345269532937294 0.7511117381074612 T T T
0.6322520923055563 0.2849672528292899 0.7481309813808323 T T T
0.3802339089432465 0.6850794216095792 0.7276446037775912 T T T
0.6767044922886569 0.5253349980986570 0.8197619925558683 T T T
0.6475113004229698 0.3558156162030812 0.8208074107862871 T T T
0.7279547863307059 0.5471223006791845 0.8579615378705228 T T T
0.6882718963371559 0.2712130416712100 0.8526217100657405 T T T

COOH/Cu_3/Cu(533) E_{ads} = −2.30 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
63 1 2 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F
0.2571614599999990 0.9524293899999989 0.3219123699999997 F F F
0.5099116399999986 0.5747781399999994 0.3415763200000015 F F F
0.5095861200000016 0.2417833900000019 0.3416938299999970 F F F
0.5096986000000001 0.9088501900000026 0.3416314700000029 F F F
0.7627858999999972 0.5310134699999978 0.3609394899999998 F F F
0.7629538699999969 0.1970798500000015 0.3608490599999996 F F F
0.7629705100000024 0.8638077299999978 0.3608832600000014 F F F
0.0188077500000006 0.4844866199999984 0.3845455499999986 F F F

0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0469276767303249	0.2942885994219622	0.4664021182023765	T	T	T
0.0466543788845451	0.6282140348640910	0.4666340783681889	T	T	T
0.0468102097191665	0.9610646039589114	0.4663854107755127	T	T	T
0.3031871497436046	0.2475497005289774	0.4871784354260388	T	T	T
0.3030028069389124	0.5809382234324221	0.4871137579380517	T	T	T
0.3033927627310478	0.9140910584244173	0.4869575777630302	T	T	T
0.5579502376420042	0.2023305808819849	0.5066570836829912	T	T	T
0.5587337992779517	0.5346700720693311	0.5063983435944440	T	T	T
0.5586469046610189	0.8678736481636131	0.5064895163155514	T	T	T
0.8158878379764938	0.1530906658408525	0.5273967600887977	T	T	T
0.8160791179736762	0.4870596895485831	0.5273659612025856	T	T	T
0.8156616620704579	0.8208473238230724	0.5274058182648322	T	T	T
0.0725479964741171	0.1059995404487829	0.5487967779512408	T	T	T
0.0720514599234187	0.4406803622417956	0.5488964579992461	T	T	T
0.0720877377208121	0.7741056404436799	0.5493574181485011	T	T	T
0.3268536119619069	0.0610396628672131	0.5693018940976308	T	T	T
0.3250949499996553	0.3969964681565013	0.5699755847144418	T	T	T
0.3266064758628456	0.7281916525925611	0.5691796275374783	T	T	T
0.5830465351524039	0.0151625306570747	0.5875471545483172	T	T	T
0.5839995642745007	0.3485070607049268	0.5880664496995749	T	T	T
0.5846326079520546	0.6787342083658506	0.5879013318013840	T	T	T
0.8429472335229515	0.6325396615386575	0.6094944178230592	T	T	T
0.8432385948525372	0.2968857887395145	0.6093325690837345	T	T	T
0.8431052569339674	0.9638396199008881	0.6099570457881475	T	T	T
0.0931417647323167	0.5895668739212413	0.6352643701726489	T	T	T
0.0969095157472625	0.2530249232950418	0.6328127182064435	T	T	T
0.0974899143781376	0.9196933726240215	0.6348952717157244	T	T	T
0.3485673681879189	0.5428672729142386	0.6523210800062911	T	T	T
0.3480306351212576	0.2107346051839488	0.6516758713459212	T	T	T
0.3492953726741422	0.8774685734664625	0.6516875458997928	T	T	T
0.6064134995793912	0.4968346377881432	0.6715148845399022	T	T	T
0.6024728928456629	0.1618087084219994	0.6687708307068435	T	T	T
0.6025809974353684	0.8353575334674870	0.6683299996882890	T	T	T
0.8624577281559873	0.4498859335007986	0.6901059368071499	T	T	T
0.8600956865677543	0.1148640007221046	0.6912837555396693	T	T	T
0.8487378935842437	0.7920168906645129	0.6935394781594689	T	T	T
0.6372499238176078	0.6729057657120440	0.7479631346451905	T	T	T
0.6257438243323004	0.2877020807408162	0.7470591533272231	T	T	T
0.3687036289612516	0.6960440992713846	0.7311094901510942	T	T	T
0.4655029124172506	0.6358353772926509	0.7976940666711047	T	T	T
0.5145181574414810	0.4349479642596747	0.8209517336425166	T	T	T
0.5273104563450096	0.7215797813455641	0.8162121758012154	T	T	T
0.5893723382972264	0.4049780364411791	0.8485773568282637	T	T	T

COOH/Cu(533) $E_{ads} = -2.30$ eV
1.00000000000000

10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 2 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0473273372967769 0.2931323415843552 0.4659982184441825 T T T
0.0472543827747916 0.6267538939151058 0.4659004660820656 T T T
0.0471246939349589 0.9600034669291519 0.4658887599593384 T T T
0.3042156288325331 0.2457473400555777 0.4866423299763035 T T T
0.3042841557657072 0.5789010946161350 0.4867546974437912 T T T
0.3040340961989196 0.9122261393627509 0.4866282434463518 T T T
0.5602102223019110 0.1986625881991951 0.5069291550838954 T T T
0.5603968968686547 0.5320320666010167 0.5069983947788020 T T T
0.5603040268804407 0.8652003316946144 0.5070231824082762 T T T
0.8171622472868171 0.1502790874065438 0.5282053381414058 T T T
0.8170358373425565 0.4848121160694512 0.5276657077727115 T T T
0.8171038537613620 0.8178204719833766 0.5278452776167515 T T T
0.0731410489403330 0.1036866721121702 0.5482599840131889 T T T
0.0732786086283739 0.4374227147016073 0.5481883585748978 T T T
0.0730248631085025 0.7711422101114874 0.5482027890968283 T T T
0.3290383595647794 0.0572126619774287 0.5688598210786681 T T T
0.3289789150809651 0.3907474914601148 0.5690112349035463 T T T
0.3285101589111905 0.7245163107150926 0.5691315359600433 T T T
0.5865207482437089 0.0091920521368928 0.5888331809032439 T T T
0.5859919592897985 0.3428421690172721 0.5887875648658009 T T T
0.5864483677500474 0.6760748593247915 0.5890120680237678 T T T
0.8451927485408344 0.6267319339789480 0.6108386948059777 T T T
0.8445291503250406 0.2961270206799159 0.6100613875426076 T T T
0.8452701393619267 0.9568115335800088 0.6110415497968992 T T T
0.1014120128828965 0.5796559954595926 0.6317677311631702 T T T
0.1015424289082139 0.2464817421390417 0.6317695808731584 T T T
0.1001062972082910 0.9144174801388975 0.6325822599137187 T T T

0.3536281613661502	0.5358498016768799	0.6519073082445440	T	T	T
0.3543993337150000	0.2021802440642590	0.6516501161758170	T	T	T
0.3536391105606927	0.8695007757235368	0.6521170818940659	T	T	T
0.6067983637545816	0.4917756946554271	0.6712905847123893	T	T	T
0.6080856324819275	0.1564511206937597	0.6715415046721257	T	T	T
0.6086247389564922	0.8233113532249881	0.6708945489716740	T	T	T
0.8683707285301047	0.4318219559134542	0.6926867340972960	T	T	T
0.8609195622548985	0.1134110591550548	0.6898895329644468	T	T	T
0.8694625020475840	0.7795704063644586	0.6935673260695912	T	T	T
0.9353857345223799	0.4701282133806686	0.7571287363977260	T	T	T
0.9874924013863066	0.3261694789973215	0.7955936626822433	T	T	T
0.9370841764637989	0.6341764597697706	0.7630849413807714	T	T	T
0.0206325553984676	0.3787931217289677	0.8231735926124530	T	T	T

COOH/Defected-Cu(533) $E_{ads} = -2.26$ eV
1.00000000000000
10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H
59 1 2 1
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0469206947450971	0.2941774712366012	0.4660672692236147	T	T	T
0.0469887366328550	0.6270403428544071	0.4657552455971938	T	T	T
0.0468742452651156	0.9610327082883572	0.4659748079552202	T	T	T
0.3037727274513813	0.2463836311673475	0.4866454704931655	T	T	T
0.3042278821957680	0.5797951643050325	0.4863383971188071	T	T	T
0.3033461167611904	0.9138399432862059	0.4866958127170591	T	T	T
0.5597188771529460	0.2008338687400766	0.5069848996753308	T	T	T
0.5597188862040596	0.5330200093009481	0.5068288502934593	T	T	T
0.5590379055959787	0.8663368490511303	0.5071655185772030	T	T	T
0.8160648302405136	0.1527634669053128	0.5275560065106362	T	T	T

0.8154233140899905	0.4862254105469930	0.5277579868114941	T	T	T
0.8162257402031727	0.8190628341646971	0.5273628839441287	T	T	T
0.0712780530944528	0.1075333759371304	0.5485566187789175	T	T	T
0.0716074920041692	0.4398155159877462	0.5484208963702173	T	T	T
0.0729929068079755	0.7717347864393318	0.5474952687919696	T	T	T
0.3266143643896058	0.0609765387796628	0.5689168693891133	T	T	T
0.3278679226105794	0.3935602050430376	0.5685364984731436	T	T	T
0.3278848917699619	0.7261855440259311	0.5684588719653476	T	T	T
0.5847022138328128	0.0126736814466568	0.5880961781911154	T	T	T
0.5862147392528314	0.3462669019563052	0.5898603892471641	T	T	T
0.5855313478557420	0.6754937250992725	0.5897306633478436	T	T	T
0.8420421526199249	0.6256872045129711	0.6101298695482313	T	T	T
0.8425968238457742	0.2974031142138855	0.6117034147935030	T	T	T
0.8450119034630319	0.9620529567020171	0.6093640911798417	T	T	T
0.0979423985359205	0.5842507697242212	0.6319206622240543	T	T	T
0.0941349864958241	0.2545412805117024	0.6332823896675208	T	T	T
0.0981151907633020	0.9180365557299268	0.6313911548213866	T	T	T
0.3509177907156555	0.5400964738316105	0.6509061506987450	T	T	T
0.3495390775947413	0.2089768413751543	0.6514327948650305	T	T	T
0.3485855220326073	0.8768101441670950	0.6509034552900843	T	T	T
0.6036948806188462	0.5018771164913431	0.6732482579420278	T	T	T
0.6063300925420805	0.1566137061976178	0.6701867779685955	T	T	T
0.6040443322693463	0.8316851601918387	0.6694049738605230	T	T	T
0.8710488626555701	0.0931441493664593	0.6917687449125367	T	T	T
0.8608937071330800	0.7722188204029479	0.6881908081251495	T	T	T
0.7639452395861710	0.2536883507171055	0.7530719889686424	T	T	T
0.8068304329761844	0.1612868334021229	0.7992273177741396	T	T	T
0.6434477297276473	0.4559958744162316	0.7500872366414129	T	T	T
0.7294202750675041	0.2773943824817522	0.8235542014268589	T	T	T

COOH/Defected-Cu(533) $E_{ads} = -2.24$ eV
1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H
59 1 2 1
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F

0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0472465109605102 0.2927379117570257 0.4659663747000274 T T T
0.0470271022380592 0.6258107344556049 0.4658058219686694 T T T
0.0471753638021013 0.9596669472159989 0.4657761987308489 T T T
0.3038106992355881 0.2452277766927515 0.4867468029027669 T T T
0.3048490093231277 0.5777105749955362 0.4864686150847246 T T T
0.3039350464484975 0.9114375540180305 0.4867156913644542 T T T
0.5601564581139178 0.1974309367590105 0.5072551987065427 T T T
0.5599443215703073 0.5321949228303394 0.5068886020439588 T T T
0.5591792332537812 0.8652113199891802 0.5071990748923694 T T T
0.8165217402318009 0.1505583340692516 0.5273645742384251 T T T
0.8160028392186531 0.4845821993469286 0.5275009262075682 T T T
0.8159155130757831 0.8180722546659281 0.5276484267108302 T T T
0.0722010793622056 0.1036056692733876 0.5483135523942689 T T T
0.0714879239128280 0.4371089394526559 0.5484767947053610 T T T
0.0732334288952494 0.7695556657609024 0.5475585899630390 T T T
0.3270379962050606 0.0574449073654492 0.5689592296330740 T T T
0.3289666658379569 0.3890873124577048 0.5685460296131114 T T T
0.3287207828231908 0.7227389623578064 0.5688301016564800 T T T
0.5852802717558385 0.0058653878423913 0.5899713777119269 T T T
0.5856135889106693 0.3439535067932544 0.5890171386857477 T T T
0.5863221726376472 0.6746966399905682 0.5902050160391856 T T T
0.8424174625248330 0.6242742746146237 0.6108026750625868 T T T
0.8427998076981511 0.2981501962495694 0.6100822347295725 T T T
0.8440281615595713 0.9609235364924896 0.6089338627267313 T T T
0.0999221400232285 0.5776654609672871 0.6312165118818267 T T T
0.0947924261962112 0.2500066936067565 0.6331844620552002 T T T
0.0987311617955641 0.9145842415181592 0.6318941256144031 T T T
0.3505794339562769 0.5353022528054983 0.6509480437436643 T T T
0.3513639426935361 0.2025228562863841 0.6512888104130004 T T T
0.3503361383549132 0.8705319038109930 0.6505833869487598 T T T
0.6062478038339485 0.4840070038593562 0.6726075959096103 T T T
0.6075507395927732 0.1544617495507385 0.6707805540702600 T T T
0.6103626074731405 0.8237877288596576 0.6738151506351723 T T T
0.8632990032004868 0.1112477739552888 0.6882758677491893 T T T
0.8681894456785808 0.7791386576441125 0.6880059892126059 T T T
0.6116040613269633 0.5664810654360203 0.7411738055268581 T T T
0.5942907932964401 0.4752091537895459 0.7817157433860895 T T T
0.6255759604792067 0.7182689915088283 0.7485918041732793 T T T
0.5933261333686174 0.5530164357856285 0.8118142401263786 T T T

COOH/Defected-Cu(533) E_{ads} = −2.21 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
59 1 2 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F

0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0466636676540929	0.2950174165719968	0.4659353920912425	T	T	T
0.0469471452253414	0.6280163257407553	0.4659772276626127	T	T	T
0.0470616136549393	0.9618831580951896	0.4660843224450459	T	T	T
0.3032613013384287	0.2482301546063199	0.4866943869197832	T	T	T
0.3038009233705312	0.5811220522859205	0.4864490328074734	T	T	T
0.3034159226488701	0.9150322183910470	0.4866955904892473	T	T	T
0.5597681117363539	0.2016223747873839	0.5068581881568820	T	T	T
0.5597447820305057	0.5346627952359195	0.5068408231846239	T	T	T
0.5589343550009589	0.8690511679759754	0.5071079625595678	T	T	T
0.8163996851500585	0.1539480112741732	0.5275148850007810	T	T	T
0.8158092534383868	0.4889864029231348	0.5278360299956715	T	T	T
0.8161263316694938	0.8209937019711546	0.5275947669101221	T	T	T
0.0717476244549127	0.1092656523100414	0.5485590270248962	T	T	T
0.0712239246889252	0.4417357567172692	0.5483914194711295	T	T	T
0.0724129020816530	0.7745769573545156	0.5479862254579755	T	T	T
0.3265502395117604	0.0635470439741025	0.5691614924781677	T	T	T
0.3280583029142835	0.3954462836729189	0.5687616288659332	T	T	T
0.3278904878360434	0.7287089770988042	0.5687449866411246	T	T	T
0.5852004359972879	0.0152921133241533	0.5887718385392748	T	T	T
0.5860138263595848	0.3471287557326302	0.5887368628682775	T	T	T
0.5852405520325951	0.6815258543438775	0.5887215172176159	T	T	T
0.8425878238350664	0.6316707729299968	0.6115459862627601	T	T	T
0.8423459998216540	0.3025808557412286	0.6104726789257803	T	T	T
0.8443243708700715	0.9654742865561307	0.6105220711291216	T	T	T
0.0989749754389725	0.5853142503630829	0.6314361302414511	T	T	T
0.0945415669175483	0.2570110102923746	0.6333218638803458	T	T	T
0.0984963569892173	0.9210864071607576	0.6316791092197949	T	T	T
0.3514155200155713	0.5428189026915222	0.6517049508295764	T	T	T
0.3510049265881621	0.2103736544315484	0.6519375445990402	T	T	T
0.3502504786427926	0.8781157881896641	0.6518594242047620	T	T	T
0.6049627718159236	0.5007507938461742	0.6697476320137322	T	T	T
0.6075328775383535	0.1636889413436809	0.6708780498084383	T	T	T
0.6056732086961127	0.8309922768916335	0.6699268190670652	T	T	T
0.8628836729982756	0.1310830815346628	0.6910286184329508	T	T	T
0.8646953290762504	0.7712183729106089	0.6907998874567912	T	T	T
0.9107780709363068	0.0244135125974249	0.7598598226949118	T	T	T

0.9076449876034209 0.8343937618672875 0.7620315463024923 T T T
0.9485989465613671 0.0706370905846091 0.7976288030145990 T T T
0.9452142578058029 0.7612160414930653 0.7952590694805729 T T T

COOH/Defected-Cu(533) E_{ads} = −2.20 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
59 1 2 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0472597269769569 0.2942952005540003 0.4660475820378839 T T T
0.0469514721025498 0.6271637094224336 0.4657912883667364 T T T
0.0469938001132360 0.9610778639012405 0.4659405128100855 T T T
0.3039788490333276 0.2468980659370951 0.4867223230193481 T T T
0.3045802267360240 0.5797270933797434 0.4864937033148943 T T T
0.3040613631648046 0.9132460770487824 0.4866987287777192 T T T
0.5600657176065208 0.2002591501210478 0.5072270737696577 T T T
0.5600340888765515 0.5332492527249965 0.5066753374170146 T T T
0.5595614989725767 0.8670976310354597 0.5068897528413168 T T T
0.8164449001613918 0.1525516211397722 0.5276297970155968 T T T
0.8163638244608196 0.4860361382582408 0.5275386278952607 T T T
0.8164240182472826 0.8204839841370930 0.5279495125871634 T T T
0.0725341048337391 0.1064536581979755 0.5483210086536574 T T T
0.0722094025556382 0.4399748082187424 0.5485723315535546 T T T
0.0732103376414383 0.7720449181024920 0.5476713184718959 T T T
0.3278758011626466 0.0604548199679557 0.5689080141264329 T T T
0.3288138981217909 0.3928791707459746 0.5687752924724564 T T T
0.3291457415128817 0.7254979061144891 0.5688034564038190 T T T
0.5857939794384529 0.0111636105675432 0.5890634636860080 T T T
0.5862848539107625 0.3471574808215832 0.5896834536550907 T T T

0.5863660449079964	0.6770594226032911	0.5889369729036511	T	T	T
0.8432010191703476	0.6264174403401783	0.6102090633725741	T	T	T
0.8438180877969831	0.2987917746131964	0.6106071550051175	T	T	T
0.8451929998302014	0.9647056552890196	0.6102933882149332	T	T	T
0.0996431052852437	0.5830452831988180	0.6320273493045953	T	T	T
0.0958156739314500	0.2541876594249357	0.6327512350422744	T	T	T
0.1000830722395499	0.9173339638914217	0.6314577675162931	T	T	T
0.3523346395778950	0.5389130595849217	0.6512089707985362	T	T	T
0.3526713122740006	0.2062180019755443	0.6516517753547054	T	T	T
0.3500194416476060	0.8764453910652334	0.6506421346271671	T	T	T
0.6052160668280718	0.4990742893314908	0.6728795202701654	T	T	T
0.6079403463953509	0.1584434647193878	0.6711881865136022	T	T	T
0.6092248620319152	0.8241819862037870	0.6709988934183966	T	T	T
0.8708768609222934	0.1039608061331943	0.6906042399371027	T	T	T
0.8625985789616057	0.7790989655045152	0.6883480054591130	T	T	T
0.6562607085595559	0.5144504130896386	0.7432425871715912	T	T	T
0.8173283070298420	0.3093889500892523	0.7522694053780539	T	T	T
0.5851127455466441	0.6350840486534102	0.7788576569067815	T	T	T
0.8412871825681673	0.2939590342513904	0.7886877641857674	T	T	T

COOH/Cu(533) E_{ads} = −2.11 eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H

60 1 2 1

Selective dynamics

Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0471834821759047	0.2948921435103857	0.4660604775694903	T	T	T
0.0467055437664284	0.6284674764998097	0.4658602667242512	T	T	T
0.0468184146135017	0.9616942349968572	0.4660132290280719	T	T	T
0.3036256202383194	0.2482846088649248	0.4867616610270066	T	T	T

0.3033147031122945	0.5815580150290068	0.4867121235268329	T	T	T
0.3034994292692847	0.9147681276864889	0.4866751291724237	T	T	T
0.5589778551913328	0.2025736326604779	0.5069898726484673	T	T	T
0.5591900940878126	0.5355633631826993	0.5070089619567559	T	T	T
0.5593355263351443	0.8684084387802919	0.5069398084233508	T	T	T
0.8155409799607741	0.1550298864325715	0.5277323594608491	T	T	T
0.8158166256643437	0.4881083854180644	0.5274063124147820	T	T	T
0.8155642213825323	0.8227428713408225	0.5280004322468533	T	T	T
0.0716739662516753	0.1087495126829758	0.5482967459075287	T	T	T
0.0718690716608647	0.4424667584274968	0.5482176030561192	T	T	T
0.0714554884302530	0.7754621701243732	0.5482298093992031	T	T	T
0.3270856658367881	0.0630651326676166	0.5690752169274972	T	T	T
0.3264286425077706	0.3972170028420918	0.5692121285361651	T	T	T
0.3269039385795880	0.7298938847343812	0.5690004464670945	T	T	T
0.5836538977688652	0.0168080120616520	0.5887082273293175	T	T	T
0.5838204873421325	0.3499788345866229	0.5889648847166572	T	T	T
0.5845277682937979	0.6824341756009636	0.5889532993705148	T	T	T
0.8420770313472318	0.6329647477126868	0.6096122020101512	T	T	T
0.8426531829164710	0.3012246631948896	0.6103316387635129	T	T	T
0.8424485490347036	0.9705183221539411	0.6106092335476526	T	T	T
0.0969668985991931	0.5889876113397340	0.6326158004328627	T	T	T
0.0980250775423845	0.2546593179799201	0.6320763522680838	T	T	T
0.0983374715166772	0.9210913214071040	0.6320008947249389	T	T	T
0.3504518213520366	0.5444497822853049	0.6520297415603855	T	T	T
0.3500596850255381	0.2120481793043979	0.6519000129815575	T	T	T
0.3505876953691870	0.8774850323994046	0.6518785307327164	T	T	T
0.6048840390626302	0.4997956858757890	0.6709919841633208	T	T	T
0.6040037308097773	0.1676081683989880	0.6715361670548620	T	T	T
0.6027135896060181	0.8354569114789268	0.6710881455407319	T	T	T
0.8613999904257407	0.4603218691858159	0.6917814340505711	T	T	T
0.8639231398663256	0.1124740014907706	0.6923913885118537	T	T	T
0.8575095866582587	0.7901350602397572	0.6894792867303788	T	T	T
0.9144071330256872	0.3588994531423457	0.7611389805822404	T	T	T
0.9068077547102402	0.1755381134232523	0.7657243261536694	T	T	T
0.9585057799239970	0.4064023080087495	0.7971695479986917	T	T	T
0.9494521320816014	0.1017015434453097	0.7987314808626371	T	T	T

COOH/Cu(533) $E_{ads} = -2.08$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 2 1
Selective dynamics
Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F

0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0472803537374639	0.2939507895990653	0.4659525489126434	T	T	T
0.0471047908184297	0.6272492288406097	0.4658108499326367	T	T	T
0.0469614864818266	0.9606406389239319	0.4658436392766903	T	T	T
0.3038346969927981	0.2468082475903345	0.4867343917874932	T	T	T
0.3037829858935485	0.5800787227203326	0.4868667168681592	T	T	T
0.3038057378393786	0.9128803167039907	0.4866501584436556	T	T	T
0.5591369143858156	0.2008579568309119	0.5069911566313349	T	T	T
0.5587015637751624	0.5344198180470319	0.5069892046346444	T	T	T
0.5590563579772684	0.8664343708233733	0.5072402090897574	T	T	T
0.8152629427004191	0.1543186981064766	0.5274927055966017	T	T	T
0.8152566732188355	0.4870953528907664	0.5274498881037767	T	T	T
0.8156197794324185	0.8196117076085686	0.5278515324609824	T	T	T
0.0717408066010825	0.1062200889327683	0.5480373796925760	T	T	T
0.0715606841183360	0.4403862190617616	0.5480841727655646	T	T	T
0.0718144754536925	0.7730161847270018	0.5481060882480768	T	T	T
0.3266564264348641	0.0601710021167267	0.5687970273608314	T	T	T
0.3268550550632921	0.3937138027928909	0.5690897524969072	T	T	T
0.3261485519805019	0.7278740238128582	0.5693214188137493	T	T	T
0.5835866916546020	0.0129003515505847	0.5885842714145206	T	T	T
0.5837915888718114	0.3484676334584941	0.5894872809715116	T	T	T
0.5839979583963536	0.6766141923344128	0.5900705201032900	T	T	T
0.8426630053077377	0.6280695542197903	0.6101205514937303	T	T	T
0.8421510976285145	0.2999119335764621	0.6098079633311436	T	T	T
0.8419836376252268	0.9661954675558549	0.6088877926419979	T	T	T
0.0975177379320297	0.5842099043710570	0.6324562823837128	T	T	T
0.0983282980849889	0.2502882410616658	0.6318426563792761	T	T	T
0.0960061121126878	0.9201098605719215	0.6326914504869378	T	T	T
0.3485955655124966	0.5414519196322078	0.6513804220319149	T	T	T
0.3501853826232476	0.2064752872162200	0.6516579732708251	T	T	T
0.3507901562872197	0.8731417962120708	0.6516640382635018	T	T	T
0.6014044742988042	0.4958366297156694	0.6758508842998482	T	T	T
0.6024646094161146	0.1602312863687787	0.6708327164307146	T	T	T
0.6047628077177297	0.8293831204232488	0.6708661971190566	T	T	T
0.8738234885384747	0.4483809380158663	0.6920903893762183	T	T	T
0.8574538047264182	0.1142019507234174	0.6890041602674224	T	T	T
0.8596947398413068	0.7870479889934364	0.6889270502902060	T	T	T
0.6800489358323767	0.4143615547421861	0.7464439087629277	T	T	T
0.5959831575075307	0.3954960551621645	0.7817514565367800	T	T	T
0.7990375641782963	0.4077191482427909	0.7611527355944203	T	T	T
0.6468519298805016	0.3784464334324102	0.8146917650546417	T	T	T

COOH/Cu(533) E_{ads} = −2.08 eV

1.00000000000000

10.3878408006999994 0.0000000000000000 0.0000000000000000

4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
63 1 2 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F
0.2571614599999990 0.9524293899999989 0.3219123699999997 F F F
0.5099116399999986 0.5747781399999994 0.3415763200000015 F F F
0.5095861200000016 0.2417833900000019 0.3416938299999970 F F F
0.5096986000000001 0.9088501900000026 0.3416314700000029 F F F
0.7627858999999972 0.5310134699999978 0.3609394899999998 F F F
0.7629538699999969 0.1970798500000015 0.3608490599999996 F F F
0.7629705100000024 0.8638077299999978 0.3608832600000014 F F F
0.0188077500000006 0.4844866199999984 0.3845455499999986 F F F
0.0188649600000019 0.1508076399999965 0.3844206699999972 F F F
0.0189457299999987 0.8174492599999965 0.3845321800000008 F F F
0.2777182000000025 0.4350678200000004 0.4051130599999979 F F F
0.2779364200000032 0.1018241299999971 0.4049400600000013 F F F
0.2778532499999997 0.7683188099999967 0.4050370400000034 F F F
0.5346647900000008 0.3873898000000011 0.4243529600000002 F F F
0.5347255300000029 0.0542446099999978 0.4245416400000011 F F F
0.5343893300000033 0.7214487199999979 0.4243017399999971 F F F
0.7896143700000025 0.3418778500000030 0.4451831499999983 F F F
0.7893677400000030 0.0085227100000012 0.4452920299999974 F F F
0.7895473399999986 0.6754118300000016 0.4453449800000016 F F F
0.0467274591672674 0.2945907015400776 0.4663996542503943 T T T
0.0454029899613299 0.6295767997331893 0.4664081091092364 T T T
0.0459789147298861 0.9616601161926825 0.4664372678267490 T T T
0.3025535018608323 0.2492321358267258 0.4868087333626260 T T T
0.3023811124809178 0.5809050253587841 0.4874509161893201 T T T
0.3022906155315061 0.9138368260228407 0.4869586532003797 T T T
0.5573743371329870 0.2019517110457633 0.5066715753008330 T T T
0.5582199803593305 0.5348290799783268 0.5062299622842172 T T T
0.5587057819424430 0.8669450367851212 0.5060668154672077 T T T
0.8151303079042872 0.1542016836316830 0.5276601528300452 T T T
0.8159049081462665 0.4868102502234090 0.5275355624696894 T T T
0.8145047660332145 0.8218563882579585 0.5280894153669838 T T T
0.0708866030979547 0.1066302646323095 0.5489696754164556 T T T
0.0703731805368820 0.4436050406879653 0.5484166601321216 T T T
0.0706997771872491 0.7752419321600156 0.5493214540402952 T T T
0.3258939009790482 0.0640327033717242 0.5674726966019247 T T T
0.3252251995584283 0.3968247502825808 0.5710203383616135 T T T
0.3251753534527828 0.7266325764632656 0.5698447458685609 T T T
0.5816884202588749 0.0113717173057070 0.5877474518544500 T T T
0.5818928238394767 0.3477340771140663 0.5873598850046058 T T T
0.5841114017487292 0.6794186759670443 0.5875552359597146 T T T
0.8395207673845432 0.6343668762638099 0.6104715345144853 T T T
0.8414163104820128 0.2985855692683824 0.6104043262820965 T T T
0.8428476238283508 0.9667706291135052 0.6104718294536772 T T T
0.0949215042337295 0.5887328448631864 0.6342071542152683 T T T
0.0968440893075602 0.2555322906090778 0.6308906103481794 T T T
0.0940968040753992 0.9232508722179755 0.6360929305914693 T T T
0.3457592181707300 0.5443925433568019 0.6570522845486928 T T T

0.3474046786848925	0.2109025077527921	0.6528362527105508	T	T	T
0.3466554032807607	0.8858957743870547	0.6471320429066363	T	T	T
0.6013000226127836	0.4971904313663270	0.6673965680074069	T	T	T
0.6045462462007165	0.1508481023629754	0.6671738462534571	T	T	T
0.5999547809664645	0.8285754363499562	0.6738058260344256	T	T	T
0.8738638185309187	0.4433808255084858	0.6904071745184636	T	T	T
0.8491016634807957	0.1239037317043214	0.6942243007744856	T	T	T
0.8560423589952052	0.7882628578376247	0.6913197192235693	T	T	T
0.6629868897340859	0.5690757484920870	0.7500272075919745	T	T	T
0.5605768540135682	0.3460867940550986	0.7415660050534636	T	T	T
0.3797604004468674	0.7438507749149035	0.7281005505388111	T	T	T
0.8824225624676055	0.3986838085950181	0.7795527693059319	T	T	T
0.9536120332239364	0.1710132995799250	0.7804235693552534	T	T	T
0.9400873951026389	0.4702999584670045	0.8043835668827538	T	T	T
0.0495491300534787	0.0977982960357058	0.8025626932750297	T	T	T

COOH/Defected-Cu(533) $E_{ads} = -2.06$ eV
1.00000000000000
10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H
59 1 2 1
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0470780414861253	0.2937530312078139	0.4661858690080329	T	T	T
0.0469183212612376	0.6267548379875082	0.4657822513322321	T	T	T
0.0468364341390179	0.9605948417233980	0.4659149840551152	T	T	T
0.3033126674068200	0.2465580370951395	0.4867576311275046	T	T	T
0.3040649934937533	0.5792824217225989	0.4865110836834574	T	T	T
0.3033037370631713	0.9129761972638648	0.4866623660287349	T	T	T
0.5589426900943398	0.2001565460132150	0.5066608604070802	T	T	T
0.5591756396974794	0.5334289208131877	0.5067180081656120	T	T	T

0.5588144616046564	0.8664643045570977	0.5072875436031580	T	T	T
0.8158388705031108	0.1522175129968988	0.5273896438547356	T	T	T
0.8153465135101394	0.4868039483978636	0.5273603958503460	T	T	T
0.8157557208414874	0.8192969984580950	0.5275588557377949	T	T	T
0.0721884315016137	0.1050447111409522	0.5484417896099500	T	T	T
0.0709829315119071	0.4397644531331633	0.5486332085238831	T	T	T
0.0726077381664340	0.7713462585963333	0.5477375799745996	T	T	T
0.3261301505114725	0.0598485957703938	0.5688855518235257	T	T	T
0.3272042333911733	0.3926535525142760	0.5688520074299366	T	T	T
0.3267843337643107	0.7259968091716062	0.5689151093791469	T	T	T
0.5839666951846699	0.0121214648917711	0.5885859019061667	T	T	T
0.5848064745412339	0.3448527225527396	0.5886662931832422	T	T	T
0.5850422180820632	0.6756370368959818	0.5895372374662836	T	T	T
0.8418036734631212	0.6264748287289168	0.6105351757572379	T	T	T
0.8432835909577792	0.2988395110248026	0.6094164804715269	T	T	T
0.8436809903362457	0.9631293215461137	0.6094505945456143	T	T	T
0.0975681103774705	0.5828966519248930	0.6321295686230309	T	T	T
0.0947349583060681	0.2516108415628785	0.6330609069264155	T	T	T
0.0950867019222354	0.9190540755511442	0.6329438017566071	T	T	T
0.3500453618468981	0.5399916717201880	0.6510869177184168	T	T	T
0.3489084012285387	0.2062744750455479	0.6515348470700646	T	T	T
0.3508657803758506	0.8713557156507801	0.6514973781334480	T	T	T
0.6076944214638595	0.4932271326337015	0.6721967280661195	T	T	T
0.6019119120812766	0.1585104811616753	0.6706623809310799	T	T	T
0.6053533457264876	0.8267633016341558	0.6701477537084474	T	T	T
0.8530315730746602	0.1254588094425579	0.6899989077031677	T	T	T
0.8603813256911904	0.7818374809331817	0.6883232115197687	T	T	T
0.7176175769922706	0.3416161232927398	0.7469649171236984	T	T	T
0.6143526696318423	0.3060216117717087	0.7690435651887022	T	T	T
0.7703202548750950	0.4227370375862278	0.7710555539590460	T	T	T
0.5953910963012744	0.3607398843870125	0.8040744509419876	T	T	T

COOH/Defected-Cu(533) $E_{ads} = -1.96$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
59 1 2 1
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F

0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0479131102358433	0.2929886333546131	0.4658652031791134	T	T	T
0.0479300192109322	0.6258440657695323	0.4660579332766543	T	T	T
0.0478120060310875	0.9599722304064968	0.4659224260933954	T	T	T
0.3053542995233995	0.2452633150671373	0.4870588378806910	T	T	T
0.3051261470361921	0.5782349356349203	0.4865604260495061	T	T	T
0.3045627399867565	0.9114266077161922	0.4869640182379684	T	T	T
0.5610036082765689	0.1988918832152305	0.5068461042961401	T	T	T
0.5611414689937414	0.5311708676252346	0.5068379234684990	T	T	T
0.5605218399884618	0.8639533367794211	0.5072686193870392	T	T	T
0.8178207896704212	0.1503219161364834	0.5275550864860721	T	T	T
0.8181071528724135	0.4828286928778600	0.5275759502678945	T	T	T
0.8179410569749969	0.8163526793461876	0.5275413425727877	T	T	T
0.0737159140638727	0.1038900268934144	0.5483364894139436	T	T	T
0.0745984875562282	0.4354897666307543	0.5483887980809392	T	T	T
0.0753017092501815	0.7689832534840302	0.5479248250650368	T	T	T
0.3296337683237460	0.0564925582208501	0.5690509940460575	T	T	T
0.3314512588319417	0.3913744172799065	0.5700337509965118	T	T	T
0.3321846073334374	0.7190851791153494	0.5696484350836559	T	T	T
0.5868765069551571	0.0096843474457992	0.5881571148109914	T	T	T
0.5879590802167272	0.3431383895925267	0.5897364308558412	T	T	T
0.5893813765724413	0.6708258234558959	0.5897974463921195	T	T	T
0.8465100629525796	0.6200132547557384	0.6102782204533804	T	T	T
0.8465785057382120	0.2937481171157836	0.6110060746114789	T	T	T
0.8466658218349118	0.9575683920457934	0.6090591012915069	T	T	T
0.1017790426904395	0.5773903418780106	0.6314294990737116	T	T	T
0.0989389969749645	0.2476432047954333	0.6333092743236788	T	T	T
0.1047035932130757	0.9111244390462089	0.6309575914943057	T	T	T
0.3545156274797239	0.5331243088072757	0.6562082419015507	T	T	T
0.3550877728527227	0.1994361691096000	0.6515094883887433	T	T	T
0.3560528536570844	0.8692557176264172	0.6508389942145267	T	T	T
0.6260286602530186	0.4856482564405631	0.6735954458701070	T	T	T
0.6136067336026569	0.1491657119068907	0.6707166687528842	T	T	T
0.6117648249542679	0.8240971716186558	0.6696594811132077	T	T	T
0.8740907535616169	0.0935617740499919	0.6881483935466031	T	T	T
0.8662688502114265	0.7712878024577399	0.6884143149054116	T	T	T
0.4023016207702151	0.5205112994715930	0.7284012288396038	T	T	T
0.3069940302298529	0.5224757437390853	0.7631650160097878	T	T	T
0.5177085546396919	0.5185213359688269	0.7440106783151038	T	T	T
0.3498888744777508	0.5200153619478387	0.7966372948791597	T	T	T

COOH/Cu(533) $E_{ads} = -1.95$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 2 1
Selective dynamics
Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0475462334372463	0.2932840923960909	0.4658022114834762	T	T	T
0.0476176567154857	0.6268236815958721	0.4658371479416372	T	T	T
0.0472604961996298	0.9603787091861842	0.4659507981280136	T	T	T
0.3046065171723421	0.2461930840467872	0.4868958988153157	T	T	T
0.3041428421055913	0.5790532406022939	0.4869957436177287	T	T	T
0.3045183023797324	0.9116296824472436	0.4870964344239089	T	T	T
0.5595912041381801	0.1998706944840644	0.5069206539916677	T	T	T
0.5595897701329490	0.5323357286566518	0.5072347414359878	T	T	T
0.5601682030555548	0.8656413742308646	0.5068372237890862	T	T	T
0.8156904836508039	0.1524459189812867	0.5277722941399553	T	T	T
0.8168317143023001	0.4848471252020399	0.5276500623402071	T	T	T
0.8169128067398621	0.8185322748867858	0.5274741307584618	T	T	T
0.0735643745785498	0.1042361834599160	0.5480566387324738	T	T	T
0.0734717817019756	0.4381030441092369	0.5478609281317803	T	T	T
0.0721384503773689	0.7725632832031337	0.5482093118779984	T	T	T
0.3291807913687075	0.0581985318294759	0.5687731875162808	T	T	T
0.3292257075411738	0.3923255964268507	0.5700802660782631	T	T	T
0.3285959515070561	0.7227199563501656	0.5702120039066032	T	T	T
0.5864929754025611	0.0109041834338104	0.5889203039905463	T	T	T
0.5835653210808707	0.3436771437777531	0.5902624973856451	T	T	T
0.5854734708279470	0.6770524892329729	0.5887369371171360	T	T	T
0.8448153938566823	0.6280142056032976	0.6093174155401536	T	T	T
0.8446741126883456	0.2938104816181905	0.6092875733677515	T	T	T
0.8414916809568548	0.9633568169850871	0.6101260822348485	T	T	T
0.0998295835502056	0.5820486062931772	0.6311930869155253	T	T	T
0.1016144803236893	0.2478418470628053	0.6320080932701242	T	T	T
0.0987644969778335	0.9176813148132693	0.6319164920923820	T	T	T
0.3479020940677482	0.5462103276307460	0.6550381853189461	T	T	T
0.3553716785665619	0.1990321067819210	0.6508323513794513	T	T	T
0.3548812839687694	0.8707008946630268	0.6514836171080955	T	T	T
0.6120611316490536	0.4903437577294669	0.6710387816573090	T	T	T
0.6099622855317949	0.1517611384824358	0.6755040083136602	T	T	T
0.6113059406266191	0.8189596863602374	0.6713627340281619	T	T	T
0.8664134385799476	0.4416579828941500	0.6897301800332549	T	T	T

0.8651973686415949 0.1103650151824130 0.6899553241659099 T T T
0.8691554689830854 0.7710228554868115 0.6899537957322798 T T T
0.4708771128594421 0.2744691603163811 0.7351453597090876 T T T
0.5074456018818637 0.1473136371508153 0.7764137893709772 T T T
0.3490224634674481 0.4741148500592096 0.7362681783822493 T T T
0.4235218683794334 0.2423401549653189 0.8019650136600438 T T T

COOH/Cu(533) $E_{ads} = -1.93$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 2 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0475543548174643 0.2936886359151474 0.4658247782137347 T T T
0.0476681683528276 0.6270063941526585 0.4657382142330078 T T T
0.0477541507782920 0.9603031375197292 0.4657386541127286 T T T
0.3048657539701480 0.2459917940017134 0.4866959221425010 T T T
0.3050026134578451 0.5791184236372565 0.4866695109933971 T T T
0.3045344652589607 0.9129332084096653 0.4867309227137483 T T T
0.5603389945216851 0.2002982415442396 0.5070545327586551 T T T
0.5602221298932035 0.5329351964925100 0.5072148529138105 T T T
0.5605679433004106 0.8661185444484165 0.5074656230149818 T T T
0.8170089904812463 0.1525702388891850 0.5274871112987963 T T T
0.8166314009974250 0.4861194766181063 0.5277485094514104 T T T
0.8170406746025162 0.8190888650474314 0.5273698574787393 T T T
0.0728417169315480 0.1061438172074066 0.5481689238218771 T T T
0.0735986032252132 0.4389021740059201 0.5479797684625596 T T T
0.0736138991731533 0.7721280957402195 0.5478043754304733 T T T
0.3296154567946743 0.0592499221854102 0.5687699760638429 T T T
0.3296732696815066 0.3920896231043350 0.5689041603020168 T T T

0.3289507924074371 0.7260424140131366 0.5688475493070150 T T T
0.5867358760773838 0.0142070082634285 0.5897382487776578 T T T
0.5869179206037928 0.3445166404122565 0.5902920685548141 T T T
0.5859153697327454 0.6768955741741961 0.5898330632949202 T T T
0.8450030421587217 0.6301434272660756 0.6091582885315404 T T T
0.8429643691438915 0.2971929167378982 0.6098728266810519 T T T
0.8443645270589778 0.9632212421384128 0.6091743359022360 T T T
0.1014642549754596 0.5826383630458010 0.6319020728212833 T T T
0.1017268130799380 0.2491870395403570 0.6317437411945076 T T T
0.1012885883894957 0.9163316972212655 0.6317594521488510 T T T
0.3527961381649025 0.5394859547317489 0.6503383305914446 T T T
0.3545399885368717 0.2050150145074047 0.6515168080413735 T T T
0.3532148733103811 0.8743728910010725 0.6511393839874975 T T T
0.6061615000551158 0.5023655704071344 0.6745922276644357 T T T
0.6091828728567961 0.1559612413665490 0.6756056923035308 T T T
0.6104283130910834 0.8255321691263775 0.6711481095263767 T T T
0.8684667413070204 0.4450815691740796 0.6891858038770993 T T T
0.8710582778820961 0.1067603581088145 0.6889578396546786 T T T
0.8686708749820972 0.7746236266240797 0.6893515617156000 T T T
0.5851290276473403 0.2684161864281011 0.7440213044247517 T T T
0.5891474883386352 0.1573049137134386 0.7844967775461741 T T T
0.5613204201135871 0.4502386634966711 0.7511645396147605 T T T
0.5708601962778852 0.2471474966871091 0.8145584865509424 T T T

COOH/Cu(533) $E_{ads} = -1.92$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 2 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F

0.0471136569069176 0.2938422327131256 0.4659044459947904 T T T
0.0468950941437120 0.6271863040516098 0.4660039943118481 T T T
0.0471261264889046 0.9604558106463962 0.4656700594875145 T T T
0.3043461532149886 0.2454705819913151 0.4866703794682042 T T T
0.3046065977705270 0.5787295333176051 0.4867544403087126 T T T
0.3045945762174597 0.9125987891538287 0.4868832488720157 T T T
0.5599243415461621 0.1986860328602735 0.5069521365299030 T T T
0.5596660491020614 0.5323708611489678 0.5070322064395003 T T T
0.5596781719543475 0.8662958360026458 0.5071398173088389 T T T
0.8166409396117359 0.1508499898631708 0.5278805858047232 T T T
0.8158474522050237 0.4859324850171169 0.5275903570454180 T T T
0.8146609133203148 0.8198036062363812 0.5279230756537837 T T T
0.0737760176112991 0.1043422026438091 0.5476965528783866 T T T
0.0735495168757911 0.4373052850595886 0.5478767259763923 T T T
0.0729089681444646 0.7728619061269175 0.5473738564988815 T T T
0.3289169395043051 0.0600399737998446 0.5701067992439950 T T T
0.3306229596901019 0.3887431007792102 0.5692468703702346 T T T
0.3288007596070641 0.7247766506701070 0.5690465433370732 T T T
0.5807891544125268 0.0139340833204217 0.5904236554153823 T T T
0.5864899602622758 0.3415548433247525 0.5890869217887933 T T T
0.5855889728128306 0.6774825348256561 0.5891406102524754 T T T
0.8448955153387249 0.6277395024831083 0.6097143241411429 T T T
0.8451841199870745 0.2924414373684535 0.6091049040046823 T T T
0.8448052556951179 0.9577896647897464 0.6103169481315813 T T T
0.1019827496041268 0.5845767511904271 0.6282101260046777 T T T
0.0994524519041669 0.2465836834657050 0.6311194665765439 T T T
0.1023538134443265 0.9135974421543820 0.6321701132704276 T T T
0.3584129586226411 0.5337462860779096 0.6514460557903736 T T T
0.3443289019985113 0.2139571673840818 0.6590398999373615 T T T
0.3566053466758987 0.8676901037804228 0.6516899555347417 T T T
0.6086668984935723 0.4889192304936296 0.6722108881160784 T T T
0.6144744403086826 0.1489356083073856 0.6724698271925672 T T T
0.6135201436332479 0.8204789947396252 0.6718991595069950 T T T
0.8612029279082927 0.4394478439447389 0.6892506980215481 T T T
0.8648614139765692 0.1086271256700612 0.6895698689137892 T T T
0.8833732443973383 0.7568984344996458 0.6922572699900926 T T T
0.2253399027841981 0.3190143415242001 0.7245027652563396 T T T
0.3130285910793202 0.1660702182520969 0.7612390022436254 T T T
0.0907419518668350 0.4931591618049539 0.7371990005058805 T T T
0.2485146146736744 0.2255880455592890 0.7925655933525798 T T T

COOH/Cu(533) E_{ads} = −1.91 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 2 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F

0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0476981598613024	0.2939223548422762	0.4658851764105251	T	T	T
0.0475122513345614	0.6272038084839209	0.4658075475174460	T	T	T
0.0474311875033769	0.9607275344692549	0.4658000688212456	T	T	T
0.3046157945361876	0.2465303914433282	0.4867222911935769	T	T	T
0.3044634046093823	0.5799514615541542	0.4867921561658552	T	T	T
0.3048031996065860	0.9127991506233865	0.4867484091576952	T	T	T
0.5599815341375288	0.2009168738518052	0.5071917390245430	T	T	T
0.5597022156493960	0.5338472805788982	0.5069643693801638	T	T	T
0.5601008180391531	0.8662872982807687	0.5071906886450278	T	T	T
0.8164824654904655	0.1532839387126920	0.5274931612524035	T	T	T
0.8167087004876101	0.4856797172648949	0.5274986081720102	T	T	T
0.8167993331240393	0.8199671389970564	0.5277834319629331	T	T	T
0.0732605014307018	0.1061429355012104	0.5479799866568691	T	T	T
0.0734707092905847	0.4395060374795792	0.5481087434524833	T	T	T
0.0731344262599403	0.7728380650024135	0.5479875176658602	T	T	T
0.3284406618233681	0.0601750613695529	0.5690102959915532	T	T	T
0.3286447147850104	0.3938499874259730	0.5690599926508910	T	T	T
0.3285334872091218	0.7269009457653632	0.5692344579498615	T	T	T
0.5855132075248645	0.0130293968888872	0.5887214844716914	T	T	T
0.5860232844212092	0.3483178939461764	0.5899366695516024	T	T	T
0.5860854144191437	0.6765080533665916	0.5898256064296475	T	T	T
0.8441403149263135	0.6294217434410152	0.6088728169587007	T	T	T
0.8441226325191246	0.2954046549252883	0.6098992016172716	T	T	T
0.8449282421074610	0.9652038935004360	0.6098267015714575	T	T	T
0.1005221407867941	0.5839625810954173	0.6323456272130228	T	T	T
0.0995705859813711	0.2511815345333585	0.6322841706326048	T	T	T
0.1002049740499066	0.9176975426520353	0.6320409986525285	T	T	T
0.3531733610021915	0.5400657848764355	0.6516883208697377	T	T	T
0.3531455624744027	0.2070859960388317	0.6517128256312142	T	T	T
0.3520120512467502	0.8750475777348611	0.6511825470544621	T	T	T
0.6049075040679499	0.4981561815424509	0.6765826118287613	T	T	T
0.6077312288504050	0.1603454080680844	0.6710320190794006	T	T	T
0.6066401938970845	0.8313077988536229	0.6711904896833504	T	T	T
0.8635266691894458	0.4514291814902358	0.6887026963069818	T	T	T
0.8725105727630548	0.0999953262666786	0.6912739942813181	T	T	T
0.8628788882063086	0.7788956849248883	0.6889879669168639	T	T	T
0.6334300964956722	0.4804886011516771	0.7507136239910231	T	T	T
0.7807361420001968	0.2672653749280520	0.7642186195349411	T	T	T
0.5500063589773948	0.6073568245083116	0.7841539150492360	T	T	T
0.7908769444214876	0.2531272666318320	0.8013025673887115	T	T	T

COOH/Cu(533) E_{ads} = −1.90 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 2 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0476302661909190 0.2931539494683122 0.4657832529678712 T T T
0.0481225319793589 0.6261820439246366 0.4660444545885186 T T T
0.0478944357986149 0.9596944617616335 0.4659734520966985 T T T
0.3055600070078899 0.2449240914205020 0.4867495337096429 T T T
0.3049163970499342 0.5786819179153645 0.4867480559686972 T T T
0.3048076023552121 0.9113765137776501 0.4870448438329152 T T T
0.5608973104823071 0.1992633384789668 0.5069343371341526 T T T
0.5608263363731533 0.5318885147813155 0.5069321153532449 T T T
0.5609777939504179 0.8642847501324092 0.5071622062589768 T T T
0.8174327258748948 0.1514112487293828 0.5277636275643827 T T T
0.8177631246912348 0.4840174183412403 0.5277798357920751 T T T
0.8180725847740088 0.8174916345494779 0.5275273535555794 T T T
0.0738893231489634 0.1037225830286426 0.5481968702130888 T T T
0.0756765155278133 0.4355100426279451 0.5479319615093803 T T T
0.0749627132586490 0.7698650442856703 0.5483415137292698 T T T
0.3310172635315238 0.0556162024821928 0.5687430947339307 T T T
0.3311749677460735 0.3909844664280803 0.5697253549334078 T T T
0.3313835857337242 0.7200007441769118 0.5699215382579412 T T T
0.5876345620405272 0.0093861524866825 0.5884572317504031 T T T
0.5867906041998858 0.3442998913121866 0.5898701288293459 T T T
0.5879072077250842 0.6730867285265068 0.5899251200413625 T T T
0.8475593353298118 0.6253462531005788 0.6091494559068011 T T T
0.8447000856835892 0.2944663811910905 0.6103119980105761 T T T
0.8467106991012182 0.9601141023692521 0.6095224969750623 T T T
0.1023283566663275 0.5779244419324445 0.6316753032512165 T T T

0.1042906408920082 0.2439120378351825 0.6317495895495537 T T T
0.1041519606297152 0.9116565255425592 0.6317144674339645 T T T
0.3538404154993770 0.5323449979416151 0.6553249400764517 T T T
0.3578325616332451 0.1965228756209013 0.6513611253124039 T T T
0.3572337978500579 0.8685488760756533 0.6510092682813936 T T T
0.6163167947543257 0.4894726380939982 0.6756062031171826 T T T
0.6140750762052197 0.1491404071708075 0.6708812124020854 T T T
0.6139770644695084 0.8210418431261199 0.6714976671953443 T T T
0.8725997937355878 0.4406931344790722 0.6897523006880542 T T T
0.8720734333372187 0.1037089963011805 0.6895696059475473 T T T
0.8681895504048464 0.7750881206881902 0.6897801820479436 T T T
0.3892605884628599 0.5138842259299307 0.7283074380851425 T T T
0.2901170785203566 0.5109247948852410 0.7604941211830867 T T T
0.5009333974867705 0.5137057306664631 0.7464451017549839 T T T
0.3275927982009122 0.5074004274798598 0.7949926495426306 T T T

COOH/Cu(533) E_{ads} = −1.86 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
59 1 2 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0472521541848777 0.2940049856517837 0.4658059533848269 T T T
0.0474814608980145 0.6269087053856599 0.4659853591623703 T T T
0.0476235012971361 0.9605574216502528 0.4660005643952443 T T T
0.3046858036749476 0.2465635128608280 0.4869636492343778 T T T
0.3045305057771633 0.5793494754892327 0.4865301479170410 T T T
0.3041743447320092 0.9129190801989332 0.4869054734927080 T T T
0.5605782054696709 0.1999316333491838 0.5066617111239692 T T T
0.5606760872883376 0.5328445491308441 0.5067850226239882 T T T

0.5598669214669544 0.8663706565557272 0.5071278271767760 T T T
0.8172256644955980 0.1522953436162187 0.5276185957859910 T T T
0.8175581792784462 0.4851217859259386 0.5277184526766788 T T T
0.8173105941570524 0.8188685486175605 0.5276347547822970 T T T
0.0735328744798975 0.1062286261896203 0.5481994643115223 T T T
0.0740243781427791 0.4378921326132182 0.5481998316627706 T T T
0.0747202583782682 0.7712378738699347 0.5479929386351386 T T T
0.3288727664922109 0.0592418876168895 0.5692795239483845 T T T
0.3305818681938679 0.3933445164674833 0.5697413298228647 T T T
0.3312799023147949 0.7223426471763141 0.5695384257968424 T T T
0.5865469985231255 0.0122944914660974 0.5886326751265646 T T T
0.5858388691878271 0.3450432830063924 0.5890336952033745 T T T
0.5879770328919258 0.6761959100233732 0.5889905994220227 T T T
0.8460950751811656 0.6243432293021477 0.6105352738640446 T T T
0.8461606342503377 0.2976320800693578 0.6109479379644193 T T T
0.8462163598997565 0.9615248304464863 0.6095823567110785 T T T
0.1014857028043145 0.5801080895646484 0.6309990198828965 T T T
0.0992140816281824 0.2507410362744074 0.6333147247543298 T T T
0.1019445551448334 0.9181113265074972 0.6303913841473127 T T T
0.3534223538511799 0.5393605019301014 0.6566412665579068 T T T
0.3557293290187418 0.2028678554154264 0.6516768617657759 T T T
0.3566842956485473 0.8711152625558369 0.6518811387663889 T T T
0.6153136404103093 0.4899824027024643 0.6702670916374455 T T T
0.6141577901336757 0.1530143638571215 0.6717128765554602 T T T
0.6121526889516703 0.8222551105481378 0.6703773623273941 T T T
0.8697033222721142 0.1064113644660118 0.6888532721687715 T T T
0.8663633715572183 0.7756847995122893 0.6885948668198281 T T T
0.3088026745017143 0.5687257616453958 0.7297628468173377 T T T
0.4389240645982270 0.4008139867886658 0.7576978827476119 T T T
0.1827041519886474 0.7124387217186736 0.7509168527083977 T T T
0.4043460798482985 0.4270975974655753 0.7933516533812792 T T T

COOH/Cu(533) $E_{ads} = -1.85$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 2 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F

0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0476295779158248	0.2938571599383397	0.4658986037234779	T	T	T
0.0474213566273348	0.6271666173719750	0.4658916037820004	T	T	T
0.0474460784779358	0.9606220996352122	0.4658269040935040	T	T	T
0.3043399525926865	0.2466013372034641	0.4868722901752444	T	T	T
0.3043289594764286	0.5799239394950378	0.4868700906732726	T	T	T
0.3045445819293012	0.9127179753702012	0.4867876431301158	T	T	T
0.5598741505030145	0.2003430029019375	0.5070970542946994	T	T	T
0.5596347015934937	0.5338823165392792	0.5069875795502889	T	T	T
0.5599018182877373	0.8664409679123237	0.5073543275303819	T	T	T
0.8165548676016680	0.1531210240294568	0.5275219548052457	T	T	T
0.8165935167495063	0.4862388183964561	0.5275081923075513	T	T	T
0.8164647026349932	0.8195407534982405	0.5277805046760500	T	T	T
0.0730539021717914	0.1058228550012331	0.5481264460522228	T	T	T
0.0730887250141279	0.4393836515430562	0.5482901462369522	T	T	T
0.0730535710834024	0.7728272876147702	0.5481658768798843	T	T	T
0.3284208504978461	0.0593613646928738	0.5690972275580375	T	T	T
0.3287558759876268	0.3934214993838622	0.5692180070136023	T	T	T
0.3285357524689029	0.7264094981126158	0.5694277878433740	T	T	T
0.5850724229581622	0.0128432460807338	0.5890998497699748	T	T	T
0.5858378502255490	0.3470852600391271	0.5895827530737194	T	T	T
0.5859251128871499	0.6764690357780274	0.5900213047512048	T	T	T
0.8440319967931434	0.6293978917518902	0.6095323167047659	T	T	T
0.8433873626313396	0.2973927536470748	0.6095237299761472	T	T	T
0.8442529263738069	0.9642467169947112	0.6093681857492409	T	T	T
0.1008850126966083	0.5829333201624360	0.6323282898479100	T	T	T
0.1006750694181545	0.2493946892525437	0.6322236373602522	T	T	T
0.1000866332609179	0.9172522614050789	0.6325155379476796	T	T	T
0.3531893844655435	0.5391556070975844	0.6518280406788041	T	T	T
0.3534181431318008	0.2055299099177529	0.6517251988676254	T	T	T
0.3533520933671285	0.8724221035686534	0.6516665297881181	T	T	T
0.6066004822183800	0.4934151345519875	0.6763146458526279	T	T	T
0.6078406432806271	0.1583479018979183	0.6716436980149224	T	T	T
0.6082377774883316	0.8290642385015289	0.6716409013615989	T	T	T
0.8672471478694582	0.4455415166722249	0.6894134065622669	T	T	T
0.8652310548825046	0.1113037370522180	0.6895152020308722	T	T	T
0.8644425992046085	0.7802664074001686	0.6894140672690734	T	T	T
0.5869464684207437	0.5152240335674019	0.7503793647663111	T	T	T
0.5632828414390383	0.3733811676705918	0.7728285707225458	T	T	T
0.5906603380378960	0.6471888258496742	0.7755618115113462	T	T	T
0.5506445682469393	0.4062291079826588	0.8093388522278290	T	T	T

COOH/Cu(533) $E_{ads} = -1.82$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 2 1
Selective dynamics

Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0481940185081917	0.2935711930471250	0.4657777709636030	T	T	T
0.0485083560659285	0.6265457918642988	0.4659645320058389	T	T	T
0.0486589409380018	0.9596972691446686	0.4660079097668496	T	T	T
0.3062144145335506	0.2455175453137214	0.4869349931431582	T	T	T
0.3055654487175353	0.5789998872615568	0.4868588759666365	T	T	T
0.3058436851068317	0.9118395867584959	0.4869996597422712	T	T	T
0.5616964605788696	0.1990702734275346	0.5068580899626935	T	T	T
0.5618009090541640	0.5320061751657853	0.5068165747138884	T	T	T
0.5618357529521132	0.8654025700637205	0.5070842587576173	T	T	T
0.8190356926732525	0.1509883867144910	0.5276213425478353	T	T	T
0.8192575597695548	0.4842727308209827	0.5276928903355752	T	T	T
0.8193516157243270	0.8178228596658019	0.5275992994843534	T	T	T
0.0761983822498829	0.1040484187280497	0.5480612509463028	T	T	T
0.0770585197472575	0.4367552157291761	0.5480245189160697	T	T	T
0.0762354387170127	0.7704566134353134	0.5484612326459885	T	T	T
0.3321576828431904	0.0573748619143057	0.5690844777863379	T	T	T
0.3327461854100396	0.3922765548686632	0.5700350228158957	T	T	T
0.3329971692796000	0.7213286384521573	0.5699613053636803	T	T	T
0.5896189947265894	0.0101122428714319	0.5890252456983017	T	T	T
0.5884990965463029	0.3430096344696795	0.5891266890820186	T	T	T
0.5892133574917094	0.6755343041023728	0.5888640950061450	T	T	T
0.8497820125586000	0.6257549670776748	0.6092599358992019	T	T	T
0.8482800596308214	0.2933373968251652	0.6096342267453225	T	T	T
0.8482628872229699	0.9605951455815990	0.6098463325928920	T	T	T
0.1060098851983188	0.5795779096901296	0.6321292688626730	T	T	T
0.1054483370788742	0.2468874814108706	0.6321950744145800	T	T	T
0.1049267637357692	0.9147894195977878	0.6313548799568196	T	T	T
0.3584609833784234	0.5365066239172434	0.6564245315630142	T	T	T
0.3594641920675026	0.2002347982150893	0.6514387061377476	T	T	T
0.3595941011876336	0.8709480577744018	0.6515153649697284	T	T	T
0.6149685717817214	0.4895512891149802	0.6716260505432471	T	T	T
0.6174076138015343	0.1497661918061543	0.6722577091242151	T	T	T
0.6149391717448706	0.8205088067684879	0.6716049793899832	T	T	T

0.8691433075284010	0.4428089154000524	0.6897332507515636	T	T	T
0.8713367593466171	0.1081099970462204	0.6898876179096045	T	T	T
0.8709596375042276	0.7730471669710354	0.6897526214982872	T	T	T
0.3568067933928727	0.5510158102871997	0.7309653332617678	T	T	T
0.4594930307654648	0.3429449275819749	0.7534802587562928	T	T	T
0.2725556052567165	0.7162925403279795	0.7568509932962763	T	T	T
0.4481628836636829	0.3642355234175767	0.7904428345809624	T	T	T

COOH/Cu(533) $E_{ads} = -1.82$ eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H

60 1 2 1

Selective dynamics

Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0474179371707088	0.2938910563916053	0.4658548444873917	T	T	T
0.0478289096394366	0.6269158399510754	0.4660038973606738	T	T	T
0.0478624679875486	0.9600870798973323	0.4659773294219223	T	T	T
0.3049941657390453	0.2458718138701089	0.4868204661389459	T	T	T
0.3045169544751067	0.5795627061165260	0.4868439715586744	T	T	T
0.3047363031825366	0.9124377087148714	0.4870732868585990	T	T	T
0.5602200929855069	0.1999133802342649	0.5067585920900073	T	T	T
0.5602019978238554	0.5331407180069132	0.5067352734301334	T	T	T
0.5601253546821755	0.8661577985468788	0.5070569944075897	T	T	T
0.8169995405788535	0.1522797645540015	0.5275668871380808	T	T	T
0.8172188385617586	0.4853890712229220	0.5277133502002707	T	T	T
0.8172378588907003	0.8189133797992655	0.5275072796359652	T	T	T
0.0741183445466359	0.1047588696216372	0.5480318615405602	T	T	T
0.0748028348390606	0.4380242684002009	0.5480559455831228	T	T	T
0.0742298653385817	0.7715878396487629	0.5484057249033888	T	T	T
0.3294975353485902	0.0588378045797821	0.5692817560708957	T	T	T

0.3298680550333717 0.3933110026277100 0.5697812364284457 T T T
0.3300731708294324 0.7232312845174946 0.5701173099969375 T T T
0.5863124386178130 0.0121639051718710 0.5888093281862963 T T T
0.5850978588149809 0.3457816308088811 0.5888727543146125 T T T
0.5860436135550570 0.6774651299513996 0.5890559909553508 T T T
0.8463852080925778 0.6279786601555635 0.6092131060169268 T T T
0.8458217068455385 0.2947661493138990 0.6094805054134267 T T T
0.8452608474450761 0.9624363124779970 0.6094930851564000 T T T
0.1016017533426717 0.5820866846977828 0.6321138548620224 T T T
0.1019579922513547 0.2485252360298064 0.6319772105274273 T T T
0.1014673714129305 0.9161592096001256 0.6318001864178368 T T T
0.3549214691117963 0.5366085981484910 0.6559857555103495 T T T
0.3558925598531720 0.2015468005704111 0.6517294020254311 T T T
0.3558510503145239 0.8728056409223075 0.6519296527435511 T T T
0.6126801230983007 0.4905553858366822 0.6714449397633506 T T T
0.6117439608997998 0.1559644646203240 0.6715006104090870 T T T
0.6111891318714467 0.8237379360349716 0.6716077850071381 T T T
0.8661120275493351 0.4451820614564596 0.6896536806677280 T T T
0.8657051286289438 0.1116725193327239 0.6898040894515628 T T T
0.8646890218727682 0.7790114369229008 0.6896625017092912 T T T
0.3291657943934173 0.5649977435076415 0.7298934160438424 T T T
0.3198307107783133 0.4102504700506001 0.7527597897134122 T T T
0.3153735493173018 0.7120983166328952 0.7544350421517085 T T T
0.3022170990236958 0.4467734944527464 0.7890558819372387 T T T

COOH/Cu(533) $E_{ads} = -1.78$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 2 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F

0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0476130544065483	0.2929548048665315	0.4658690739097490	T	T	T
0.0480299263805553	0.6260193135921083	0.4660364516076899	T	T	T
0.0480175370832871	0.9592450127659146	0.4658879098284301	T	T	T
0.3051435803143299	0.2449184839220391	0.4867184954453417	T	T	T
0.3046233128810444	0.5783293034445804	0.4869002657239985	T	T	T
0.3049105775538014	0.9112918382139439	0.4872440521745635	T	T	T
0.5603730403864708	0.1988997282747598	0.5067904954705630	T	T	T
0.5603991118037766	0.5321050581967495	0.5066842046859186	T	T	T
0.5604004023120071	0.8648580517352421	0.5069208655000188	T	T	T
0.8175813049216634	0.1506051746616249	0.5275462146443618	T	T	T
0.8177493478474234	0.4837519200449834	0.5276550262212194	T	T	T
0.8175297983422809	0.8174675079493290	0.5274727015780338	T	T	T
0.0747236259242988	0.1020282054827141	0.5480204757778483	T	T	T
0.0752563502152864	0.4356564127633624	0.5480663273377641	T	T	T
0.0744401618366299	0.7697802716587430	0.5483918963840563	T	T	T
0.3300961796186429	0.0570044314993517	0.5692962388569682	T	T	T
0.3305100928851094	0.3900087119363347	0.5699210671425093	T	T	T
0.3307452538451453	0.7193951748784904	0.5702300813960759	T	T	T
0.5865801010689107	0.0100316923630433	0.5887175768292414	T	T	T
0.5861956464367548	0.3433736627218377	0.5887680068353635	T	T	T
0.5870089369278115	0.6750167317123418	0.5887753657378909	T	T	T
0.8471354370452127	0.6253395559766686	0.6091824903657764	T	T	T
0.8468599478079666	0.2916704923382568	0.6094459459321805	T	T	T
0.8455887346612022	0.9602651018684838	0.6095326016732839	T	T	T
0.1017822083855051	0.5792176439684855	0.6316253506898896	T	T	T
0.1023630595357571	0.2440839591347041	0.6318039288849561	T	T	T
0.1036930499861022	0.9105305437422226	0.6322770151919096	T	T	T
0.3560441657583584	0.5330220492989671	0.6566544884409862	T	T	T
0.3558036466328429	0.1957100902948317	0.6521504623022115	T	T	T
0.3573994899905841	0.8660982953627304	0.6513764208421216	T	T	T
0.6145391253778443	0.4888128068585066	0.6712762792652810	T	T	T
0.6123110193022255	0.1545894612747885	0.6713531442228309	T	T	T
0.6127771457436427	0.8197259242568942	0.6712429014515640	T	T	T
0.8677768423521767	0.4422698829809063	0.6897570526939755	T	T	T
0.8675677550210718	0.1084399351474664	0.6897245461352066	T	T	T
0.8650820520323104	0.7771849132970884	0.6895895062282181	T	T	T
0.3678578185766239	0.4556915846709190	0.7293127172747454	T	T	T
0.3019182802757915	0.3431220533511626	0.7381334604727178	T	T	T
0.4112667793242114	0.5099902787070221	0.7646391982336643	T	T	T
0.3101020005842147	0.3110267473376120	0.7745882185385378	T	T	T

COOH/Cu(533) $E_{ads} = -1.69$ eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H

60 1 2 1

Selective dynamics

Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F

0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0474836311156363	0.2944965797464552	0.4659192009787314	T	T	T
0.0469682637071485	0.6274266042906196	0.4661427610824354	T	T	T
0.0470632580190798	0.9595995102116995	0.4662341520994996	T	T	T
0.3038100068987898	0.2475905816683855	0.4868202969451610	T	T	T
0.3037464265830871	0.5799171364351717	0.4868120461379038	T	T	T
0.3040206960275034	0.9129922708613525	0.4866816823452490	T	T	T
0.5586378448461021	0.2015076688610548	0.5069309520063291	T	T	T
0.5589515778283524	0.5340558746614472	0.5067322805222431	T	T	T
0.5595310139184020	0.8672644349031839	0.5067240444285652	T	T	T
0.8151572146581643	0.1532372585453115	0.5276806360290184	T	T	T
0.8161850016509222	0.4865066403533650	0.5272396423582327	T	T	T
0.8156724743709960	0.8200400585245224	0.5275329915037108	T	T	T
0.0724737365127207	0.1058061420280690	0.5472005450768495	T	T	T
0.0731985227067769	0.4404114028763421	0.5490708907157140	T	T	T
0.0729675146255515	0.7695662288832978	0.5493012922106563	T	T	T
0.3279863779324176	0.0605398882051120	0.5683585284974871	T	T	T
0.3264840629490417	0.3960888685579225	0.5701251507553146	T	T	T
0.3274223454143821	0.7258504126570914	0.5691964428411297	T	T	T
0.5839801630657213	0.0143920837095184	0.5885350234368545	T	T	T
0.5829377793914139	0.3480503756821081	0.5891328457611309	T	T	T
0.5848479253551483	0.6798450255548698	0.5882655611602685	T	T	T
0.8433979747450829	0.6304509957578017	0.6090464058894693	T	T	T
0.8438309640433198	0.2971688626539742	0.6088254399425019	T	T	T
0.8451946295270567	0.9610671187464700	0.6092156503983970	T	T	T
0.1014521509685414	0.5763714315548893	0.6380004985712621	T	T	T
0.1002004210034670	0.2444100359499497	0.6306878372670581	T	T	T
0.0993727576224050	0.9186520891541996	0.6307998198028408	T	T	T
0.3583396374521918	0.5420808458600459	0.6536798178654765	T	T	T
0.3558783039380338	0.2002179238162949	0.6511324285068432	T	T	T
0.3552682704855104	0.8725078239360307	0.6508798509175117	T	T	T
0.6103702256120888	0.4948759292323311	0.6716549583163632	T	T	T
0.6100150959075636	0.1590158044256855	0.6711588277436126	T	T	T
0.6080588528456672	0.8277443153257578	0.6715684774230528	T	T	T
0.8622257756199496	0.4481089994731244	0.6892121655118050	T	T	T
0.8617800835339645	0.1173492994908071	0.6889864873271470	T	T	T
0.8564708861206372	0.7892434156293996	0.6906028998304995	T	T	T
0.1663736599564565	0.5177255149198950	0.7116646127157366	T	T	T
0.1139714390776649	0.4331746304121734	0.7447031119610780	T	T	T
0.2516077687208271	0.5679734715968311	0.7291650859988218	T	T	T
0.1583878049036891	0.4271771377678934	0.7781495437211109	T	T	T

COOH/Cu(111) E_{ads} = −2.06 eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
3.8289832201000000 6.6319934786000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu C O H
45 1 2 1
Selective dynamics
Direct
0.8888888887999968 0.2222222223999992 0.3170124957488483 F F F
0.2222222221000010 0.2222222223999992 0.3170124957488483 F F F
0.5555555553999980 0.2222222223999992 0.3170124957488483 F F F
0.8888888890000004 0.5555555553000033 0.3170124957488483 F F F
0.2222222222999974 0.5555555553000033 0.3170124957488483 F F F
0.5555555556000016 0.5555555553000033 0.3170124957488483 F F F
0.8888888891999969 0.8888888882000003 0.3170124957488483 F F F
0.2222222225000010 0.8888888882000003 0.3170124957488483 F F F
0.5555555557999980 0.8888888882000003 0.3170124957488483 F F F
0.0000000000000000 0.0000000000000000 0.3975777759823913 F F F
0.3333333332999970 0.0000000000000000 0.3975777759823913 F F F
0.6666666666000012 0.0000000000000000 0.3975777759823913 F F F
0.0000000002103135 0.3333333328999970 0.3975777759823913 F F F
0.3333333335000006 0.3333333328999970 0.3975777759823913 F F F
0.6666666668999994 0.3333333328999970 0.3975777759823913 F F F
0.9999999996666986 0.6666666672999995 0.3975777759823913 F F F
0.3333333329999988 0.6666666672999995 0.3975777759823913 F F F
0.6666666663000029 0.6666666672999995 0.3975777759823913 F F F
0.1111111113999996 0.1111111104999978 0.4771948603999974 F F F
0.4444444447999985 0.1111111104999978 0.4771948603999974 F F F
0.7777777781000026 0.1111111104999978 0.4771948603999974 F F F
0.1111111108999978 0.4444444449000002 0.4771948603999974 F F F
0.4444444442000020 0.4444444449000002 0.4771948603999974 F F F
0.7777777774999990 0.4444444449000002 0.4771948603999974 F F F
0.1111111111000014 0.7777777777999972 0.4771948603999974 F F F
0.4444444443999984 0.7777777777999972 0.4771948603999974 F F F
0.7777777777000026 0.7777777777999972 0.4771948603999974 F F F
0.8865881800753357 0.2228487844755307 0.5574695137135421 T T T
0.2235942988779129 0.2227424790433830 0.5569773873311874 T T T
0.5552364849278106 0.2231865337853307 0.5575536437173270 T T T
0.8894900215200039 0.5546457274296017 0.5566569099603456 T T T
0.2236512034598803 0.5520386420754804 0.5571584594274910 T T T
0.5560837090407915 0.5527283253987463 0.5573630897787396 T T T
0.8885644237754136 0.8887517883071610 0.5565518377865075 T T T
0.2220213247576979 0.8888296549191352 0.5562904076146538 T T T
0.5547231508918600 0.8891043229052258 0.5563487434576189 T T T
0.0017904807546358 0.9973409589954159 0.6365028569864322 T T T
0.3332475762964791 0.9967809047661902 0.6366824610432502 T T T
0.6681281921633442 0.9943459993354793 0.6359897100636331 T T T
0.0000337341092873 0.3331226008509276 0.6365280459316338 T T T
0.3290185795444742 0.3311645234701928 0.6401050033599702 T T T
0.6735831806151822 0.3334961400239251 0.6401971049592063 T T T
0.9988159587256575 0.6668146742866981 0.6369394621258024 T T T
0.3303264280004186 0.6702881084986814 0.6359475961213690 T T T
0.6671239065562347 0.6675490647257121 0.6366456864180563 T T T
0.4337399581389221 0.3045101585478633 0.7110950625201227 T T T
0.3458361411218434 0.2690390018169637 0.7521987408902717 T T T
0.5863655104040717 0.3211775345076902 0.7194789114991949 T T T
0.4248722679489063 0.2604928588681901 0.7837025988583619 T T T

COOH/Cu(111) E_{ads} = −1.94 eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
3.8289832201000000 6.6319934786000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu C O H
45 1 2 1
Selective dynamics
Direct
0.8888888887999968 0.2222222223999992 0.3170124957488483 F F F
0.2222222221000010 0.2222222223999992 0.3170124957488483 F F F
0.5555555553999980 0.2222222223999992 0.3170124957488483 F F F
0.8888888890000004 0.5555555553000033 0.3170124957488483 F F F
0.2222222222999974 0.5555555553000033 0.3170124957488483 F F F
0.5555555556000016 0.5555555553000033 0.3170124957488483 F F F
0.8888888891999969 0.8888888882000003 0.3170124957488483 F F F
0.2222222225000010 0.8888888882000003 0.3170124957488483 F F F
0.5555555557999980 0.8888888882000003 0.3170124957488483 F F F
0.0000000000000000 0.0000000000000000 0.3975777759823913 F F F
0.3333333332999970 0.0000000000000000 0.3975777759823913 F F F
0.6666666666000012 0.0000000000000000 0.3975777759823913 F F F
0.0000000002103135 0.3333333328999970 0.3975777759823913 F F F
0.3333333335000006 0.3333333328999970 0.3975777759823913 F F F
0.6666666668999994 0.3333333328999970 0.3975777759823913 F F F
0.9999999996666986 0.6666666672999995 0.3975777759823913 F F F
0.3333333329999988 0.6666666672999995 0.3975777759823913 F F F
0.6666666663000029 0.6666666672999995 0.3975777759823913 F F F
0.1111111113999996 0.1111111104999978 0.4771948603999974 F F F
0.4444444447999985 0.1111111104999978 0.4771948603999974 F F F
0.7777777781000026 0.1111111104999978 0.4771948603999974 F F F
0.1111111108999978 0.4444444449000002 0.4771948603999974 F F F
0.4444444442000020 0.4444444449000002 0.4771948603999974 F F F
0.7777777774999990 0.4444444449000002 0.4771948603999974 F F F
0.1111111111000014 0.7777777777999972 0.4771948603999974 F F F
0.4444444443999984 0.7777777777999972 0.4771948603999974 F F F
0.7777777777000026 0.7777777777999972 0.4771948603999974 F F F
0.8891097248886339 0.2221049760056957 0.5567301418642074 T T T
0.2232560837601341 0.2227878916378216 0.5571752807412764 T T T
0.5532254030847810 0.2231917025717038 0.5572626496934419 T T T
0.8895814525366177 0.5549734848456183 0.5567149409337802 T T T
0.2234987270492681 0.5530815596217877 0.5575535578780375 T T T
0.5548454341641147 0.5550254938221499 0.5569711751957129 T T T
0.8887520658811496 0.8887902774703775 0.5567714149014904 T T T
0.2222114577117438 0.8887527915633768 0.5569634242229000 T T T
0.5550126217079807 0.8895854274355131 0.5568437750165032 T T T
0.9995351366081948 0.9998665776160678 0.6369963650091677 T T T
0.3335036837529728 0.9972297790477782 0.6372374943374552 T T T
0.6681393144395500 0.9983519888847638 0.6370870261908763 T T T
0.9984924920405760 0.3335118363616445 0.6370272657926535 T T T
0.3336005567281646 0.3308508005950799 0.6411817511924056 T T T
0.6688051381539211 0.3324610955244367 0.6368585053847582 T T T
0.9973068758411614 0.6680606235659141 0.6368510802461174 T T T
0.3334726430062815 0.6687996599647121 0.6373714094086509 T T T
0.6671044500090417 0.6659732704058996 0.6370586253301909 T T T
0.3321101202042271 0.3393106378464452 0.7181815560668738 T T T
0.3411763752036450 0.1754227590746282 0.7425194597242850 T T T
0.3239216026704952 0.4782191337928268 0.7435431795775855 T T T
0.3395026353423845 0.1984013452629867 0.7806702896092474 T T T

COOH/Cu(100) E_{ads} = −2.16 eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu C O H
45 1 2 1
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.3173193249345303 F F F
0.3333333332999970 0.0000000000000000 0.3173193249345303 F F F
0.6666666666000012 0.0000000000000000 0.3173193249345303 F F F
0.0000000000000000 0.3333333332999970 0.3173193249345303 F F F
0.3333333332999970 0.3333333332999970 0.3173193249345303 F F F
0.6666666666000012 0.3333333332999970 0.3173193249345303 F F F
0.0000000000000000 0.6666666666000012 0.3173193249345303 F F F
0.3333333332999970 0.6666666666000012 0.3173193249345303 F F F
0.6666666666000012 0.6666666666000012 0.3173193249345303 F F F
0.1666666667000030 0.1666666667000030 0.3854655552433357 F F F
0.5000000000000000 0.1666666667000030 0.3854655552433357 F F F
0.8333333332999970 0.1666666667000030 0.3854655552433357 F F F
0.1666666667000030 0.5000000000000000 0.3854655552433357 F F F
0.5000000000000000 0.5000000000000000 0.3854655552433357 F F F
0.8333333332999970 0.5000000000000000 0.3854655552433357 F F F
0.1666666667000030 0.8333333332999970 0.3854655552433357 F F F
0.5000000000000000 0.8333333332999970 0.3854655552433357 F F F
0.8333333332999970 0.8333333332999970 0.3854655552433357 F F F
0.0000000000000000 0.0000000000000000 0.4552941175999976 F F F
0.3333333332999970 0.0000000000000000 0.4552941175999976 F F F
0.6666666666000012 0.0000000000000000 0.4552941175999976 F F F
0.0000000000000000 0.3333333332999970 0.4552941175999976 F F F
0.3333333332999970 0.3333333332999970 0.4552941175999976 F F F
0.6666666666000012 0.3333333332999970 0.4552941175999976 F F F
0.0000000000000000 0.6666666666000012 0.4552941175999976 F F F
0.3333333332999970 0.6666666666000012 0.4552941175999976 F F F
0.6666666666000012 0.6666666666000012 0.4552941175999976 F F F
0.1667542480253071 0.1666175580970871 0.5248970012810545 T T T
0.5013699648585490 0.1683137841888929 0.5248566976822293 T T T
0.8317147746047049 0.1687172634604336 0.5250452028976642 T T T
0.1667860782162435 0.4991913041317625 0.5248117977532857 T T T
0.5020481091109997 0.5004759629825617 0.5252435520817430 T T T
0.8309576005718418 0.5002878838071085 0.5254172644584468 T T T
0.1664732345449417 0.8343888153824195 0.5243894583489939 T T T
0.5015367843001655 0.8316902937145491 0.5252826312795084 T T T
0.8317536531967009 0.8316000357745486 0.5253323113827931 T T T
-0.0000987819647083 0.0001932769878460 0.5928400900924949 T T T
0.3332531462301226 0.0000510873617437 0.5927389177326372 T T T
0.6666573756977298 0.0005430201716283 0.5925839564058731 T T T
0.0018025355145966 0.3327279326667338 0.5928900580416623 T T T
0.3319576634972699 0.3325841681021523 0.5929854900773655 T T T
0.6667062740432076 0.3250765519824015 0.5971829583912162 T T T
0.0032930689967890 0.6675164590385363 0.5922490527529161 T T T
0.3295727765165284 0.6679657816987997 0.5921263310843002 T T T
0.6671698637848149 0.6765176443052255 0.5967982477915666 T T T
0.6552546525192969 0.4248486720149858 0.6668624298428172 T T T
0.6471726438867169 0.3243004828847225 0.7100221338436948 T T T
0.6575929559337153 0.5876824857495155 0.6733324998301499 T T T
0.6445520183046406 0.4037663025053186 0.7405214977080344 T T T

COOH/Cu(100) E_{ads} = −2.11 eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu C O H
45 1 2 1
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.3173193249345303 F F F
0.3333333332999970 0.0000000000000000 0.3173193249345303 F F F
0.6666666666000012 0.0000000000000000 0.3173193249345303 F F F
0.0000000000000000 0.3333333332999970 0.3173193249345303 F F F
0.3333333332999970 0.3333333332999970 0.3173193249345303 F F F
0.6666666666000012 0.3333333332999970 0.3173193249345303 F F F
0.0000000000000000 0.6666666666000012 0.3173193249345303 F F F
0.3333333332999970 0.6666666666000012 0.3173193249345303 F F F
0.6666666666000012 0.6666666666000012 0.3173193249345303 F F F
0.1666666667000030 0.1666666667000030 0.3854655552433357 F F F
0.5000000000000000 0.1666666667000030 0.3854655552433357 F F F
0.8333333332999970 0.1666666667000030 0.3854655552433357 F F F
0.1666666667000030 0.5000000000000000 0.3854655552433357 F F F
0.5000000000000000 0.5000000000000000 0.3854655552433357 F F F
0.8333333332999970 0.5000000000000000 0.3854655552433357 F F F
0.1666666667000030 0.8333333332999970 0.3854655552433357 F F F
0.5000000000000000 0.8333333332999970 0.3854655552433357 F F F
0.8333333332999970 0.8333333332999970 0.3854655552433357 F F F
0.0000000000000000 0.0000000000000000 0.4552941175999976 F F F
0.3333333332999970 0.0000000000000000 0.4552941175999976 F F F
0.6666666666000012 0.0000000000000000 0.4552941175999976 F F F
0.0000000000000000 0.3333333332999970 0.4552941175999976 F F F
0.3333333332999970 0.3333333332999970 0.4552941175999976 F F F
0.6666666666000012 0.3333333332999970 0.4552941175999976 F F F
0.0000000000000000 0.6666666666000012 0.4552941175999976 F F F
0.3333333332999970 0.6666666666000012 0.4552941175999976 F F F
0.6666666666000012 0.6666666666000012 0.4552941175999976 F F F
0.1673721115759402 0.1684582128227313 0.5254715940376726 T T T
0.5001203984196607 0.1663754154448886 0.5239581949332049 T T T
0.8320180661643272 0.1690509697262926 0.5256268898783341 T T T
0.1689358643373948 0.4992291593166974 0.5255946076178294 T T T
0.5000336431036361 0.5014975175839274 0.5235454901722939 T T T
0.8308469781770156 0.4991719022520040 0.5256620406710931 T T T
0.1670574563631182 0.8320285818473931 0.5252793288210454 T T T
0.5000353052329884 0.8319872350969528 0.5250034214235161 T T T
0.8330192882081985 0.8320324502499949 0.5252653951835565 T T T
-0.0001310745348653 0.0004781332440420 0.5935365026066021 T T T
0.3325090324632095 0.0003361006467670 0.5922650264738425 T T T
0.6673777612539863 0.0002386788216932 0.5922902560389913 T T T
0.0001137428227992 0.3336536461956049 0.5932188868949312 T T T
0.3371412281669998 0.3300305116231219 0.5953685354427568 T T T
0.6626661426344894 0.3299525963325603 0.5961088513547980 T T T
0.0001759579559271 0.6662530583773626 0.5930126022899296 T T T
0.3285149657955345 0.6708115434696922 0.5947368910180690 T T T
0.6718298237735892 0.6718307131484753 0.5947597279473472 T T T
0.5070134661493378 0.4253604799867103 0.6551786223894537 T T T
0.4999752243229534 0.3320379312893996 0.7000397594641896 T T T
0.5001005648830678 0.5921655194867602 0.6604286752152938 T T T
0.4884583608895474 0.4159963213395579 0.7292108024786562 T T T

COOH/Cu(100) E_{ads} = −1.95 eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu C O H
45 1 2 1
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.3173193249345303 F F F
0.3333333332999970 0.0000000000000000 0.3173193249345303 F F F
0.6666666666000012 0.0000000000000000 0.3173193249345303 F F F
0.0000000000000000 0.3333333332999970 0.3173193249345303 F F F
0.3333333332999970 0.3333333332999970 0.3173193249345303 F F F
0.6666666666000012 0.3333333332999970 0.3173193249345303 F F F
0.0000000000000000 0.6666666666000012 0.3173193249345303 F F F
0.3333333332999970 0.6666666666000012 0.3173193249345303 F F F
0.6666666666000012 0.6666666666000012 0.3173193249345303 F F F
0.1666666667000030 0.1666666667000030 0.3854655552433357 F F F
0.5000000000000000 0.1666666667000030 0.3854655552433357 F F F
0.8333333332999970 0.1666666667000030 0.3854655552433357 F F F
0.1666666667000030 0.5000000000000000 0.3854655552433357 F F F
0.5000000000000000 0.5000000000000000 0.3854655552433357 F F F
0.8333333332999970 0.5000000000000000 0.3854655552433357 F F F
0.1666666667000030 0.8333333332999970 0.3854655552433357 F F F
0.5000000000000000 0.8333333332999970 0.3854655552433357 F F F
0.8333333332999970 0.8333333332999970 0.3854655552433357 F F F
0.0000000000000000 0.0000000000000000 0.4552941175999976 F F F
0.3333333332999970 0.0000000000000000 0.4552941175999976 F F F
0.6666666666000012 0.0000000000000000 0.4552941175999976 F F F
0.0000000000000000 0.3333333332999970 0.4552941175999976 F F F
0.3333333332999970 0.3333333332999970 0.4552941175999976 F F F
0.6666666666000012 0.3333333332999970 0.4552941175999976 F F F
0.0000000000000000 0.6666666666000012 0.4552941175999976 F F F
0.3333333332999970 0.6666666666000012 0.4552941175999976 F F F
0.6666666666000012 0.6666666666000012 0.4552941175999976 F F F
0.1678007428112618 0.1681453446989052 0.5253487343534307 T T T
0.5000795726668747 0.1657331089538408 0.5242423458647650 T T T
0.8314371054615388 0.1684254275932331 0.5255301407111639 T T T
0.1683992084640008 0.4982864529961355 0.5256446183312538 T T T
0.5000517699730416 0.5008188210407405 0.5243487862041598 T T T
0.8309223687321350 0.4980100421494205 0.5257999961555282 T T T
0.1659877258458315 0.8333572332553432 0.5249718214324021 T T T
0.4999277041898849 0.8333432110832580 0.5250726802874172 T T T
0.8342083545927090 0.8333766154762045 0.5248409663822983 T T T
-0.0001076954543398 0.0006590142228347 0.5931937172126771 T T T
0.3314666735048246 -0.0025200187132088 0.5930516261431560 T T T
0.6686783302941796 -0.0024075337475082 0.5929619321925781 T T T
-0.0011637229695299 0.3330497009648342 0.5930894382526721 T T T
0.3361527174739877 0.3321264759955426 0.5953303801544613 T T T
0.6605201600096993 0.3322211063956890 0.5964332895197131 T T T
-0.0000636243007356 0.6659730865979010 0.5932499756590620 T T T
0.3319762275508903 0.6695445001369249 0.5930308080035929 T T T
0.6682874078010478 0.6694935638441757 0.5928903677380081 T T T
0.4881429020712753 0.3363296595960801 0.6628281093057933 T T T
0.4864156693582779 0.1753164605233093 0.6876291867977514 T T T
0.4869701006305710 0.4705635121757264 0.6892065610562336 T T T
0.4821427291822629 0.1979654115660278 0.7257033956440031 T T T

COOH/Cu(211) E_{ads} = −2.36 eV
1.00000000000000
6.2527034153000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.3164343000000009
Cu C O H
45 1 2 1
Selective dynamics
Direct
0.0061862950247047 0.1666666667000030 0.3120745335338029 F F F
0.0061862950247047 0.5000000000000000 0.3120745335338029 F F F
0.0061862950247047 0.8333333332999970 0.3120745335338029 F F F
0.3355456677560653 0.0000000000000000 0.3354619372229379 F F F
0.3355456677560653 0.3333333332999970 0.3354619372229379 F F F
0.3355456677560653 0.6666666666000012 0.3354619372229379 F F F
0.6630854692850079 0.1666666667000030 0.3607350091654666 F F F
0.6630854692850079 0.5000000000000000 0.3607350091654666 F F F
0.6630854692850079 0.8333333332999970 0.3607350091654666 F F F
0.9944057463905267 0.0000000000000000 0.3915351276171819 F F F
0.9944057463905267 0.3333333332999970 0.3915351276171819 F F F
0.9944057463905267 0.6666666666000012 0.3915351276171819 F F F
0.3330656692422309 0.1666666667000030 0.4179888222780335 F F F
0.3330656692422309 0.5000000000000000 0.4179888222780335 F F F
0.3330656692422309 0.8333333332999970 0.4179888222780335 F F F
0.6656564241704075 0.0000000000000000 0.4448469552356400 F F F
0.6656564241704075 0.3333333332999970 0.4448469552356400 F F F
0.6656564241704075 0.6666666666000012 0.4448469552356400 F F F
0.0003515212697778 0.1666666667000030 0.4732099031121066 F F F
0.0003515212697778 0.5000000000000000 0.4732099031121066 F F F
0.0003515212697778 0.8333333332999970 0.4732099031121066 F F F
0.3333333329999988 0.0000000000000000 0.5000000000000000 F F F
0.3333333329999988 0.3333333332999970 0.5000000000000000 F F F
0.3333333329999988 0.6666666666000012 0.5000000000000000 F F F
0.6663151448302216 0.1666666667000030 0.5267900968878934 F F F
0.6663151448302216 0.5000000000000000 0.5267900968878934 F F F
0.6663151448302216 0.8333333332999970 0.5267900968878934 F F F
0.9975826197754843 0.0002787647621268 0.5550496871432820 T T T
0.9982282911718463 0.3329195683676716 0.5550719579861326 T T T
0.9979291471036768 0.6663547633725233 0.5550182407790746 T T T
0.3306059368617492 0.1664114253715520 0.5815676968932827 T T T
0.3314764136702706 0.4996743318034554 0.5817377238463262 T T T
0.3307727420246361 0.8329317952231390 0.5816254811561010 T T T
0.6660831645663818 0.9964636103863226 0.6097381794904845 T T T
0.6662176205630497 0.3357083182691994 0.6089833083141764 T T T
0.6668055806483072 0.6665122371941512 0.6097983679770711 T T T
0.9951382624400567 0.1659478427289299 0.6388784974619973 T T T
0.9963750850080652 0.4995468684306817 0.6385793820769943 T T T
0.9974464961247448 0.8328931180877700 0.6383372414431734 T T T
0.3245935240910061 0.9991366473456377 0.6635892000882473 T T T
0.3225428461143655 0.3324661051455405 0.6634630692719949 T T T
0.3251823962195449 0.6660579043355415 0.6629031556278777 T T T
0.6509859693223348 0.1669246422178464 0.6881593489779395 T T T
0.6557927010666255 0.4909686745738661 0.6914507558343541 T T T
0.6604438005148355 0.8409230414561710 0.6919806834877349 T T T
0.6659481412849557 0.5875334860084629 0.7591170185218660 T T T
0.6529123746506017 0.4913908325710041 0.8016463699552309 T T T
0.6833475086659299 0.7506381323634589 0.7642762404167536 T T T
0.6586555312639915 0.5728189815297265 0.8307517946650118 T T T

11.2 *HCOO Adsorption

HCOO/Cu_3/Cu(533)	E_{ads} = −3.78 eV				
1.00000000000000					
10.3878408006999994	0.0000000000000000	0.0000000000000000			
4.5828709415000004	6.0103788927000004	0.0000000000000000			
0.0000000000000000	0.0000000000000000	26.5000000000000000			
Cu C O H					
63 1 2 1					
Selective dynamics					
Direct					
0.0032853599999996	0.9972806999999975	0.3042624500000031	F	F	F
0.0028217400000017	0.3308767700000033	0.3042691500000032	F	F	F
0.0026800899999984	0.6645640400000019	0.3042978000000005	F	F	F
0.2572489900000008	0.6186597399999982	0.3218759499999990	F	F	F
0.2571973700000001	0.2857762699999995	0.3217927099999969	F	F	F
0.2571614599999990	0.9524293899999989	0.3219123699999997	F	F	F
0.5099116399999986	0.5747781399999994	0.3415763200000015	F	F	F
0.5095861200000016	0.2417833900000019	0.3416938299999970	F	F	F
0.5096986000000001	0.9088501900000026	0.3416314700000029	F	F	F
0.7627858999999972	0.5310134699999978	0.3609394899999998	F	F	F
0.7629538699999969	0.1970798500000015	0.3608490599999996	F	F	F
0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F
0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0467888680771154	0.2944055760044364	0.4664103899851924	T	T	T
0.0465214740036473	0.6280543774143155	0.4666477500119015	T	T	T
0.0472610783853540	0.9607002826059414	0.4662939990066022	T	T	T
0.3031543464831543	0.2473265196214385	0.4870968721761031	T	T	T
0.3036891607145904	0.5803378790037215	0.4869680557567833	T	T	T
0.3039135905724493	0.9136819568230337	0.4869267888832027	T	T	T
0.5588579541136198	0.2010504224006908	0.5066760307396123	T	T	T
0.5594773152173076	0.5340716954678939	0.5063849652574888	T	T	T
0.5590830908270163	0.8678417653476629	0.5068580081222223	T	T	T
0.8170746701768437	0.1521386798838478	0.5272463467913084	T	T	T
0.8164026768918760	0.4868163129547867	0.5275284697758096	T	T	T
0.8158000569465358	0.8208215599062285	0.5278536293414433	T	T	T
0.0733430943919373	0.1053733666093351	0.5487565004410513	T	T	T
0.0719135995937208	0.4405305516359306	0.5489497471369731	T	T	T
0.0729553473087705	0.7732150093740131	0.5490392199513536	T	T	T
0.3272306358730006	0.0607497212103567	0.5693097077643188	T	T	T
0.3267387857647819	0.3945145601607152	0.5693614023736444	T	T	T
0.3283285676726067	0.7265562075668583	0.5689853889153724	T	T	T
0.5840383670494660	0.0137526438882318	0.5887458996396617	T	T	T
0.5860406680392032	0.3456744959904654	0.5879216003729155	T	T	T
0.5855849732776548	0.6789175232825215	0.5882724058421331	T	T	T
0.8430485718398160	0.6317480727475555	0.6101334655143660	T	T	T
0.8440837832599826	0.2961584301377371	0.6093829374830833	T	T	T

0.8440165536270925 0.9640615539719946 0.6101154472269386 T T T
0.0962631917930850 0.5864206108877781 0.6341253497440675 T T T
0.0971986089106807 0.2527429275929833 0.6332675833656509 T T T
0.0999328114259157 0.9171667574860507 0.6339732407230159 T T T
0.3515109569075818 0.5371697249549570 0.6508285106774849 T T T
0.3505228567529883 0.2074254677323637 0.6519107817117344 T T T
0.3507342909771012 0.8770817772565849 0.6512030269368552 T T T
0.6046848338931454 0.4973783738782060 0.6702434924847722 T T T
0.6046871904657607 0.1588984331381411 0.6705172653733271 T T T
0.6046179117091768 0.8320487192395163 0.6715139883866925 T T T
0.8601612046965101 0.4509146946321394 0.6909537896346762 T T T
0.8655970317676562 0.1117882732834588 0.6910457962187024 T T T
0.8566775132413653 0.7866390116073418 0.6922446091186174 T T T
0.6287258811528105 0.6418059587340608 0.7499779049443092 T T T
0.6304876776162374 0.3039133814211326 0.7464534148684905 T T T
0.3627374213991175 0.6904087132075389 0.7285358694440802 T T T
0.3893284136319579 0.8154951331662517 0.8252603670013059 T T T
0.5302399481107329 0.7564059538779517 0.8159072716196434 T T T
0.2966700809383838 0.8039193062317551 0.7966491243611742 T T T
0.3411659613217353 0.8856170142887407 0.8633322028021837 T T T

HCOO/Cu_3/Cu(533) E_{ads} = −3.73 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
63 1 2 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F
0.2571614599999990 0.9524293899999989 0.3219123699999997 F F F
0.5099116399999986 0.5747781399999994 0.3415763200000015 F F F
0.5095861200000016 0.2417833900000019 0.3416938299999970 F F F
0.5096986000000001 0.9088501900000026 0.3416314700000029 F F F
0.7627858999999972 0.5310134699999978 0.3609394899999998 F F F
0.7629538699999969 0.1970798500000015 0.3608490599999996 F F F
0.7629705100000024 0.8638077299999978 0.3608832600000014 F F F
0.0188077500000006 0.4844866199999984 0.3845455499999986 F F F
0.0188649600000019 0.1508076399999965 0.3844206699999972 F F F
0.0189457299999987 0.8174492599999965 0.3845321800000008 F F F
0.2777182000000025 0.4350678200000004 0.4051130599999979 F F F
0.2779364200000032 0.1018241299999971 0.4049400600000013 F F F
0.2778532499999997 0.7683188099999967 0.4050370400000034 F F F
0.5346647900000008 0.3873898000000011 0.4243529600000002 F F F
0.5347255300000029 0.0542446099999978 0.4245416400000011 F F F
0.5343893300000033 0.7214487199999979 0.4243017399999971 F F F
0.7896143700000025 0.3418778500000030 0.4451831499999983 F F F
0.7893677400000030 0.0085227100000012 0.4452920299999974 F F F
0.7895473399999986 0.6754118300000016 0.4453449800000016 F F F
0.0467142637675906 0.2946176367471764 0.4663022263618828 T T T
0.0462061032035095 0.6286834250122553 0.4666659591116158 T T T
0.0468721029823698 0.9612267814851307 0.4664250183142897 T T T

0.3030327691535533 0.2476194467908570 0.4871819059538112 T T T
0.3030168993825058 0.5811529248802287 0.4870718643569916 T T T
0.3033350807963444 0.9144795634454397 0.4869832820282767 T T T
0.5582104169354665 0.2019186412540037 0.5067831398317182 T T T
0.5590252067562886 0.5347366903745723 0.5062848265338076 T T T
0.5586967196275623 0.8684151637125765 0.5067201895927340 T T T
0.8159200997849254 0.1534890366137986 0.5273746121116218 T T T
0.8158050991166448 0.4876226885526904 0.5274261526864237 T T T
0.8148057450156543 0.8217724877725487 0.5278052399406619 T T T
0.0722893247997902 0.1069029711477754 0.5487951528915787 T T T
0.0713970573800253 0.4412298587722105 0.5487516283889704 T T T
0.0718868228487253 0.7745842796348867 0.5492260135162752 T T T
0.3272608520552609 0.0614171570523467 0.5693387883970971 T T T
0.3258178977034234 0.3958183866347227 0.5694910027399516 T T T
0.3279015322634820 0.7277059138101762 0.5690213880209427 T T T
0.5828813091143701 0.0157853635475220 0.5890119364165614 T T T
0.5844854521760965 0.3477067520752755 0.5881398906652606 T T T
0.5846646939324245 0.6799485334779192 0.5881722948371930 T T T
0.8416344077176987 0.6336814163426610 0.6098668568641372 T T T
0.8429570104592869 0.2981456787896590 0.6093344746353466 T T T
0.8420110781545205 0.9659317264832481 0.6100403825240832 T T T
0.0944358604106057 0.5885150403989670 0.6341130562611141 T T T
0.0970045737339902 0.2540339499000979 0.6327284028834441 T T T
0.0988524621437534 0.9190377965112333 0.6339065508097121 T T T
0.3494445593073792 0.5392079659144784 0.6507271536129196 T T T
0.3494567328884060 0.2099452311280530 0.6521825029560517 T T T
0.3501895384522271 0.8798068927529030 0.6512011050118929 T T T
0.6074061276165779 0.4948500780630596 0.6707945949495624 T T T
0.6029678955621591 0.1641169006560759 0.6719468671542543 T T T
0.6031235502280126 0.8342551152526951 0.6714234497161868 T T T
0.8619935127482492 0.4514263159057990 0.6902486216972150 T T T
0.8627629053078465 0.1140712200227512 0.6905830108553914 T T T
0.8543051056838067 0.7895979692931760 0.6920815220255605 T T T
0.6279652255378920 0.6522369071122185 0.7495402723517088 T T T
0.6311792201305195 0.3033416516953267 0.7501891365179674 T T T
0.3737801445837547 0.6873714869321503 0.7267852607943013 T T T
0.6355790513874879 0.4761243153976267 0.8436728900221198 T T T
0.6303307821299811 0.6308784792525657 0.8224564593730435 T T T
0.6339801176743975 0.3259191666934953 0.8230790158013548 T T T
0.6422029591060863 0.4717812637666654 0.8854195083252492 T T T

HCOO/Cu_3/Cu(533) E_{ads} = −3.51 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
63 1 2 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F
0.2571614599999990 0.9524293899999989 0.3219123699999997 F F F
0.5099116399999986 0.5747781399999994 0.3415763200000015 F F F

0.5095861200000016	0.2417833900000019	0.3416938299999970	F	F	F
0.5096986000000001	0.9088501900000026	0.3416314700000029	F	F	F
0.7627858999999972	0.5310134699999978	0.3609394899999998	F	F	F
0.7629538699999969	0.1970798500000015	0.3608490599999996	F	F	F
0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F
0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0470997520715599	0.2938097491170808	0.4663575682975178	T	T	T
0.0463902314701841	0.6285079847542079	0.4666163597380475	T	T	T
0.0465041286116161	0.9611258638082703	0.4663894663313783	T	T	T
0.3032495968193061	0.2476811890255135	0.4868854127263376	T	T	T
0.3032684484456993	0.5806148629230208	0.4873794590921108	T	T	T
0.3035733379098033	0.9132326281280498	0.4869955038169067	T	T	T
0.5588264859247190	0.2009698789518310	0.5068945809290852	T	T	T
0.5595990240871771	0.5334384472303100	0.5062285376399771	T	T	T
0.5600350526607940	0.8659584491712735	0.5066184249068897	T	T	T
0.8167157486550423	0.1511890058708403	0.5278626103024990	T	T	T
0.8172970740772882	0.4855295597752942	0.5275622957181128	T	T	T
0.8160171706629598	0.8203419263458116	0.5278664276218237	T	T	T
0.0732256071137130	0.1045585914937206	0.5488590539856801	T	T	T
0.0719925888420576	0.4408140775299501	0.5485725630322946	T	T	T
0.0723340845405147	0.7738763378617080	0.5494762760789342	T	T	T
0.3286523943191497	0.0605575552968816	0.5682388089897401	T	T	T
0.3273081224298835	0.3942982780469109	0.5699149034520588	T	T	T
0.3285093442845977	0.7253657811659622	0.5695550569866015	T	T	T
0.5848732868446760	0.0114343969073047	0.5883821578353405	T	T	T
0.5854527406922401	0.3455659899527816	0.5882393974515310	T	T	T
0.5868274166806700	0.6768867479973437	0.5879798838020065	T	T	T
0.8433270932153079	0.6327776948173351	0.6107166602575731	T	T	T
0.8444539753724456	0.2940445297589989	0.6094182347267321	T	T	T
0.8450653678315376	0.9595390997114066	0.6117501994813352	T	T	T
0.0977800911959008	0.5851721173651967	0.6337548338931569	T	T	T
0.1002747790729259	0.2516388391705817	0.6313977514793265	T	T	T
0.0991299869286166	0.9182774324806857	0.6353865053234742	T	T	T
0.3508049987133930	0.5382206857379757	0.6529020038925140	T	T	T
0.3516732247258858	0.2075302130833592	0.6522448594461423	T	T	T
0.3510449927085588	0.8807395756550349	0.6492928539421285	T	T	T
0.6071582063790970	0.4965623817421942	0.6697368227502523	T	T	T
0.6075759278441737	0.1525180816133016	0.6694977007165477	T	T	T
0.6058795052049604	0.8289014543389328	0.6713569398415018	T	T	T
0.8709060739111578	0.4369166029879352	0.6886945722300766	T	T	T
0.8585887404906813	0.1177286767404127	0.6919584342373781	T	T	T
0.8642118388863977	0.7757909620835548	0.6960829222141172	T	T	T
0.6462435940746118	0.6183556837054951	0.7500927916837554	T	T	T
0.6072409657438058	0.3225877746799029	0.7454022605306960	T	T	T
0.3757511897291437	0.7090790293766531	0.7273474702951219	T	T	T
0.8538833921964581	0.6878696635773096	0.8052978076107493	T	T	T
0.9188621361998628	0.7139167640175117	0.7686778085017210	T	T	T

0.7431981660228644	0.6636295046359209	0.8052309561413367	T	T	T
0.9003595961589781	0.6850487938194760	0.8432334996287452	T	T	T

HCOO/Defected-Cu(533) E_{ads} = −3.46 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
59 1 2 1
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0471937523698429	0.2939261848279031	0.4659878641612565	T	T	T
0.0468609584901429	0.6269454839906885	0.4657962565866427	T	T	T
0.0471070875543944	0.9606681599425428	0.4658799794414037	T	T	T
0.3039301772639575	0.2463035215110381	0.4865746978076686	T	T	T
0.3045538808830841	0.5792181154416980	0.4863559853065524	T	T	T
0.3040054036357702	0.9128102783237111	0.4865954218625248	T	T	T
0.5602550004671230	0.1992929586468435	0.5074484030371664	T	T	T
0.5600167127936899	0.5330799928437955	0.5068194617212143	T	T	T
0.5595996197961028	0.8663882718910756	0.5069435401893330	T	T	T
0.8164339090893193	0.1521325313737592	0.5275005357524094	T	T	T
0.8161811017775022	0.4859546883170438	0.5275268414210998	T	T	T
0.8163470520337270	0.8202401291785151	0.5280075993695803	T	T	T
0.0723884057834425	0.1057805613150435	0.5482757172669253	T	T	T
0.0719327828484353	0.4393622112531048	0.5483987124679217	T	T	T
0.0730204989166054	0.7714793240818238	0.5476340256450598	T	T	T
0.3275602095217494	0.0597546608897659	0.5687104081602570	T	T	T
0.3286543646672371	0.3914698322707082	0.5684567960544555	T	T	T
0.3286599835538766	0.7247377303550238	0.5684804561523435	T	T	T
0.5858271720193216	0.0087238843316442	0.5895732404524310	T	T	T
0.5858437451656258	0.3458006881276035	0.5894167466125282	T	T	T
0.5866212267119408	0.6770479540685699	0.5894325991703866	T	T	T

0.8432413614664540	0.6262973506278726	0.6104070586507078	T	T	T
0.8436586822549685	0.2986405926046274	0.6103754813001956	T	T	T
0.8447779880240489	0.9657301770513982	0.6103289513513204	T	T	T
0.0999130052802002	0.5812581705395772	0.6316489661348754	T	T	T
0.0953939441511693	0.2534465253530769	0.6326910494487663	T	T	T
0.0991700009388765	0.9167359829262267	0.6314246249910695	T	T	T
0.3511609669741205	0.5377285448084734	0.6510015960400750	T	T	T
0.3523422313986089	0.2042512783199371	0.6515856556197619	T	T	T
0.3493494076160530	0.8750334846636463	0.6499642198128441	T	T	T
0.6038663710136163	0.4910415463983853	0.6708384379689321	T	T	T
0.6075298443453576	0.1570354947748456	0.6711538935082828	T	T	T
0.6099228314930443	0.8244464580831519	0.6726078933075712	T	T	T
0.8673151376322608	0.1107209707130465	0.6913316464516583	T	T	T
0.8653803098732453	0.7811042458198045	0.6879602060888388	T	T	T
0.7739414982220012	0.4527814940766959	0.7614165435900802	T	T	T
0.6501873781460148	0.5956014843762460	0.7344587287107061	T	T	T
0.8707070934038654	0.2461783484461293	0.7544620863307756	T	T	T
0.7958524463402341	0.5207156159769752	0.7945172610750859	T	T	T

HCOO/Defected-Cu(533) E_{ads} = −3.40 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
59 1 2 1
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0466357585143223	0.2945386507584020	0.4661152351559071	T	T	T
0.0467151016532854	0.6274851215912290	0.4659389921089979	T	T	T
0.0465515971836216	0.9615910034161479	0.4658441670906589	T	T	T
0.3031181836590658	0.2477378318862807	0.4866450411231345	T	T	T
0.3034694724330711	0.5807414671380373	0.4863898904620782	T	T	T

0.3029282460659581	0.9140944317291894	0.4866236578044157	T	T	T
0.5587727546521889	0.2013453855101889	0.5071847682411154	T	T	T
0.5585527187226634	0.5352345408466879	0.5068425408941793	T	T	T
0.5583530171512892	0.8677015497779214	0.5068523100749114	T	T	T
0.8149029549356650	0.1535916143399850	0.5276919297466719	T	T	T
0.8144103503052795	0.4881116726082705	0.5273121764058801	T	T	T
0.8150107120089928	0.8219615929290706	0.5276725381676883	T	T	T
0.0704277891893826	0.1080018358896113	0.5484146977806846	T	T	T
0.0705728489833802	0.4416420385166108	0.5484610431865565	T	T	T
0.0711190238480947	0.7745448161348666	0.5477773732419386	T	T	T
0.3254737842315537	0.0622973721368292	0.5686291090014888	T	T	T
0.3261206231791071	0.3955757600119756	0.5685864782496817	T	T	T
0.3258006858188389	0.7288986418183659	0.5685914878587871	T	T	T
0.5829923820395522	0.0126281196873138	0.5888998932515032	T	T	T
0.5834133951217043	0.3497896474002476	0.5889345786798541	T	T	T
0.5839775503911925	0.6803387088395879	0.5897801323948186	T	T	T
0.8409091903159033	0.6301041458678873	0.6097672638073293	T	T	T
0.8409200297290238	0.3025672646038987	0.6098860097840341	T	T	T
0.8423328406656062	0.9651310767009990	0.6107058553518386	T	T	T
0.0962748762895013	0.5861616445123442	0.6320200562992943	T	T	T
0.0927528140617094	0.2563609513671757	0.6324621510217502	T	T	T
0.0960085962358228	0.9213554618507673	0.6320513202023664	T	T	T
0.3484440006582236	0.5435779773121031	0.6512467837060923	T	T	T
0.3475289564661055	0.2104918404689372	0.6512935884660420	T	T	T
0.3474111778637732	0.8779486903844629	0.6512792817088616	T	T	T
0.6018336178516644	0.4985968033379874	0.6717873235523285	T	T	T
0.6018418809752154	0.1654618855225897	0.6693411771408248	T	T	T
0.6018298150442227	0.8326679940300696	0.6716081523725860	T	T	T
0.8625375285618685	0.1141383735648654	0.6899273270159110	T	T	T
0.8624974877615019	0.7822013391574875	0.6897989639664058	T	T	T
0.8095049836652526	0.4927841775755906	0.7520301689534572	T	T	T
0.7536161170962954	0.6886535101089989	0.7383344750562442	T	T	T
0.7536018811593024	0.3901538353392160	0.7382590961004841	T	T	T
0.9147662683765896	0.4048896158389381	0.7778217926845877	T	T	T

HCOO/Cu(533) E_{ads} = −3.40 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 2 1
Selective dynamics
Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F

0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0472603423146793	0.2946936849542183	0.4659723876915578	T	T	T
0.0470153357489806	0.6280537441196401	0.4658406516154230	T	T	T
0.0471593698984236	0.9612269303435212	0.4659582597823970	T	T	T
0.3041462576207579	0.2474959895526112	0.4866884614137703	T	T	T
0.3038982965199679	0.5808340470856095	0.4866326717408711	T	T	T
0.3039038706304922	0.9142725078818685	0.4866538246436747	T	T	T
0.5600581332986465	0.2011657028956435	0.5069160531458223	T	T	T
0.5598998318733592	0.5344251026500260	0.5069656074314324	T	T	T
0.5600622387656600	0.8674703276039040	0.5069048358761847	T	T	T
0.8167629796100897	0.1541000039777884	0.5277565131594031	T	T	T
0.8168557020123970	0.4866569078346359	0.5277078338754677	T	T	T
0.8169708569271563	0.8204732940416548	0.5282685482112797	T	T	T
0.0725290931393729	0.1075261369650988	0.5483206193465833	T	T	T
0.0729139347261452	0.4408768623805841	0.5481720358924989	T	T	T
0.0726605840345584	0.7739373888435139	0.5482279631002811	T	T	T
0.3281341208631900	0.0614956495117553	0.5689858104306182	T	T	T
0.3279850196100753	0.3950476524160464	0.5690180664290594	T	T	T
0.3278549157815434	0.7283343365989481	0.5689211310100077	T	T	T
0.5854500532624414	0.0141574553977719	0.5885837815782722	T	T	T
0.5854453873313403	0.3476626525160071	0.5887742937145291	T	T	T
0.5856827308680579	0.6802972438173995	0.5886885777776172	T	T	T
0.8443597956472786	0.6287390334926570	0.6103148420233921	T	T	T
0.8445437358410075	0.2982430586075537	0.6111740249088413	T	T	T
0.8442659507226438	0.9686182839418862	0.6105253858842516	T	T	T
0.0993586717412995	0.5860398095698542	0.6323565047519466	T	T	T
0.0998852694422752	0.2520585089253515	0.6320986345422526	T	T	T
0.0997624248293292	0.9190397409309341	0.6321927956391420	T	T	T
0.3523807985611214	0.5419411540964418	0.6518521931923829	T	T	T
0.3524491794930000	0.2085743216298823	0.6517349734390407	T	T	T
0.3527349355296820	0.8746962124327524	0.6516407372877993	T	T	T
0.6070871967820892	0.4965436453645395	0.6706721098103614	T	T	T
0.6056731101282651	0.1645860532000327	0.6710244281676481	T	T	T
0.6058209064825988	0.8308244961136850	0.6708653293329050	T	T	T
0.8649819226689743	0.4533147227639702	0.6927588999079006	T	T	T
0.8651229494322052	0.1109667540717538	0.6932014436133755	T	T	T
0.8601685423603840	0.7860128187222415	0.6890002809100721	T	T	T
0.9227271559817325	0.2365497880788112	0.7859508728867297	T	T	T
0.9083997266634753	0.3987373302091441	0.7652032623122835	T	T	T
0.9086205544866743	0.0972700081328242	0.7657104167848701	T	T	T
0.9513403630944168	0.2137541872995428	0.8268181469585016	T	T	T

HCOO/Cu_3/Cu(533) E_{ads} = −3.33 eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H
63 1 2 1
Selective dynamics
Direct

0.0032853599999996	0.9972806999999975	0.3042624500000031	F	F	F
0.0028217400000017	0.3308767700000033	0.3042691500000032	F	F	F
0.0026800899999984	0.6645640400000019	0.3042978000000005	F	F	F
0.2572489900000008	0.6186597399999982	0.3218759499999990	F	F	F
0.2571973700000001	0.2857762699999995	0.3217927099999969	F	F	F
0.2571614599999990	0.9524293899999989	0.3219123699999997	F	F	F
0.5099116399999986	0.5747781399999994	0.3415763200000015	F	F	F
0.5095861200000016	0.2417833900000019	0.3416938299999970	F	F	F
0.5096986000000001	0.9088501900000026	0.3416314700000029	F	F	F
0.7627858999999972	0.5310134699999978	0.3609394899999998	F	F	F
0.7629538699999969	0.1970798500000015	0.3608490599999996	F	F	F
0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F
0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0461896836169373	0.2947377531665794	0.4666251643730561	T	T	T
0.0456674011029250	0.6295342705787235	0.4666697638960144	T	T	T
0.0456791387235569	0.9623739366880812	0.4664796889124005	T	T	T
0.3018270609609814	0.2495417374693218	0.4866375457209031	T	T	T
0.3023637505883556	0.5817942795031712	0.4872668776283504	T	T	T
0.3017151229785640	0.9148658288956852	0.4871540707226956	T	T	T
0.5578638395852522	0.2022728061559320	0.5064898165944882	T	T	T
0.5581208130860844	0.5354741202518767	0.5059602139863983	T	T	T
0.5582249534687378	0.8676123499377297	0.5060895807334731	T	T	T
0.8154891092658403	0.1545549075696897	0.5281058619453773	T	T	T
0.8154523183662974	0.4877433591629554	0.5278195622371129	T	T	T
0.8147277951771628	0.8218281688636111	0.5278179538952159	T	T	T
0.0701227971530116	0.1076386609450992	0.5497932845007227	T	T	T
0.0691944718120538	0.4436611638167989	0.5488206845788071	T	T	T
0.0709893382519269	0.7765346101505486	0.5493610404327924	T	T	T
0.3242398280808345	0.0660003229285238	0.5677455677382923	T	T	T
0.3255954321075052	0.3962412801637640	0.5696471590029972	T	T	T
0.3251249449780715	0.7280205496899157	0.5697358187155217	T	T	T
0.5821079313469113	0.0122790558718435	0.5872430346762556	T	T	T
0.5826629358511326	0.3486809408409073	0.5872072102100105	T	T	T
0.5834218662515696	0.6811914768441412	0.5873065992477677	T	T	T
0.8390737733902611	0.6370033968622622	0.6116736952102215	T	T	T
0.8407635442542656	0.3022497328272493	0.6112208876899032	T	T	T
0.8436106798449856	0.9644134885757225	0.6106317050612446	T	T	T
0.0956624095951284	0.5881098762292112	0.6326391086043586	T	T	T
0.0932326142108550	0.2593125225131843	0.6329196108643131	T	T	T
0.0943304736015662	0.9234581243803817	0.6384040624940539	T	T	T
0.3467995532695127	0.5394280452261739	0.6534871972364940	T	T	T
0.3471828678646816	0.2114326079172741	0.6522488593380373	T	T	T
0.3461191208717693	0.8887496279298048	0.6473233385639503	T	T	T

0.5960508512659004	0.5056864204507647	0.6677547742949486	T	T	T
0.6053835533212180	0.1503774448706778	0.6666455104959255	T	T	T
0.6008468880597988	0.8322652552037795	0.6719245438483981	T	T	T
0.8635081906379511	0.4489629754106446	0.6929846366801655	T	T	T
0.8422238248950080	0.1355054251678851	0.6922421861119616	T	T	T
0.8658385047873054	0.7861657337665093	0.6935582457577780	T	T	T
0.6173098151241447	0.6180538080849090	0.7500601789259846	T	T	T
0.5549845528951209	0.3529684696038089	0.7403504848521649	T	T	T
0.3447534083701953	0.7457273728867193	0.7251808655298504	T	T	T
0.8800088587196271	0.6269975632697609	0.7928726546723084	T	T	T
0.9126032683846930	0.7356116193140636	0.7678048757447016	T	T	T
0.8375212702648227	0.5103084248974170	0.7752759767256876	T	T	T
0.8894982299576739	0.6278739364016204	0.8345218269292332	T	T	T

HCOO/Defected-Cu(533) $E_{ads} = -3.21$ eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H

59 1 2 1

Selective dynamics

Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0467213769598942	0.2945049282252370	0.4659735026075111	T	T	T
0.0470020976394210	0.6271502227612658	0.4658005010343942	T	T	T
0.0467534567816656	0.9615532332569217	0.4657763565049393	T	T	T
0.3035402926931852	0.2471708318630874	0.4866907347063645	T	T	T
0.3043399662904065	0.5798783626083264	0.4863787991963804	T	T	T
0.3031212706908946	0.9140497073412064	0.4866583685905326	T	T	T
0.5597558219175767	0.2002633600942332	0.5073609081182724	T	T	T
0.5593740899454360	0.5345726401532076	0.5069252555361956	T	T	T
0.5586155027309090	0.8670895241330712	0.5069964486633083	T	T	T
0.8156820950039929	0.1535485404729471	0.5275536990360905	T	T	T

0.8149487486501172	0.4874898412596025	0.5276240249126545	T	T	T
0.8155977303152397	0.8204948364252189	0.5274994967634612	T	T	T
0.0705073373160872	0.1083769092509783	0.5484406413489253	T	T	T
0.0708003062592297	0.4407263081150106	0.5484839178906356	T	T	T
0.0723908499752710	0.7732660919135554	0.5474965114381050	T	T	T
0.3260082175052972	0.0615921481255981	0.5688179366348933	T	T	T
0.3280499085985085	0.3936059410376771	0.5683883829111736	T	T	T
0.3277378073762662	0.7273599613830299	0.5684860617923491	T	T	T
0.5842693402331918	0.0100714802305504	0.5893367564572287	T	T	T
0.5847104026464223	0.3494457390471268	0.5893339913291129	T	T	T
0.5851987339742024	0.6792264431661295	0.5904722792896422	T	T	T
0.8410818213694427	0.6288578773203071	0.6106404803743715	T	T	T
0.8413080602831045	0.3029916829627197	0.6107714644722790	T	T	T
0.8431488183687605	0.9642970736142757	0.6089591565082912	T	T	T
0.0985204740531387	0.5835922332321957	0.6313567405086005	T	T	T
0.0930600250363938	0.2560501772971122	0.6334365131483395	T	T	T
0.0986901915735316	0.9192282747971277	0.6313889341660825	T	T	T
0.3501545963328923	0.5408065044610737	0.6506671101521988	T	T	T
0.3494625784222620	0.2093013041248426	0.6507393895742837	T	T	T
0.3490753394947035	0.8764130137617840	0.6504769625099769	T	T	T
0.6058875581860548	0.4927835278207127	0.6731576584603687	T	T	T
0.6071493968188051	0.1606259769673457	0.6695777031421173	T	T	T
0.6059917223434965	0.8305785134509449	0.6731784268005825	T	T	T
0.8662715287088147	0.1085280239798507	0.6881136752011940	T	T	T
0.8656983079410665	0.7815468780545132	0.6880464047066965	T	T	T
0.6189732700683663	0.6508562123439674	0.7695289060364914	T	T	T
0.6157334706024429	0.8041278972720676	0.7485776831332842	T	T	T
0.6164301373581935	0.5025759244504400	0.7484365505324533	T	T	T
0.6241024240476634	0.6462348339142494	0.8113373323158086	T	T	T

HCOO/Cu(533) E_{ads} = −3.14 eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H

60 1 2 1

Selective dynamics

Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F

0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0471199730549449 0.2940534995084295 0.4657609803624779 T T T
0.0471784896622850 0.6273602589889894 0.4658464037820128 T T T
0.0471211748475868 0.9604927789991512 0.4657332953106992 T T T
0.3040031653722862 0.2462096795339070 0.4866540731725112 T T T
0.3042740304015857 0.5795790983986842 0.4865020739214821 T T T
0.3040289758839691 0.9131209049472053 0.4866122276066434 T T T
0.5601112876878727 0.1984416432607981 0.5071755995697822 T T T
0.5598014875307765 0.5339371339400169 0.5070476526437835 T T T
0.5593772788979430 0.8667412394489734 0.5070145285086213 T T T
0.8166700251951617 0.1530065023137094 0.5278167170822329 T T T
0.8161040418468735 0.4862446103161375 0.5275651052744739 T T T
0.8160532219672055 0.8186497382333471 0.5277724092126020 T T T
0.0725947679215709 0.1057603554872267 0.5479032620193721 T T T
0.0716579287400735 0.4397850423643269 0.5480326684914765 T T T
0.0728988542060923 0.7722548471936931 0.5479207061750708 T T T
0.3271257021381589 0.0602440059054940 0.5689273214651323 T T T
0.3283399046878829 0.3921738347728769 0.5685380638716391 T T T
0.3280660157993781 0.7260912219451694 0.5686603578919883 T T T
0.5853813386433221 0.0083453713391634 0.5901293579770224 T T T
0.5853420905232678 0.3448054595176069 0.5882812679697133 T T T
0.5853263028254029 0.6802843120792356 0.5897527543531640 T T T
0.8422702144632520 0.6282787374616668 0.6107853268056778 T T T
0.8447673735912431 0.2984906652346889 0.6102520132791505 T T T
0.8439687246998110 0.9620743822224785 0.6088842556267188 T T T
0.1002410935281354 0.5822014706254307 0.6315605974692893 T T T
0.0981832392326848 0.2513122307686688 0.6322894495641280 T T T
0.0996830773603035 0.9162891168470358 0.6320203168418627 T T T
0.3528362647995903 0.5382107399328014 0.6512498547505442 T T T
0.3514000658183887 0.2069541764432733 0.6509216248453917 T T T
0.3510503918843612 0.8726543138422095 0.6508078585734605 T T T
0.6070588533426974 0.4902584036406118 0.6699286235118201 T T T
0.6071973250207992 0.1609865403393282 0.6709722223625906 T T T
0.6031424228042557 0.8297780442493522 0.6759294762281484 T T T
0.8695914470533240 0.4387740779588241 0.6931884343289860 T T T
0.8623950242127558 0.1113242427263268 0.6889887962573765 T T T
0.8667859877482225 0.7813814255065987 0.6885676446506489 T T T
0.6860111597892343 0.6765009742452229 0.7793147556857837 T T T
0.5739964462786745 0.8299777616662344 0.7516165798190887 T T T
0.8238286730115799 0.5036649068317077 0.7659272677253383 T T T
0.6610258686826544 0.6952319246837583 0.8204232526834694 T T T

HCOO/Cu(533) E_{ads} = −2.98 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 2 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F

0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0478185900648000	0.2936364566665119	0.4657788224747037	T	T	T
0.0479665587686355	0.6269305981709223	0.4658178499140675	T	T	T
0.0477916140055683	0.9603499767279970	0.4657769478663667	T	T	T
0.3052496599034171	0.2457108482983088	0.4866301738914487	T	T	T
0.3054356817570394	0.5790761802629376	0.4866933539362037	T	T	T
0.3050535754629635	0.9125478928144233	0.4867238168278760	T	T	T
0.5616799426698265	0.1986999119054857	0.5076402087175751	T	T	T
0.5614096536450717	0.5330212824229363	0.5072504693882891	T	T	T
0.5613013753521727	0.8651561151485652	0.5072294013434941	T	T	T
0.8179897138426639	0.1518849507689737	0.5276806566103431	T	T	T
0.8177456275727337	0.4853573368302762	0.5277984219600995	T	T	T
0.8181502448254889	0.8182648641123009	0.5276642289774145	T	T	T
0.0738265086072190	0.1055425662801639	0.5480814254054778	T	T	T
0.0740935715393718	0.4385159219429653	0.5481003423446325	T	T	T
0.0751327512271800	0.7710327329902995	0.5479978417123945	T	T	T
0.3311992109399498	0.0575565026077598	0.5686844905964819	T	T	T
0.3314761571362439	0.3906014794857740	0.5686250051438506	T	T	T
0.3312076375899622	0.7245805459208796	0.5687478461062412	T	T	T
0.5883632108989474	0.0072262159496077	0.5899671641606119	T	T	T
0.5883786896187004	0.3462554820133761	0.5899718765509050	T	T	T
0.5886576045792893	0.6765450475933008	0.5910564499347402	T	T	T
0.8449394000869859	0.6294625216810985	0.6100859232716189	T	T	T
0.8448669488129568	0.2965003335224665	0.6100527662685451	T	T	T
0.8476048507426199	0.9606499524808640	0.6092955415265067	T	T	T
0.1042954340969473	0.5797998973311493	0.6317210212743802	T	T	T
0.1045142012740641	0.2468516503659757	0.6313534567979744	T	T	T
0.1041502999806383	0.9138429894369651	0.6317355774276763	T	T	T
0.3563815745621426	0.5358912425512941	0.6509951898830835	T	T	T
0.3567689217128844	0.2038197280981109	0.6510183184755292	T	T	T
0.3555366182845034	0.8707421687610477	0.6504198387687339	T	T	T
0.6100770894905381	0.4898690651582882	0.6761563199581460	T	T	T
0.6143169061352083	0.1551528435758627	0.6705372773714160	T	T	T
0.6107060070070460	0.8271556073030197	0.6762818605906986	T	T	T
0.8764942872082173	0.4366369026369625	0.6890302565333357	T	T	T
0.8720978960480394	0.1054355289025963	0.6894494191284721	T	T	T

0.8725003522307020	0.7752593513897565	0.6894593763865231	T	T	T
0.5487798290560733	0.7094626900099428	0.7713813712378723	T	T	T
0.5641648326242503	0.8474472048516901	0.7510988994952967	T	T	T
0.5601178826342874	0.5494312574988953	0.7507260006019720	T	T	T
0.5227533127101864	0.7308310363635826	0.8124378282480933	T	T	T

HCOO/Cu(533) E_{ads} = −2.98 eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H

60 1 2 1

Selective dynamics

Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0474854642846686	0.2942151804764621	0.4655755912139685	T	T	T
0.0478111667727815	0.6273316217333397	0.4658218040400131	T	T	T
0.0472510059658201	0.9613657633034107	0.4659863156730418	T	T	T
0.3050482266960785	0.2471599429931160	0.4867598485413576	T	T	T
0.3051547106836584	0.5797897915127986	0.4867740884542001	T	T	T
0.3051701194040806	0.9124440651992028	0.4869063263755480	T	T	T
0.5607544201322920	0.2006436635300112	0.5071717970651498	T	T	T
0.5605743548698597	0.5334417964779915	0.5071013891343267	T	T	T
0.5608978123548094	0.8667101781962990	0.5068658758729844	T	T	T
0.8161895236104613	0.1543843841020261	0.5279205561074387	T	T	T
0.8181588538061316	0.4856794666305555	0.5282977127158993	T	T	T
0.8176763398130151	0.8195516710576963	0.5274565654269380	T	T	T
0.0744785585398206	0.1066841953059890	0.5477399919439911	T	T	T
0.0746907685756145	0.4381984116107801	0.5476896710380292	T	T	T
0.0747284021996701	0.7724105362133197	0.5478025542103859	T	T	T
0.3301937056620602	0.0596769339452747	0.5687474860954714	T	T	T
0.3311628580564301	0.3939262499154843	0.5699220772981628	T	T	T
0.3311502600669309	0.7239534368812948	0.5700063167889426	T	T	T

0.5880975667511288 0.0115970075575724 0.5887780339442549 T T T
0.5836268484839930 0.3488578989997760 0.5902256172933097 T T T
0.5880643141413201 0.6783859406435865 0.5888327652380240 T T T
0.8473971391776106 0.6311450412247893 0.6101927015318563 T T T
0.8466408097122141 0.2941041165054622 0.6102428621415782 T T T
0.8467792019901986 0.9629969144633793 0.6094714444657562 T T T
0.1031141489134777 0.5804065379084137 0.6298474771286611 T T T
0.1037500201916391 0.2485952249230761 0.6325218008981247 T T T
0.1030671366504916 0.9186700453500822 0.6298828266303107 T T T
0.3485213782757180 0.5449510115611998 0.6578035280872918 T T T
0.3583623406402082 0.2014454798161385 0.6513784897797466 T T T
0.3599882572399882 0.8705094891139350 0.6513661313526025 T T T
0.6139737051651680 0.4899519461746731 0.6717672788376460 T T T
0.6136656922901303 0.1564573117249388 0.6707142424712109 T T T
0.6142978409307426 0.8253894852941996 0.6720330776766534 T T T
0.8664058935983560 0.4470783677952374 0.6896303695307350 T T T
0.8733992603210649 0.1114215087272091 0.6915148098727009 T T T
0.8754289456136295 0.7696835640670457 0.6916945500354833 T T T
0.1356751165924202 0.7304894969276130 0.7580414206660180 T T T
0.9859734060929816 0.8484926217612719 0.7436537167528010 T T T
0.2615901868730667 0.6215096232965276 0.7320972535912533 T T T
0.1511957198438992 0.7290256450684790 0.7995489142307651 T T T

HCOO/Cu(533) E_{ads} = −2.92 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 2 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0468405711585760 0.2954065772077001 0.4656548648656909 T T T

0.0465736315951659 0.6291147289924766 0.4658435862161809 T T T
0.0463825774525120 0.9623937675120970 0.4659479323945774 T T T
0.3034447922528472 0.2494448046236215 0.4867958783345046 T T T
0.3026740513802082 0.5824695124470054 0.4868739789609435 T T T
0.3035830712875480 0.9143988249676340 0.4868528942992754 T T T
0.5580147038869114 0.2037721004056081 0.5070432972670176 T T T
0.5581752286243784 0.5356874064861330 0.5070018768998636 T T T
0.5586638743488734 0.8700686187701621 0.5069926944805871 T T T
0.8132317406590417 0.1572080668161817 0.5278599568083919 T T T
0.8150443180562590 0.4893281908020626 0.5274796559512112 T T T
0.8143161347772079 0.8238925519719871 0.5276039557862333 T T T
0.0712608859212835 0.1098574650083179 0.5476496358285914 T T T
0.0712771669826111 0.4433460694740319 0.5476915344413840 T T T
0.0692120654156767 0.7784007427914972 0.5482437178885178 T T T
0.3263933176283089 0.0646687190543886 0.5683668379756810 T T T
0.3260621270277113 0.4002002254731707 0.5699314474164439 T T T
0.3264156427308222 0.7287717791336732 0.5699166280198114 T T T
0.5829351010363695 0.0200015318908200 0.5897706640380846 T T T
0.5797041827681326 0.3517617072287749 0.5905822720392422 T T T
0.5827482565867470 0.6842276278106496 0.5882353070936901 T T T
0.8417357091890949 0.6358366579012014 0.6090452054907658 T T T
0.8413361279655689 0.3022894299675869 0.6090179011986834 T T T
0.8372462364527777 0.9728096560782831 0.6104419523099764 T T T
0.0960037028352971 0.5901125159090626 0.6309804025134795 T T T
0.0978308941589390 0.2557732612818100 0.6316910031861696 T T T
0.0955393537223870 0.9260189496906364 0.6307045967097125 T T T
0.3454267164968314 0.5521789542199116 0.6555147597985496 T T T
0.3504217908998513 0.2099799493567431 0.6502954133139554 T T T
0.3519963352683106 0.8801718652300039 0.6507653205342123 T T T
0.6090007183747446 0.5008457260295529 0.6703440291955474 T T T
0.6033355006317862 0.1675312499219004 0.6768416869272400 T T T
0.6069861855287542 0.8304285198829859 0.6711244774850229 T T T
0.8626277824731190 0.4527539201832127 0.6894372001462443 T T T
0.8644996828264766 0.1193551174578289 0.6894510377023479 T T T
0.8642541020972772 0.7821467972188287 0.6894631291563300 T T T
0.3945057465419737 0.4356839601709623 0.7601860232274262 T T T
0.2964768690615784 0.5936464948143296 0.7306361468897364 T T T
0.5253569588035347 0.2478424587814061 0.7492054200900355 T T T
0.3618611779093115 0.4653321451979693 0.8007904892645854 T T T

HCOO/Cu(533) E_{ads} = −2.88 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 2 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F

0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0476287173546339	0.2937251586175549	0.4657773590855427	T	T	T
0.0477685161649504	0.6269547992524664	0.4657490037946488	T	T	T
0.0476147281647101	0.9603706915137877	0.4659550002427295	T	T	T
0.3053275186836970	0.2455701501601126	0.4872910828630310	T	T	T
0.3051630080351941	0.5795380143373947	0.4869958668511671	T	T	T
0.3048956196962536	0.9120355144036196	0.4870406585470377	T	T	T
0.5601525260731748	0.1998713542280086	0.5069334245897608	T	T	T
0.5599652521228506	0.5334416945841838	0.5070569015445585	T	T	T
0.5602281629532584	0.8662941145649086	0.5068849898932655	T	T	T
0.8165420078854737	0.1528411907597018	0.5276292945044290	T	T	T
0.8167700435637713	0.4858521865854186	0.5277017183119170	T	T	T
0.8177816742234540	0.8184283820221552	0.5274943088542585	T	T	T
0.0747688139773928	0.1044898618327821	0.5478763520717465	T	T	T
0.0753383096132012	0.4372528304994532	0.5476458041278462	T	T	T
0.0753902452092703	0.7707451707174400	0.5478708053370269	T	T	T
0.3306907513091986	0.0551668208711007	0.5700203828289716	T	T	T
0.3306029454304493	0.3938073559317203	0.5700750195641930	T	T	T
0.3307322441588099	0.7245680623185820	0.5711947677480396	T	T	T
0.5876791146466616	0.0102751282334310	0.5886652493903526	T	T	T
0.5847549797417457	0.3460794821908664	0.5894508195688175	T	T	T
0.5844815991570798	0.6796333982848921	0.5895178951282247	T	T	T
0.8472552887223443	0.6271912950735512	0.6091296842657314	T	T	T
0.8467902889606975	0.2946754811051946	0.6090851933074646	T	T	T
0.8471920582880443	0.9604642133015702	0.6090356146285316	T	T	T
0.1027501701996201	0.5802564513463935	0.6313189673456350	T	T	T
0.1028035050450384	0.2489730061809681	0.6312676739733405	T	T	T
0.1009431636137919	0.9162006810076946	0.6307023678721038	T	T	T
0.3556767869804034	0.5350173775377414	0.6562483762969151	T	T	T
0.3591826764144557	0.2006850568736027	0.6507019274244996	T	T	T
0.3552328515787622	0.8731839975672173	0.6564990695286284	T	T	T
0.6172626136740291	0.4861689738155235	0.6705526132841584	T	T	T
0.6152759595495354	0.1519552062979912	0.6712539383484355	T	T	T
0.6153553092712229	0.8221686312937280	0.6714113800863402	T	T	T
0.8690839371667423	0.4427740823790316	0.6895855106404412	T	T	T
0.8673385880184270	0.1100759120406423	0.6893414156142725	T	T	T
0.8692864954619282	0.7755838664747898	0.6897061643958509	T	T	T
0.2904028774048371	0.7579735962726275	0.7514338590374265	T	T	T
0.3045050742535906	0.8970978374492447	0.7311307658700201	T	T	T
0.3063394883955013	0.5941586315331406	0.7310542319494857	T	T	T
0.2600564811584860	0.7828979677257450	0.7921971549170834	T	T	T

HCOO/Defected-Cu(533) E_{ads} = −2.85 eV

1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
59 1 2 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0473964516467267 0.2939403322547236 0.4659616353279741 T T T
0.0475746894987813 0.6266720320962689 0.4657860589381210 T T T
0.0474711296586570 0.9608549157630585 0.4659896546119155 T T T
0.3049308063383812 0.2460046232487837 0.4874401468494692 T T T
0.3052428517936818 0.5795328822168904 0.4867165900768763 T T T
0.3042573450507361 0.9127594482200373 0.4869688093951359 T T T
0.5603072505985232 0.1998415467453243 0.5066975550125739 T T T
0.5600937203672605 0.5335500364898846 0.5069248173053393 T T T
0.5597010953192113 0.8666201920800339 0.5069478007092181 T T T
0.8164905707730009 0.1529925772429991 0.5275067664982270 T T T
0.8165841362635453 0.4861048770946464 0.5275967848712609 T T T
0.8176158119245138 0.8183281445489867 0.5274711191891360 T T T
0.0741489349193836 0.1054065354496362 0.5481945742022222 T T T
0.0743963517543916 0.4375362230631614 0.5481192839903984 T T T
0.0755116995757870 0.7706781075780027 0.5474003546035212 T T T
0.3295371472600420 0.0560211844023280 0.5702681569375592 T T T
0.3307980121490413 0.3940590983150896 0.5698956821897787 T T T
0.3312508704855593 0.7242110413540136 0.5708494174898868 T T T
0.5872861760904571 0.0107433563708259 0.5882902422769147 T T T
0.5852611039760557 0.3457106506346828 0.5891266604041592 T T T
0.5859962927306984 0.6784832351374589 0.5894523698228379 T T T
0.8465415974069710 0.6240593368771306 0.6102262009782559 T T T
0.8470507105420639 0.2972250270096726 0.6099501003123756 T T T
0.8474955749794549 0.9598454278258229 0.6087073343806204 T T T
0.1023748205972527 0.5798110280823874 0.6309496802675801 T T T
0.0983040958704565 0.2523955541930809 0.6323755160795330 T T T

0.1012500348803783	0.9165688522940115	0.6301668903589672	T	T	T
0.3553904015903330	0.5353300113435336	0.6561351968732420	T	T	T
0.3580111690371717	0.2018912844298769	0.6506395646443590	T	T	T
0.3547288977846300	0.8737911674241058	0.6563134975057454	T	T	T
0.6203607185669771	0.4854861333618996	0.6692031393283063	T	T	T
0.6151074895955573	0.1522622390677303	0.6710405385968865	T	T	T
0.6164782401157149	0.8210734181621239	0.6698684368027401	T	T	T
0.8679738374147695	0.1074118384395534	0.6879723908738988	T	T	T
0.8687170427945957	0.7765154511283794	0.6884255202219365	T	T	T
0.2978055269903608	0.7518454927600575	0.7518730233079264	T	T	T
0.3105233838202763	0.8921545083562898	0.7314924098333845	T	T	T
0.3119631627035448	0.5895966226337495	0.7313659153665690	T	T	T
0.2711889388252524	0.7737382585246319	0.7928972739095411	T	T	T

HCOO/Cu(111) $E_{ads} = -3.03$ eV

1.00000000000000

7.6579664403000001	0.0000000000000000	0.0000000000000000
3.8289832201000000	6.6319934786000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.5000000000000000

Cu C O H

45 1 2 1

Selective dynamics

Direct

0.8888888887999968	0.2222222223999992	0.3170124957488483	F	F	F
0.2222222221000010	0.2222222223999992	0.3170124957488483	F	F	F
0.5555555553999980	0.2222222223999992	0.3170124957488483	F	F	F
0.8888888890000004	0.5555555553000033	0.3170124957488483	F	F	F
0.2222222222999974	0.5555555553000033	0.3170124957488483	F	F	F
0.5555555556000016	0.5555555553000033	0.3170124957488483	F	F	F
0.8888888891999969	0.8888888882000003	0.3170124957488483	F	F	F
0.2222222225000010	0.8888888882000003	0.3170124957488483	F	F	F
0.5555555557999980	0.8888888882000003	0.3170124957488483	F	F	F
0.0000000000000000	0.0000000000000000	0.3975777759823913	F	F	F
0.3333333332999970	0.0000000000000000	0.3975777759823913	F	F	F
0.6666666666000012	0.0000000000000000	0.3975777759823913	F	F	F
0.0000000002103135	0.3333333328999970	0.3975777759823913	F	F	F
0.3333333335000006	0.3333333328999970	0.3975777759823913	F	F	F
0.6666666668999994	0.3333333328999970	0.3975777759823913	F	F	F
0.9999999996666986	0.6666666672999995	0.3975777759823913	F	F	F
0.3333333329999988	0.6666666672999995	0.3975777759823913	F	F	F
0.6666666663000029	0.6666666672999995	0.3975777759823913	F	F	F
0.1111111113999996	0.1111111104999978	0.4771948603999974	F	F	F
0.4444444447999985	0.1111111104999978	0.4771948603999974	F	F	F
0.7777777781000026	0.1111111104999978	0.4771948603999974	F	F	F
0.1111111108999978	0.4444444449000002	0.4771948603999974	F	F	F
0.4444444442000020	0.4444444449000002	0.4771948603999974	F	F	F
0.7777777774999990	0.4444444449000002	0.4771948603999974	F	F	F
0.1111111111000014	0.7777777777999972	0.4771948603999974	F	F	F
0.4444444443999984	0.7777777777999972	0.4771948603999974	F	F	F
0.7777777777000026	0.7777777777999972	0.4771948603999974	F	F	F
0.8852402684083381	0.2242570436194706	0.5573706665611714	T	T	T
0.2218768236782744	0.2224327573205540	0.5560697505065051	T	T	T
0.5561544358958815	0.2244765198442011	0.5573856010418530	T	T	T
0.8852407386542028	0.5571625462921216	0.5573658751082965	T	T	T
0.2221212029224148	0.5553206426195350	0.5562160764500589	T	T	T
0.5571859616776711	0.5547115959996424	0.5581762517350382	T	T	T
0.8877556276485974	0.8894775662019782	0.5564981843579415	T	T	T

0.2220867594379107	0.8892449990561447	0.5562131567918138	T	T	T
0.5561734235511796	0.8860684815060669	0.5573642895191253	T	T	T
0.0007888193356959	0.9983943956701871	0.6363750006275725	T	T	T
0.3297950661710356	0.0029094135984878	0.6361528655767263	T	T	T
0.6661663796496979	0.0002826829290059	0.6357917584537514	T	T	T
0.0032133947320222	0.3317339849205316	0.6356815648968120	T	T	T
0.3298682021481472	0.3340000832102193	0.6362070560778216	T	T	T
0.6657938762948834	0.3311518224756043	0.6410000648865473	T	T	T
0.0007324886250466	0.6674852463622550	0.6363516106836671	T	T	T
0.3269892238664149	0.6698078423960957	0.6354939449561939	T	T	T
0.6656116706005024	0.6697536119310229	0.6409072545319255	T	T	T
0.6557413328804813	0.5056150757257756	0.7414164163628082	T	T	T
0.6572401412154977	0.6535568042261406	0.7196517221187293	T	T	T
0.6595175501841397	0.3548873378148374	0.7197718517423036	T	T	T
0.6502496581196869	0.5085846561013561	0.7848803415951577	T	T	T

HCOO/Cu(100) $E_{ads} = -3.17$ eV

1.00000000000000

7.6579664403000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.6579664403000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.5000000000000000

Cu C O H

45 1 2 1

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.3173193249345303	F	F	F
0.3333333332999970	0.0000000000000000	0.3173193249345303	F	F	F
0.6666666666000012	0.0000000000000000	0.3173193249345303	F	F	F
0.0000000000000000	0.3333333332999970	0.3173193249345303	F	F	F
0.3333333332999970	0.3333333332999970	0.3173193249345303	F	F	F
0.6666666666000012	0.3333333332999970	0.3173193249345303	F	F	F
0.0000000000000000	0.6666666666000012	0.3173193249345303	F	F	F
0.3333333332999970	0.6666666666000012	0.3173193249345303	F	F	F
0.6666666666000012	0.6666666666000012	0.3173193249345303	F	F	F
0.1666666667000030	0.1666666667000030	0.3854655552433357	F	F	F
0.5000000000000000	0.1666666667000030	0.3854655552433357	F	F	F
0.8333333332999970	0.1666666667000030	0.3854655552433357	F	F	F
0.1666666667000030	0.5000000000000000	0.3854655552433357	F	F	F
0.5000000000000000	0.5000000000000000	0.3854655552433357	F	F	F
0.8333333332999970	0.5000000000000000	0.3854655552433357	F	F	F
0.1666666667000030	0.8333333332999970	0.3854655552433357	F	F	F
0.5000000000000000	0.8333333332999970	0.3854655552433357	F	F	F
0.8333333332999970	0.8333333332999970	0.3854655552433357	F	F	F
0.0000000000000000	0.0000000000000000	0.4552941175999976	F	F	F
0.3333333332999970	0.0000000000000000	0.4552941175999976	F	F	F
0.6666666666000012	0.0000000000000000	0.4552941175999976	F	F	F
0.0000000000000000	0.3333333332999970	0.4552941175999976	F	F	F
0.3333333332999970	0.3333333332999970	0.4552941175999976	F	F	F
0.6666666666000012	0.3333333332999970	0.4552941175999976	F	F	F
0.0000000000000000	0.6666666666000012	0.4552941175999976	F	F	F
0.3333333332999970	0.6666666666000012	0.4552941175999976	F	F	F
0.6666666666000012	0.6666666666000012	0.4552941175999976	F	F	F
0.1684349500613657	0.1681292283152070	0.5250902314965015	T	T	T
0.4999435871674652	0.1695338810793908	0.5255819708871099	T	T	T
0.8310199776645139	0.1683076644308189	0.5251980197281449	T	T	T
0.1687706698893526	0.4983287886647971	0.5252136742555648	T	T	T
0.4999128147960326	0.4968215651364455	0.5257367856484679	T	T	T

0.8307285899402975	0.4982597702792217	0.5253038536955505	T	T	T
0.1661642542699233	0.8331573203035219	0.5244289749864006	T	T	T
0.5000087217235040	0.8332789142535809	0.5245159442462480	T	T	T
0.8337023412362756	0.8331193231827129	0.5244327689878390	T	T	T
-0.0001323652303552	-0.0004466754816807	0.5923219979373084	T	T	T
0.3327758717850092	-0.0032294669482187	0.5922033299567537	T	T	T
0.6670864440673815	-0.0031534135228900	0.5922619676799755	T	T	T
-0.0006048055917169	0.3335047089315933	0.5919654758365611	T	T	T
0.3282286582731465	0.3340373154282625	0.5970401947516480	T	T	T
0.6705419447341129	0.3340281345870598	0.5975161983990389	T	T	T
-0.0001040492094534	0.6667962090129582	0.5925082081714883	T	T	T
0.3330226878096706	0.6694767094732808	0.5924077332372564	T	T	T
0.6667461197412954	0.6695212275422617	0.5924812171445251	T	T	T
0.4963974321943829	0.3083112274979846	0.6965745564432861	T	T	T
0.3480730755357421	0.3125777706408960	0.6746065000375538	T	T	T
0.6453888483949647	0.3162386557453441	0.6751313982741363	T	T	T
0.4955143103615665	0.2955963222572714	0.7398804963917586	T	T	T

HCOO/Cu(100) $E_{ads} = -3.12$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu C O H
45 1 2 1
Selective dynamics
Direct

0.0000000000000000	0.0000000000000000	0.3173193249345303	F	F	F
0.3333333332999970	0.0000000000000000	0.3173193249345303	F	F	F
0.6666666666000012	0.0000000000000000	0.3173193249345303	F	F	F
0.0000000000000000	0.3333333332999970	0.3173193249345303	F	F	F
0.3333333332999970	0.3333333332999970	0.3173193249345303	F	F	F
0.6666666666000012	0.3333333332999970	0.3173193249345303	F	F	F
0.0000000000000000	0.6666666666000012	0.3173193249345303	F	F	F
0.3333333332999970	0.6666666666000012	0.3173193249345303	F	F	F
0.6666666666000012	0.6666666666000012	0.3173193249345303	F	F	F
0.1666666667000030	0.1666666667000030	0.3854655552433357	F	F	F
0.5000000000000000	0.1666666667000030	0.3854655552433357	F	F	F
0.8333333332999970	0.1666666667000030	0.3854655552433357	F	F	F
0.1666666667000030	0.5000000000000000	0.3854655552433357	F	F	F
0.5000000000000000	0.5000000000000000	0.3854655552433357	F	F	F
0.8333333332999970	0.5000000000000000	0.3854655552433357	F	F	F
0.1666666667000030	0.8333333332999970	0.3854655552433357	F	F	F
0.5000000000000000	0.8333333332999970	0.3854655552433357	F	F	F
0.8333333332999970	0.8333333332999970	0.3854655552433357	F	F	F
0.0000000000000000	0.0000000000000000	0.4552941175999976	F	F	F
0.3333333332999970	0.0000000000000000	0.4552941175999976	F	F	F
0.6666666666000012	0.0000000000000000	0.4552941175999976	F	F	F
0.0000000000000000	0.3333333332999970	0.4552941175999976	F	F	F
0.3333333332999970	0.3333333332999970	0.4552941175999976	F	F	F
0.6666666666000012	0.3333333332999970	0.4552941175999976	F	F	F
0.0000000000000000	0.6666666666000012	0.4552941175999976	F	F	F
0.3333333332999970	0.6666666666000012	0.4552941175999976	F	F	F
0.6666666666000012	0.6666666666000012	0.4552941175999976	F	F	F
0.1682900346230826	0.1675784486561905	0.5250242550631983	T	T	T
0.4990627411504076	0.1676264940977684	0.5250530609733988	T	T	T
0.8328067595621502	0.1644739122134867	0.5241652148959324	T	T	T

0.1672479702511885	0.5008806482447914	0.5252543077477854	T	T	T
0.4994160313778493	0.4998092862242214	0.5247661663827633	T	T	T
0.8359016799817176	0.5016106614692952	0.5249500834879823	T	T	T
0.1669203168607475	0.8300623446140050	0.5258739275033255	T	T	T
0.4987224944813018	0.8323282765411014	0.5251594520437597	T	T	T
0.8373087777022064	0.8314878995496593	0.5256005803551125	T	T	T
0.0008992507227385	0.0012905414669994	0.5930290116800043	T	T	T
0.3335956353203204	0.0012822928491403	0.5929121607184556	T	T	T
0.6669735955213318	-0.0005041214148525	0.5930956568685046	T	T	T
-0.0037074834036288	0.3271920376673575	0.5913768436563087	T	T	T
0.3353710447194567	0.3293915375902163	0.5949107037241466	T	T	T
0.6688787043081679	0.3319679950756455	0.5918416909483118	T	T	T
-0.0012907271673629	0.6680505653174257	0.5979369972272445	T	T	T
0.3399889902336962	0.6716096172121814	0.5950929338822842	T	T	T
0.6691503025979670	0.6675135115919678	0.5917916947025611	T	T	T
0.1826882746652045	0.5266350873869309	0.6883614078889710	T	T	T
0.0390238529029618	0.5890394035530394	0.6735815226047107	T	T	T
0.3252285560958288	0.5200042126694839	0.6619159461092297	T	T	T
0.1888734633412510	0.4695515301106596	0.7282566320667989	T	T	T

HCOO/Cu(211) $E_{ads} = -3.46$ eV
1.00000000000000
6.2527034153000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.3164343000000009
Cu C O H
45 1 2 1
Selective dynamics
Direct

0.0061862950247047	0.1666666667000030	0.3120745335338029	F	F	F
0.0061862950247047	0.5000000000000000	0.3120745335338029	F	F	F
0.0061862950247047	0.8333333332999970	0.3120745335338029	F	F	F
0.3355456677560653	0.0000000000000000	0.3354619372229379	F	F	F
0.3355456677560653	0.3333333332999970	0.3354619372229379	F	F	F
0.3355456677560653	0.6666666666000012	0.3354619372229379	F	F	F
0.6630854692850079	0.1666666667000030	0.3607350091654666	F	F	F
0.6630854692850079	0.5000000000000000	0.3607350091654666	F	F	F
0.6630854692850079	0.8333333332999970	0.3607350091654666	F	F	F
0.9944057463905267	0.0000000000000000	0.3915351276171819	F	F	F
0.9944057463905267	0.3333333332999970	0.3915351276171819	F	F	F
0.9944057463905267	0.6666666666000012	0.3915351276171819	F	F	F
0.3330656692422309	0.1666666667000030	0.4179888222780335	F	F	F
0.3330656692422309	0.5000000000000000	0.4179888222780335	F	F	F
0.3330656692422309	0.8333333332999970	0.4179888222780335	F	F	F
0.6656564241704075	0.0000000000000000	0.4448469552356400	F	F	F
0.6656564241704075	0.3333333332999970	0.4448469552356400	F	F	F
0.6656564241704075	0.6666666666000012	0.4448469552356400	F	F	F
0.0003515212697778	0.1666666667000030	0.4732099031121066	F	F	F
0.0003515212697778	0.5000000000000000	0.4732099031121066	F	F	F
0.0003515212697778	0.8333333332999970	0.4732099031121066	F	F	F
0.3333333329999988	0.0000000000000000	0.5000000000000000	F	F	F
0.3333333329999988	0.3333333332999970	0.5000000000000000	F	F	F
0.3333333329999988	0.6666666666000012	0.5000000000000000	F	F	F
0.6663151448302216	0.1666666667000030	0.5267900968878934	F	F	F
0.6663151448302216	0.5000000000000000	0.5267900968878934	F	F	F
0.6663151448302216	0.8333333332999970	0.5267900968878934	F	F	F
-0.0001742746886428	0.0002211152692423	0.5550158594985882	T	T	T

0.0000090990837334	0.3330472059382524	0.5549943315048597	T	T	T
-0.0005295543279497	0.6666850307597104	0.5550246744399734	T	T	T
0.3337646290301732	0.1665443057808992	0.5816151802123629	T	T	T
0.3334873634250322	0.5001346725059070	0.5818041351325555	T	T	T
0.3334065693278737	0.8331282329370685	0.5817938682799689	T	T	T
0.6703850954425402	-0.0036674208183966	0.6094729300270063	T	T	T
0.6704128610138634	0.3362497795561522	0.6092739117553575	T	T	T
0.6701738312049355	0.6665609111818007	0.6101101245796101	T	T	T
0.0008394687637803	0.1665062698887731	0.6386446020665286	T	T	T
0.0012346222270205	0.5001431009933587	0.6386103260823045	T	T	T
0.0012838177565410	0.8330831374910980	0.6386627202117126	T	T	T
0.3292574161858562	-0.0002686491054938	0.6635919551520333	T	T	T
0.3287014334709362	0.3329669346043265	0.6634873436576748	T	T	T
0.3300855961742958	0.6666121981398448	0.6632457145691920	T	T	T
0.6578948591479405	0.1660237162980065	0.6876526870217593	T	T	T
0.6613730919578420	0.4948445902365615	0.6912490065292891	T	T	T
0.6622169470113127	0.8367055212461544	0.6918457648222739	T	T	T
0.6707588885693545	0.6607959959146131	0.7866580688814419	T	T	T
0.6733818597683027	0.8099227927911815	0.7658247983443888	T	T	T
0.6664101222815887	0.5124872388149533	0.7653409090693547	T	T	T
0.6720283644700287	0.6597234121065194	0.8287486367075284	T	T	T

11.3 *CO Adsorption

CO/Cu_3/Cu(533) $E_{ads} = -1.22$ eV

1.00000000000000					
10.3878408006999994	0.0000000000000000	0.0000000000000000			
4.5828709415000004	6.0103788927000004	0.0000000000000000			
0.0000000000000000	0.0000000000000000	26.5000000000000000			
Cu C O					
63 1 1					
Selective dynamics					
Direct					
0.0032853599999996	0.9972806999999975	0.3042624500000031	F	F	F
0.0028217400000017	0.3308767700000033	0.3042691500000032	F	F	F
0.0026800899999984	0.6645640400000019	0.3042978000000005	F	F	F
0.2572489900000008	0.6186597399999982	0.3218759499999990	F	F	F
0.2571973700000001	0.2857762699999995	0.3217927099999969	F	F	F
0.2571614599999990	0.9524293899999989	0.3219123699999997	F	F	F
0.5099116399999986	0.5747781399999994	0.3415763200000015	F	F	F
0.5095861200000016	0.2417833900000019	0.3416938299999970	F	F	F
0.5096986000000001	0.9088501900000026	0.3416314700000029	F	F	F
0.7627858999999972	0.5310134699999978	0.3609394899999998	F	F	F
0.7629538699999969	0.1970798500000015	0.3608490599999996	F	F	F
0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F
0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F

0.7895473399999986 0.6754118300000016 0.4453449800000016 F F F
0.0465898452548637 0.2941123420651278 0.4664935070186257 T T T
0.0460313695668737 0.6284296257813253 0.4665840978660195 T T T
0.0467648712612431 0.9607284253960431 0.4664314517478117 T T T
0.3029524682587531 0.2471250637095517 0.4870156908736280 T T T
0.3030844499765148 0.5803229293392836 0.4871079522311226 T T T
0.3029111387072104 0.9137340476024877 0.4870136763145154 T T T
0.5582974236850334 0.2011176945872802 0.5067047035270902 T T T
0.5587497361521646 0.5339099199873233 0.5062807894912006 T T T
0.5587208236844378 0.8670825649290339 0.5066287712464588 T T T
0.8160014347913138 0.1523003768858151 0.5273405062673195 T T T
0.8154422603160567 0.4865352266175328 0.5275207817320866 T T T
0.8148969891756009 0.8209288837235553 0.5277351080574184 T T T
0.0717027243767329 0.1055618382321173 0.5490814199964285 T T T
0.0711415286651517 0.4404198812831997 0.5487006133111124 T T T
0.0719011218479796 0.7733232191666863 0.5491856998980245 T T T
0.3267357846471467 0.0601629404657379 0.5689331553763395 T T T
0.3256474722124604 0.3940859379008819 0.5693754872243580 T T T
0.3269317906897047 0.7267832612601217 0.5692225186427140 T T T
0.5830096821871250 0.0127716861842150 0.5884221284131370 T T T
0.5843238350158781 0.3461817602355641 0.5880013768926031 T T T
0.5841336317967476 0.6786600303227689 0.5881806019554886 T T T
0.8416182134440605 0.6319029166494876 0.6098065137766929 T T T
0.8422245907177509 0.2964344383927685 0.6096345978068236 T T T
0.8426676426117753 0.9644258124713692 0.6101138153190576 T T T
0.0945716960872245 0.5862850684888141 0.6340126049419241 T T T
0.0967510437036516 0.2523081283399451 0.6325632741832090 T T T
0.0974434269442064 0.9183157543346659 0.6348574071651961 T T T
0.3485796597178636 0.5371376292485104 0.6507295879762752 T T T
0.3492536241962846 0.2073085177282242 0.6519407834299010 T T T
0.3490280203081744 0.8792722302844418 0.6510138756332942 T T T
0.6044613685913443 0.4960498710585440 0.6700798605279663 T T T
0.6038273617047424 0.1564505954643263 0.6696773209716563 T T T
0.6035713546025649 0.8309547615296693 0.6718308503568341 T T T
0.8626945835199313 0.4487032845188191 0.6903268637383302 T T T
0.8599364320302216 0.1153477461571076 0.6919356014861238 T T T
0.8557863869820962 0.7862990321870453 0.6919754946559725 T T T
0.6276645821126045 0.6307946655129701 0.7499670894863878 T T T
0.6153560287964335 0.3096658685235519 0.7464697174371302 T T T
0.3661614316477333 0.6927321680854159 0.7272549388907190 T T T
0.6335428250349125 0.6851031167050363 0.8166453808862362 T T T
0.6389698801654352 0.7070166806420169 0.8593578025668508 T T T

CO/Defected-Cu(533) $E_{ads} = -1.15$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
59 1 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F

0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0465895932699207	0.2946552406806304	0.4660585244338839	T	T	T
0.0466498479461961	0.6271773207410283	0.4658883699296880	T	T	T
0.0468190859165420	0.9611374676454248	0.4659877518110072	T	T	T
0.3032282974551950	0.2471294306268887	0.4868431550936084	T	T	T
0.3035535388978333	0.5800021153880728	0.4864178145825734	T	T	T
0.3030403427731400	0.9140268145234310	0.4866501028454737	T	T	T
0.5595099386289001	0.2003959104802732	0.5068278838290173	T	T	T
0.5595243788084779	0.5334005323163673	0.5068930698968227	T	T	T
0.5586646378522760	0.8670531190500576	0.5068687968549633	T	T	T
0.8161096744122065	0.1529488875976033	0.5275166419520488	T	T	T
0.8157373352219263	0.4860839410228121	0.5277603063437596	T	T	T
0.8160315348928292	0.8199874461037050	0.5279101436167019	T	T	T
0.0716544581148524	0.1069852373065685	0.5485278437093460	T	T	T
0.0713840237522041	0.4399154201536074	0.5486891972907250	T	T	T
0.0724168764242407	0.7724212721543792	0.5478519300239871	T	T	T
0.3263318986759429	0.0607806991542720	0.5692099395244683	T	T	T
0.3273258626400344	0.3936528049809192	0.5689954554394103	T	T	T
0.3276367146809303	0.7263816068836392	0.5686994092980915	T	T	T
0.5841569156026095	0.0125641053829703	0.5884161267285758	T	T	T
0.5850495458745680	0.3449646333660737	0.5887877860400704	T	T	T
0.5851959483248412	0.6782412780362653	0.5888307072495989	T	T	T
0.8424645120787501	0.6263196847407344	0.6103651819533018	T	T	T
0.8429904371732924	0.2982423252600528	0.6113361776099767	T	T	T
0.8437751942816591	0.9652641680070263	0.6101833008323310	T	T	T
0.0980931773851460	0.5839802453587483	0.6322705567366484	T	T	T
0.0946670542554069	0.2534717205406503	0.6333289638251783	T	T	T
0.0989528290696193	0.9178246012200892	0.6317948258889627	T	T	T
0.3510296491848895	0.5398548120210378	0.6518093617702988	T	T	T
0.3500711558673669	0.2071781329344735	0.6518042148692651	T	T	T
0.3507589681175940	0.8737881141059375	0.6517748623678434	T	T	T
0.6054598979779273	0.4950556444213077	0.6699033303058440	T	T	T
0.6042621522169704	0.1609397788596885	0.6711844286152900	T	T	T
0.6056995234190350	0.8264443713881110	0.6701460398733096	T	T	T
0.8637391505622660	0.1112819617912525	0.6915585347483295	T	T	T
0.8590482733056364	0.7783943965226331	0.6883060648279398	T	T	T
0.8751548774539593	0.1254271839844482	0.7603707584181599	T	T	T
0.8715041559740031	0.1321945010473335	0.8037194446771141	T	T	T

CO/Defected-Cu(533) E_{ads} = −1.14 eV

1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
59 1 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0474817640241626 0.2934024358570105 0.4660580691857476 T T T
0.0472584104304462 0.6264454172875245 0.4660278092996331 T T T
0.0475129784296262 0.9602057793229589 0.4658975314185865 T T T
0.3037715056161601 0.2462226134891094 0.4869232232558177 T T T
0.3045491700263565 0.5789458816318698 0.4866042699625949 T T T
0.3043637395660390 0.9122817234779659 0.4866570188852481 T T T
0.5599201015488350 0.1998264963101848 0.5069712580398874 T T T
0.5597011701019320 0.5328868579232882 0.5070483383924987 T T T
0.5593512094591822 0.8655303749618295 0.5073699048298226 T T T
0.8169430358276625 0.1513820105227059 0.5272611696470746 T T T
0.8162719839238627 0.4858383447796994 0.5272750165625615 T T T
0.8163507174289745 0.8188737070888635 0.5277367487174958 T T T
0.0737248157514846 0.1041636669760576 0.5482759624806008 T T T
0.0718858641147097 0.4386882132114996 0.5487549769814170 T T T
0.0738171570369692 0.7707467688871017 0.5479499342498287 T T T
0.3273954887123749 0.0588521761393725 0.5693173886892093 T T T
0.3286874530938462 0.3918090002895813 0.5690162954222072 T T T
0.3282898196123361 0.7253256774843476 0.5691167852826334 T T T
0.5850060987178071 0.0108738407800393 0.5886306355323427 T T T
0.5868335953359568 0.3442042326852382 0.5894444442207381 T T T
0.5870177694408617 0.6741122570712079 0.5899274452845337 T T T
0.8437815162790474 0.6244403227393790 0.6106532266853764 T T T
0.8454969523811903 0.2969144353521168 0.6090915371393918 T T T
0.8446406146755421 0.9627106357398074 0.6092997114405826 T T T
0.0999206198361291 0.5812114107579676 0.6320989898131001 T T T
0.0961740280613943 0.2507070937103943 0.6335175708465145 T T T

0.0984223043911638	0.9174738083822267	0.6326288104918253	T	T	T
0.3529533359474230	0.5379807578255799	0.6516473923074100	T	T	T
0.3511194913883195	0.2051399089918468	0.6519801429417583	T	T	T
0.3534045543338395	0.8699469141898745	0.6521623134553148	T	T	T
0.6088595367010297	0.4950843109389560	0.6739340562841737	T	T	T
0.6045277403913311	0.1567988580649494	0.6711494576835355	T	T	T
0.6081056032726595	0.8250542872204518	0.6708202407570926	T	T	T
0.8610581577859961	0.1170797240322462	0.6894733658697151	T	T	T
0.8622873799774575	0.7815179280136973	0.6883095310693891	T	T	T
0.7072854496767476	0.3530116344587022	0.7384371325788082	T	T	T
0.6971183094288063	0.3680651727807282	0.7823436949800290	T	T	T

CO/Cu(533) $E_{ads} = -1.13$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 1
Selective dynamics
Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0466816194668451	0.2945855663535202	0.4659723150570652	T	T	T
0.0459597906173227	0.6284509879734027	0.4660227123185200	T	T	T
0.0467404253836929	0.9609593333619332	0.4659989205119563	T	T	T
0.3027885369393393	0.2479098894043316	0.4868183045284658	T	T	T
0.3026544204197311	0.5808706221339128	0.4866956420442015	T	T	T
0.3029570002676206	0.9141633973279486	0.4866000288713554	T	T	T
0.5582320422960778	0.2015135617680398	0.5069232368970079	T	T	T
0.5583146512445873	0.5346892212893075	0.5068863097688322	T	T	T
0.5582157510469462	0.8680422605926839	0.5068228518394285	T	T	T
0.8145890609830704	0.1536844338243081	0.5271956292872363	T	T	T
0.8146189203536498	0.4886538949766430	0.5272310108350665	T	T	T
0.8146868812880839	0.8210261967727379	0.5283234436952386	T	T	T

0.0710776421353737 0.1075965270831116 0.5480573577538154 T T T
0.0706645754492979 0.4415065718101680 0.5483379481339815 T T T
0.0705362554994831 0.7742658473824497 0.5483572182851895 T T T
0.3256978279110812 0.0618089669479562 0.5690524796432277 T T T
0.3255761523931430 0.3954431715694110 0.5691894282640613 T T T
0.3254376434651572 0.7289555217865825 0.5689383630389599 T T T
0.5827294426184072 0.0144304627104298 0.5888188474708453 T T T
0.5829159172304690 0.3473776064038958 0.5888700299579133 T T T
0.5828503187065662 0.6812395152682871 0.5887908312091368 T T T
0.8416036246108619 0.6295050143090164 0.6105116715534773 T T T
0.8409153243507175 0.2993472483411419 0.6082982430445449 T T T
0.8416906099441243 0.9676964985020370 0.6104856998571234 T T T
0.0967134609577607 0.5859032141924262 0.6327606540633566 T T T
0.0961830958280634 0.2534842770839493 0.6323398230665835 T T T
0.0960634722368979 0.9203423912826635 0.6322622065310175 T T T
0.3483153283283096 0.5424752732063616 0.6518754844644750 T T T
0.3502324979160039 0.2080557194877776 0.6518056013494157 T T T
0.3483038454717827 0.8773288686863744 0.6516884479886011 T T T
0.5980423731903656 0.5016728953355020 0.6704524020901532 T T T
0.6038782427909809 0.1640263412287673 0.6716872664253727 T T T
0.6038596877380732 0.8297112561772364 0.6716550227184737 T T T
0.8595498278094467 0.4482028955472185 0.6921783319163788 T T T
0.8595637093191910 0.1192978222069235 0.6921950159963768 T T T
0.8583425778298072 0.7847584682542117 0.6900825516875334 T T T
0.8609795816706044 0.2831580914109889 0.7499325911653839 T T T
0.8578919939403389 0.2848458081053662 0.7939086296392494 T T T

CO/Cu_3/Cu(533) E_{ads} = −1.12 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
63 1 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F
0.2571614599999990 0.9524293899999989 0.3219123699999997 F F F
0.5099116399999986 0.5747781399999994 0.3415763200000015 F F F
0.5095861200000016 0.2417833900000019 0.3416938299999970 F F F
0.5096986000000001 0.9088501900000026 0.3416314700000029 F F F
0.7627858999999972 0.5310134699999978 0.3609394899999998 F F F
0.7629538699999969 0.1970798500000015 0.3608490599999996 F F F
0.7629705100000024 0.8638077299999978 0.3608832600000014 F F F
0.0188077500000006 0.4844866199999984 0.3845455499999986 F F F
0.0188649600000019 0.1508076399999965 0.3844206699999972 F F F
0.0189457299999987 0.8174492599999965 0.3845321800000008 F F F
0.2777182000000025 0.4350678200000004 0.4051130599999979 F F F
0.2779364200000032 0.1018241299999971 0.4049400600000013 F F F
0.2778532499999997 0.7683188099999967 0.4050370400000034 F F F
0.5346647900000008 0.3873898000000011 0.4243529600000002 F F F
0.5347255300000029 0.0542446099999978 0.4245416400000011 F F F
0.5343893300000033 0.7214487199999979 0.4243017399999971 F F F

0.7896143700000025 0.3418778500000030 0.4451831499999983 F F F
0.7893677400000030 0.0085227100000012 0.4452920299999974 F F F
0.7895473399999986 0.6754118300000016 0.4453449800000016 F F F
0.0467163024586272 0.2943446272403860 0.4664380082001819 T T T
0.0461411318679249 0.6285689479658499 0.4666642051611069 T T T
0.0468633594984348 0.9609191206872626 0.4665595249710203 T T T
0.3028887965836931 0.2476448997874415 0.4871342607376912 T T T
0.3027690661352167 0.5807553851416574 0.4870078293306297 T T T
0.3032473044310369 0.9141481133443262 0.4869052457087255 T T T
0.5578376844365012 0.2012746248304461 0.5067501038304973 T T T
0.5588311226964017 0.5343647844842058 0.5061869407075472 T T T
0.5586010728366693 0.8685777127532612 0.5066361275078179 T T T
0.8159541674578956 0.1526589887682701 0.5273567224745671 T T T
0.8157528490222172 0.4872885266142287 0.5274426433020060 T T T
0.8147343207477442 0.8213370996890272 0.5278211475844429 T T T
0.0726390661825914 0.1056638514548204 0.5489330201509068 T T T
0.0707995707739602 0.4414225034782523 0.5488537131251310 T T T
0.0714884186781462 0.7741370267814767 0.5495074957345873 T T T
0.3263583692867600 0.0616223503478237 0.5693747622213817 T T T
0.3250344312945486 0.3955745516313819 0.5697057494405066 T T T
0.3269152555966771 0.7276607400820747 0.5690012106703003 T T T
0.5824139059598878 0.0150029633647995 0.5891214056524448 T T T
0.5839709819594796 0.3458639549405371 0.5874601938331299 T T T
0.5842685345419164 0.6807019854372474 0.5875445411772913 T T T
0.8411041067293007 0.6333152716834162 0.6101922687058670 T T T
0.8438012348226223 0.2960755918165309 0.6092096136842661 T T T
0.8416161618834614 0.9655553335462087 0.6105010011012845 T T T
0.0931779884950159 0.5887163289207215 0.6344824026588467 T T T
0.0954366020038394 0.2541192710108139 0.6330481586385730 T T T
0.0976682627590465 0.9191448908595350 0.6350100763534703 T T T
0.3483533731626685 0.5389211485297942 0.6510818107882059 T T T
0.3476509580114626 0.2103347890245792 0.6523733008262788 T T T
0.3488411535877853 0.8802095235951013 0.6512140774417355 T T T
0.6057558358071000 0.4949015679908155 0.6672112102147199 T T T
0.6015721876740966 0.1624218194410132 0.6716324863681866 T T T
0.6018116856897689 0.8351387474012983 0.6716206477115862 T T T
0.8599679683969061 0.4508255471482572 0.6912062937184462 T T T
0.8601779463778377 0.1163809408322772 0.6919753736472174 T T T
0.8528694140573682 0.7895056778601217 0.6928387554060431 T T T
0.6233699523715522 0.6447783009378901 0.7479067946368465 T T T
0.6226682044010916 0.3159293865303710 0.7481062457631555 T T T
0.3638100348325454 0.6965065058667701 0.7277445533790765 T T T
0.4946617942848440 0.5882262792491033 0.7927358948667350 T T T
0.4529229637930938 0.6226210019174127 0.8355225512403174 T T T

CO/Defected-Cu(533) E_{ads} = −1.11 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
59 1 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F

0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0467377188767992	0.2942295460065142	0.4660867709642784	T	T	T
0.0465671725031587	0.6273086047287837	0.4659713657976516	T	T	T
0.0467950794819920	0.9609808388752521	0.4658530269753954	T	T	T
0.3025111804499135	0.2475941585950609	0.4868586604777799	T	T	T
0.3036601455127628	0.5801376762298481	0.4865182861889058	T	T	T
0.3030143745756986	0.9137205320450528	0.4866815059195760	T	T	T
0.5584737568465452	0.2009010818245661	0.5066594545886164	T	T	T
0.5582915818850660	0.5347869315891003	0.5069040800489131	T	T	T
0.5579500675036586	0.8680486394928140	0.5075532261225170	T	T	T
0.8152638912213509	0.1539438502619209	0.5273718210044231	T	T	T
0.8143322399217859	0.4876093313820712	0.5273893684447479	T	T	T
0.8142505293179244	0.8208523605506568	0.5275375913056374	T	T	T
0.0708413319015404	0.1073119102235452	0.5483894971483408	T	T	T
0.0696193064847176	0.4412831808276278	0.5486032696013915	T	T	T
0.0718817593626895	0.7731922748319633	0.5477112032705151	T	T	T
0.3250475824934728	0.0622108048822020	0.5691882802725602	T	T	T
0.3264512251027537	0.3941795598317889	0.5688157871254262	T	T	T
0.3253943203515782	0.7287046518530500	0.5689446068790041	T	T	T
0.5827616625554036	0.0161422912269802	0.5895418878970416	T	T	T
0.5837517469271273	0.3463721711807481	0.5885765510092458	T	T	T
0.5835647104773189	0.6782946493554748	0.5896618321984844	T	T	T
0.8402355065954670	0.6283257647248516	0.6103164320758775	T	T	T
0.8415028956985292	0.3014755275346320	0.6101560485312819	T	T	T
0.8417683084621109	0.9650263460658268	0.6087458773630187	T	T	T
0.0963769858711161	0.5849139033747990	0.6316874907268529	T	T	T
0.0931585196908344	0.2551147953841203	0.6333894557780458	T	T	T
0.0942559574732141	0.9221449713215853	0.6325410000297044	T	T	T
0.3470446610511676	0.5437843133079068	0.6509161484385158	T	T	T
0.3489745687001504	0.2090008091662016	0.6519639337538145	T	T	T
0.3489023470281321	0.8755766014811572	0.6516757908061646	T	T	T
0.6031204770978577	0.4994613612742871	0.6724287575663151	T	T	T
0.6003168049767084	0.1655216961813158	0.6746273657222189	T	T	T
0.6046430507341631	0.8285119552813413	0.6706468706259741	T	T	T
0.8584069285607319	0.1165150812243583	0.6893145568597685	T	T	T
0.8597725818413661	0.7805118391706171	0.6878524319995402	T	T	T
0.6570229008525592	0.3011253944117139	0.7320486463840278	T	T	T
0.6298655982547757	0.3253071628729313	0.7757318058567402	T	T	T

CO/Cu(533) E_{ads} = −1.09 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0470226384859650 0.2942823429656766 0.4658368855762789 T T T
0.0465340267956085 0.6278959833668576 0.4660402121281563 T T T
0.0470430188496377 0.9608240981637252 0.4658439178346326 T T T
0.3030304524487905 0.2475620930949352 0.4868503779474697 T T T
0.3028844048843400 0.5809108136438853 0.4866825401840346 T T T
0.3035979838820134 0.9135869843800701 0.4865148951610687 T T T
0.5579830267828091 0.2024057912187168 0.5070565719093795 T T T
0.5578661326697192 0.5350242080517237 0.5070410780897282 T T T
0.5578618609122257 0.8677964490914950 0.5070789001809942 T T T
0.8143159956014026 0.1541131664347238 0.5270712987631230 T T T
0.8142899935788779 0.4888138235374377 0.5270458277190356 T T T
0.8140092255936522 0.8217284909889676 0.5277498511178549 T T T
0.0715292885891253 0.1071611191781927 0.5477432686825870 T T T
0.0704207879474015 0.4413738526191660 0.5482613018698935 T T T
0.0704052060883173 0.7748958124984257 0.5482113460232453 T T T
0.3246906058522301 0.0621639478195119 0.5691905023665361 T T T
0.3250300530905557 0.3963917202025461 0.5691285223500427 T T T
0.3246307213689760 0.7298371988834917 0.5691055684668421 T T T
0.5811024647049545 0.0158304005400619 0.5884480844632735 T T T
0.5826538589170240 0.3495432120884401 0.5895553221743739 T T T
0.5828436888791071 0.6794889434009934 0.5894887674750351 T T T
0.8404095610805213 0.6314783137646365 0.6093750215865148 T T T
0.8418723893716595 0.2986277233762983 0.6075118641724602 T T T
0.8400656207910563 0.9683864854658175 0.6093277790975141 T T T
0.0957039827359409 0.5875434533471350 0.6323837968668085 T T T

0.0942815080346788 0.2541668383385571 0.6328175146352685 T T T
0.0943961622349507 0.9222822585560859 0.6326785918352360 T T T
0.3482635479491336 0.5434957060539468 0.6519286869670510 T T T
0.3472171974017116 0.2105720400067845 0.6516014745390946 T T T
0.3483480585939939 0.8764442845842950 0.6518568434179534 T T T
0.5983760169184957 0.5013892559571772 0.6745865035982861 T T T
0.6003993363630619 0.1644471152196393 0.6710244220402669 T T T
0.6006871605721260 0.8349864960709767 0.6709620772848685 T T T
0.8566948844643002 0.4538853532251994 0.6904572227852223 T T T
0.8566426312424195 0.1186890960510298 0.6903759548266574 T T T
0.8570218477686441 0.7860640538296817 0.6888955003822933 T T T
0.7455451990696095 0.3785224365966033 0.7384509290680700 T T T
0.7195757619732281 0.4006262163577540 0.7822047106875993 T T T

CO/Cu(533) $E_{ads} = -1.08$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0468691076465698 0.2944007899837761 0.4658848661939633 T T T
0.0465233268370460 0.6282214721200687 0.4659009946106767 T T T
0.0466287509452157 0.9609477695601560 0.4659310375991083 T T T
0.3031385441688494 0.2473828943622670 0.4866930501498828 T T T
0.3030442693287748 0.5808413640696933 0.4867416851781725 T T T
0.3029492047165840 0.9141962155965718 0.4866119518379200 T T T
0.5584060457671465 0.2012737105446052 0.5066736324816815 T T T
0.5585111924394697 0.5347463571373001 0.5069282584259195 T T T
0.5585056512683824 0.8677809610720162 0.5068837036390237 T T T
0.8150713981736527 0.1547498151896673 0.5277427942439948 T T T

0.8150157671799113 0.4874360821354458 0.5273424477800422 T T T
0.8150313159036101 0.8201491186346301 0.5277462622297981 T T T
0.0711577346312597 0.1076019129856731 0.5480606036225893 T T T
0.0712440485215893 0.4407171348368723 0.5480107312233288 T T T
0.0712249329692288 0.7741549804006504 0.5482639985617365 T T T
0.3260713765392647 0.0615908117248761 0.5689752527935308 T T T
0.3258426280989515 0.3950652014980873 0.5691012323599483 T T T
0.3259217032059153 0.7287512313352493 0.5690836374203140 T T T
0.5829464476865333 0.0145296458980799 0.5885826814987855 T T T
0.5828705948298913 0.3475612587590002 0.5885764256165720 T T T
0.5833753385198556 0.6806176236139395 0.5888633845604845 T T T
0.8422385672767397 0.6290555442169294 0.6100548005565536 T T T
0.8421300662834510 0.3007283504548821 0.6100720612277826 T T T
0.8417925073053322 0.9653372725136607 0.6090712640012707 T T T
0.0968661622977397 0.5857696783759293 0.6324060100925851 T T T
0.0978318317714059 0.2521238294321345 0.6322840024745060 T T T
0.0972417913972607 0.9197366557655426 0.6324421629459762 T T T
0.3495280795664428 0.5420228527872880 0.6517872745062626 T T T
0.3498667374767154 0.2087385506215504 0.6517295281950103 T T T
0.3499280314191599 0.8753278482135456 0.6518639263641410 T T T
0.6024455371933175 0.4976209298283826 0.6710985365428636 T T T
0.6031165272215153 0.1642527200699136 0.6715754342233666 T T T
0.6026503008378805 0.8317853714893838 0.6710094188603694 T T T
0.8620436667963020 0.4485101748195774 0.6927464693855773 T T T
0.8583845362991742 0.1160175991155103 0.6892499094197980 T T T
0.8583484257190658 0.7870190352784594 0.6892299430798506 T T T
0.8709240628632363 0.4407996778089167 0.7620764978873734 T T T
0.8642665299006183 0.4463362869135042 0.8054434020705451 T T T

CO/Defected-Cu(533) $E_{ads} = -1.06$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
59 1 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F

0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0471092784526559 0.2938580278873043 0.4660405111272655 T T T
0.0469855704091568 0.6270396327778592 0.4660305829871413 T T T
0.0468885543019430 0.9610368094908328 0.4658705937959587 T T T
0.3033823000260601 0.2468456849017767 0.4867067713857801 T T T
0.3038735504811516 0.5798856100332269 0.4866257460972703 T T T
0.3035091835740882 0.9133374634028700 0.4867019872806353 T T T
0.5594332772522462 0.2011191240507375 0.5070618055138479 T T T
0.5592192553518260 0.5336174699290341 0.5067241891292651 T T T
0.5587652615915196 0.8663182890462474 0.5070883489848896 T T T
0.8157584047157271 0.1530677772093566 0.5274311403611278 T T T
0.8156364869644206 0.4862983686226792 0.5274631011179258 T T T
0.8154373207814715 0.8198602923800947 0.5276369487649695 T T T
0.0716900010402834 0.1066179723375002 0.5484315277394225 T T T
0.0709595592963520 0.4401433434341133 0.5485979798310604 T T T
0.0722850534229615 0.7729385804418598 0.5479034564475600 T T T
0.3262366508448509 0.0609355928390974 0.5689245493921981 T T T
0.3274829198250330 0.3933955218311254 0.5687118207092391 T T T
0.3279228593928655 0.7262074357969101 0.5688818521026218 T T T
0.5837268826309149 0.0125133465800713 0.5882654712844489 T T T
0.5853007630038062 0.3472542840860234 0.5896657523726013 T T T
0.5855690594776459 0.6762583371666863 0.5894343834953439 T T T
0.8418511033406116 0.6263325051117035 0.6104836885422881 T T T
0.8432397365922567 0.2992402706862998 0.6103472275895022 T T T
0.8431611903636752 0.9631403425909877 0.6090388529356868 T T T
0.0979414197293865 0.5833359616944142 0.6320345140663389 T T T
0.0944846755561062 0.2539262557560719 0.6332665813622734 T T T
0.0983347371520099 0.9183464178397110 0.6318862163081255 T T T
0.3507438892040507 0.5397615649495321 0.6511607966002489 T T T
0.3501302646337336 0.2075930609578433 0.6515415107732477 T T T
0.3501172726297735 0.8748422099052376 0.6512507545447277 T T T
0.6087989657751466 0.4942088768727805 0.6732017259673380 T T T
0.6052767394062040 0.1583083437901788 0.6711045959701744 T T T
0.6057143330651285 0.8290183187851746 0.6703265668868815 T T T
0.8625234879816435 0.1093333187150870 0.6885332737487343 T T T
0.8599927955108801 0.7811474970450129 0.6883797126974606 T T T
0.6295394662994049 0.5007106391774336 0.7420501216532730 T T T
0.6313771409407960 0.5085558942208062 0.7855123109400931 T T T

CO/Cu_3/Cu(533) $E_{ads} = -1.04$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
63 1 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F

0.2571614599999990	0.9524293899999989	0.3219123699999997	F	F	F
0.5099116399999986	0.5747781399999994	0.3415763200000015	F	F	F
0.5095861200000016	0.2417833900000019	0.3416938299999970	F	F	F
0.5096986000000001	0.9088501900000026	0.3416314700000029	F	F	F
0.7627858999999972	0.5310134699999978	0.3609394899999998	F	F	F
0.7629538699999969	0.1970798500000015	0.3608490599999996	F	F	F
0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F
0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0459339195603080	0.2946062254426433	0.4663004104563326	T	T	T
0.0452481817132242	0.6292359811864489	0.4665914342093693	T	T	T
0.0458032009037176	0.9610754134051102	0.4663911906391232	T	T	T
0.3013977305372694	0.2484065174380206	0.4868072891314867	T	T	T
0.3017819862700955	0.5812371571149015	0.4872969253129671	T	T	T
0.3015536623659738	0.9142701580595513	0.4868775177872380	T	T	T
0.5563091768038400	0.2018662183444223	0.5063264745306300	T	T	T
0.5573778217232382	0.5350224642872040	0.5061836776148684	T	T	T
0.5575057600532870	0.8672782069411105	0.5062718816740073	T	T	T
0.8140253413224677	0.1546084185910107	0.5275510620529553	T	T	T
0.8139189046838222	0.4875907955896486	0.5274386015360379	T	T	T
0.8132149918451883	0.8214809252729497	0.5277886479216670	T	T	T
0.0690891691796419	0.1072381747275691	0.5487685100622025	T	T	T
0.0683004326753691	0.4428227940930294	0.5484431622309373	T	T	T
0.0694523359966963	0.7753208460514743	0.5493759343515046	T	T	T
0.3244228381049971	0.0621088517314789	0.5682284397316995	T	T	T
0.3227156385545236	0.3965976504259239	0.5699311444914681	T	T	T
0.3240043627109494	0.7279967860800685	0.5694094956993074	T	T	T
0.5797795060985628	0.0132236313984618	0.5877551721193538	T	T	T
0.5803848013790607	0.3476151582781192	0.5871199987224730	T	T	T
0.5820196419443328	0.6797752093985377	0.5879650818671092	T	T	T
0.8372334735544779	0.6339623343766075	0.6105449403182860	T	T	T
0.8396919407224998	0.3008677765655556	0.6105468448399143	T	T	T
0.8393335854805608	0.9667677224619893	0.6095513349193846	T	T	T
0.0909127985253662	0.5893162083725569	0.6338576981616859	T	T	T
0.0958045033338807	0.2536051472840423	0.6310534531932936	T	T	T
0.0930529290393579	0.9219212036766298	0.6350063262116906	T	T	T
0.3433120987357226	0.5433882960480235	0.6534144941523403	T	T	T
0.3450002876005587	0.2111522886874058	0.6519308813720267	T	T	T
0.3441709198809779	0.8829632574240721	0.6496009458846428	T	T	T
0.6012865947737654	0.4945370908720650	0.6676931862823448	T	T	T
0.6000440040234616	0.1557635775649914	0.6680050105178611	T	T	T
0.5970077461434237	0.8320905339554601	0.6721788910464835	T	T	T
0.8797515782014745	0.4385843583709171	0.6920628842206884	T	T	T
0.8537726375560706	0.1190712926058064	0.6914720796943464	T	T	T
0.8524528257778372	0.7922538880371233	0.6915408237493876	T	T	T
0.6573336796480601	0.5848109529821489	0.7493425724372770	T	T	T
0.6040062910731855	0.3107992313682530	0.7448193150648859	T	T	T
0.3829740282366945	0.7064504440148311	0.7284833335303258	T	T	T

0.8842468529353789 0.4696534373282177 0.7642500381734531 T T T
0.9593357172080482 0.4343303230420399 0.8008468085414489 T T T

CO/Cu_3/Cu(533) $E_{ads} = -1.04$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
63 1 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F
0.2571614599999990 0.9524293899999989 0.3219123699999997 F F F
0.5099116399999986 0.5747781399999994 0.3415763200000015 F F F
0.5095861200000016 0.2417833900000019 0.3416938299999970 F F F
0.5096986000000001 0.9088501900000026 0.3416314700000029 F F F
0.7627858999999972 0.5310134699999978 0.3609394899999998 F F F
0.7629538699999969 0.1970798500000015 0.3608490599999996 F F F
0.7629705100000024 0.8638077299999978 0.3608832600000014 F F F
0.0188077500000006 0.4844866199999984 0.3845455499999986 F F F
0.0188649600000019 0.1508076399999965 0.3844206699999972 F F F
0.0189457299999987 0.8174492599999965 0.3845321800000008 F F F
0.2777182000000025 0.4350678200000004 0.4051130599999979 F F F
0.2779364200000032 0.1018241299999971 0.4049400600000013 F F F
0.2778532499999997 0.7683188099999967 0.4050370400000034 F F F
0.5346647900000008 0.3873898000000011 0.4243529600000002 F F F
0.5347255300000029 0.0542446099999978 0.4245416400000011 F F F
0.5343893300000033 0.7214487199999979 0.4243017399999971 F F F
0.7896143700000025 0.3418778500000030 0.4451831499999983 F F F
0.7893677400000030 0.0085227100000012 0.4452920299999974 F F F
0.7895473399999986 0.6754118300000016 0.4453449800000016 F F F
0.0464460109288353 0.2946978006320129 0.4663497396544644 T T T
0.0457946751655864 0.6287667473974705 0.4666302115727428 T T T
0.0466945914041536 0.9610236484843514 0.4664928901005279 T T T
0.3027727729000143 0.2477567118219555 0.4872604952725516 T T T
0.3027607079601984 0.5809359588645473 0.4870829963945268 T T T
0.3029201405965533 0.9143320090112578 0.4870105755134554 T T T
0.5576339809137293 0.2012103335020789 0.5069883792872775 T T T
0.5587418605341380 0.5344892220745551 0.5062745644161533 T T T
0.5583989040705616 0.8689472291818492 0.5067861170058968 T T T
0.8154324734976954 0.1531421243247844 0.5274520960545668 T T T
0.8150666010318938 0.4879236725732377 0.5275173129786688 T T T
0.8139630536422412 0.8218624099729462 0.5277913124588236 T T T
0.0715821823875132 0.1068386825108898 0.5487823606467356 T T T
0.0704197330303286 0.4416629668926489 0.5487350144021561 T T T
0.0709251467023824 0.7743997214207147 0.5492150266086497 T T T
0.3265496332958580 0.0615457514739869 0.5692386627871238 T T T
0.3247219516965928 0.3958546481084082 0.5696909292203649 T T T
0.3271326768656708 0.7273617078886334 0.5690537651187741 T T T
0.5823223686829891 0.0149829161673689 0.5900330349254153 T T T
0.5836926438178812 0.3459083116251471 0.5878457664611912 T T T
0.5838344086751458 0.6814038542597373 0.5879385197726834 T T T

0.8403888443184938 0.6342864056057266 0.6101218188483161 T T T
0.8422996022424680 0.2975815912107295 0.6093626159165639 T T T
0.8407838123190378 0.9655371688093825 0.6103127989377228 T T T
0.0929614739983303 0.5887508229235007 0.6344083584549212 T T T
0.0962808905846004 0.2537623928254830 0.6324522345754939 T T T
0.0980048142603122 0.9186596486735031 0.6337486793268543 T T T
0.3484804754765870 0.5383001277353433 0.6510061539109386 T T T
0.3484637479597391 0.2097267133929736 0.6524013152318529 T T T
0.3490645484552260 0.8806657822335112 0.6510512332749405 T T T
0.6047706272506582 0.4958942888574962 0.6681483632147484 T T T
0.6020316366434962 0.1628893196989146 0.6733028347286899 T T T
0.6019037026734610 0.8342126764319283 0.6734591670702712 T T T
0.8631663840095963 0.4496185658932666 0.6904027868214880 T T T
0.8632773280527525 0.1121302230827471 0.6908810314498369 T T T
0.8537069997718286 0.7886766071964514 0.6930081996104370 T T T
0.6327963052411754 0.6325664613212183 0.7496143027204063 T T T
0.6315377653573663 0.3129921352115903 0.7496764685793060 T T T
0.3691005166500665 0.6924616729565920 0.7267671769959455 T T T
0.6316630576614322 0.4735057454937611 0.8080367444905816 T T T
0.6296202841389028 0.4751784538919857 0.8521293375364255 T T T

CO/Cu(533) $E_{ads} = -1.04$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0470819960282036 0.2941066750909430 0.4658278983184444 T T T
0.0470536895965193 0.6276020420408636 0.4658533215975962 T T T
0.0471842838500871 0.9607093576053263 0.4658232395910156 T T T

0.3033378722233013 0.2470523590044985 0.4866806637018888 T T T
0.3035837374794800 0.5806124433608797 0.4867179753570011 T T T
0.3037000916421313 0.9134279787556169 0.4866551104765923 T T T
0.5583495323125205 0.2015194234257006 0.5069044056013273 T T T
0.5581082764163542 0.5349424346483501 0.5070565335474160 T T T
0.5587638999872627 0.8677751706620873 0.5074470084941428 T T T
0.8150375784104347 0.1541178638372663 0.5272774696644175 T T T
0.8146436342563153 0.4875357837788692 0.5273168185077016 T T T
0.8146454733982008 0.8214196470816550 0.5273352211545562 T T T
0.0714067924037417 0.1070901435122782 0.5479644557505963 T T T
0.0710541701727351 0.4408495270931454 0.5479195048058416 T T T
0.0715481235184338 0.7739902936765740 0.5479918777073505 T T T
0.3262649391335732 0.0613279273600964 0.5689153115088107 T T T
0.3262581118692472 0.3946884019823406 0.5688872409498941 T T T
0.3249500609472026 0.7295747120251237 0.5692286947391660 T T T
0.5829732972763141 0.0162781498612892 0.5896252366385674 T T T
0.5833089990784365 0.3475393565845072 0.5889971693164383 T T T
0.5828450123581254 0.6792722061591403 0.5896124786173899 T T T
0.8411338255703003 0.6324164474913796 0.6086176560111327 T T T
0.8414898420109287 0.2981475928657436 0.6089292104414239 T T T
0.8414978882554180 0.9663686487201554 0.6089864983014598 T T T
0.0970805372997571 0.5856728499260073 0.6318756308040593 T T T
0.0978752372943663 0.2519453138959175 0.6320194847600754 T T T
0.0941748021857067 0.9218872599632685 0.6331055245632010 T T T
0.3477881020200213 0.5437641524854298 0.6510043545720205 T T T
0.3500850551946135 0.2081943704147360 0.6518004978893669 T T T
0.3496825755441736 0.8755076440488715 0.6517415070134104 T T T
0.6006010086879877 0.5010653570556397 0.6743065885612829 T T T
0.6005004839023176 0.1652833413721532 0.6742398898760985 T T T
0.6038004685606514 0.8301871423199325 0.6717992301141447 T T T
0.8611958365118952 0.4511452305892352 0.6885744918563279 T T T
0.8576939972705010 0.1188006962888633 0.6908335768951596 T T T
0.8611201570859564 0.7805286570383654 0.6885932653476419 T T T
0.6496433429332125 0.2922464579942097 0.7328095609282607 T T T
0.6185596612871285 0.3178641451310573 0.7762286628805209 T T T

CO/Cu(533) $E_{ads} = -1.03$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F

0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0466809526412291	0.2945268012058949	0.4659595944938325	T	T	T
0.0467516234843042	0.6277479265068047	0.4659347428197436	T	T	T
0.0471063111058203	0.9608462163011673	0.4657697434046067	T	T	T
0.3031105627072736	0.2477222011558962	0.4867968624829654	T	T	T
0.3029186405331151	0.5809242769309706	0.4868851130002965	T	T	T
0.3027560690073898	0.9138462119057842	0.4868604044904394	T	T	T
0.5579482975894131	0.2011777323652921	0.5065018931111631	T	T	T
0.5582786458230558	0.5355401789651606	0.5064436507156380	T	T	T
0.5581630318276489	0.8683067597574712	0.5072642832783572	T	T	T
0.8152748599508902	0.1539161266211463	0.5272200576673121	T	T	T
0.8141853991707493	0.4880779885576890	0.5275910600239093	T	T	T
0.8142978087679996	0.8215511397136143	0.5275446013865446	T	T	T
0.0704943507667997	0.1077909643140938	0.5481708731142779	T	T	T
0.0708690217614363	0.4413505421575714	0.5480658369736967	T	T	T
0.0702057560727818	0.7750173432131241	0.5480938300457642	T	T	T
0.3255126467877694	0.0620269828803510	0.5687172745531320	T	T	T
0.3264517692847601	0.3958048942723762	0.5695426473006657	T	T	T
0.3270130968629729	0.7263254340332367	0.5694231768761727	T	T	T
0.5819716310472428	0.0170476600916714	0.5892835205914474	T	T	T
0.5833934265872207	0.3473966375866130	0.5874559852451898	T	T	T
0.5821429964691182	0.6801144963010938	0.5893691959527539	T	T	T
0.8408756652248125	0.6330037804677834	0.6091515757119675	T	T	T
0.8392580892055669	0.2999370366120834	0.6095667286036975	T	T	T
0.8392352990287936	0.9681318526182557	0.6096138009267277	T	T	T
0.0967155278598325	0.5861849187816771	0.6322000965753271	T	T	T
0.0959671813566217	0.2535502652136508	0.6320831075847703	T	T	T
0.0979215679661580	0.9185565416702832	0.6316871318056926	T	T	T
0.3474276371532271	0.5437202018392671	0.6536583019925661	T	T	T
0.3491299800588206	0.2068928463339240	0.6513161475612580	T	T	T
0.3491414215661565	0.8781117640314831	0.6513480887688876	T	T	T
0.6033965125316800	0.4984847285516426	0.6741328078122969	T	T	T
0.6030864325785582	0.1631849492085277	0.6741189862779325	T	T	T
0.6039586179543517	0.8302659084814504	0.6716730635325877	T	T	T
0.8585777383156906	0.4518929550895681	0.6893968774158555	T	T	T
0.8644689213663124	0.1130552945011380	0.6892519720075393	T	T	T
0.8587388374220315	0.7841489589493986	0.6893682521593463	T	T	T
0.4775648811694769	0.4360371488044849	0.7196605539526441	T	T	T
0.4362890078696710	0.4703432658950320	0.7622042028592836	T	T	T

CO/Defected-Cu(533) $E_{ads} = -1.03$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O

59 1 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0466516536046275 0.2945239193697156 0.4660812939126077 T T T
0.0464761082272373 0.6275982621553285 0.4659607534434799 T T T
0.0469700153284874 0.9610942207568841 0.4657935936590570 T T T
0.3029841328402516 0.2479337884705274 0.4869583873821635 T T T
0.3032619545390126 0.5803507083862256 0.4867441492113515 T T T
0.3024447919943093 0.9142233039076967 0.4868071065927704 T T T
0.5585983583756956 0.2006551984695335 0.5063500259314705 T T T
0.5587507050423653 0.5352052923898731 0.5063702578249588 T T T
0.5580653555133563 0.8679333457982616 0.5073542988536339 T T T
0.8159941790625957 0.1535325021514037 0.5272567861569256 T T T
0.8148388581261856 0.4875939782064014 0.5275842980096943 T T T
0.8146493707841451 0.8208891670928571 0.5275965938467788 T T T
0.0703137922587508 0.1082318914143867 0.5485083242770959 T T T
0.0705540239996030 0.4411507320043893 0.5484587121407343 T T T
0.0710529618791405 0.7741476756378476 0.5478086009843159 T T T
0.3254523253685998 0.0619427704690506 0.5687988150658022 T T T
0.3276195131833113 0.3949160048689126 0.5695273760188215 T T T
0.3278154332905042 0.7255097866874907 0.5691811460991920 T T T
0.5828325068605285 0.0161920838398580 0.5890762923801949 T T T
0.5845331118971053 0.3463012566183560 0.5871622811016382 T T T
0.5841211821674765 0.6781115566900140 0.5894037053407986 T T T
0.8411595402909537 0.6289310317841077 0.6104522625861001 T T T
0.8400165221113881 0.3031028837281206 0.6109760852183018 T T T
0.8403037918408564 0.9669835444005332 0.6093470409876551 T T T
0.0971251162839125 0.5848453696946568 0.6318576379526522 T T T
0.0930145196325748 0.2556259568327098 0.6329871645110383 T T T
0.0979473337661968 0.9192046950137539 0.6312807694823760 T T T
0.3471977225554237 0.5437871977617590 0.6538257385016695 T T T
0.3489092903039662 0.2069284267118883 0.6512823186221965 T T T
0.3493023622342547 0.8774212510467725 0.6511852446296563 T T T
0.6067352775366875 0.4963533693819434 0.6720754269033385 T T T

0.6033614625650388 0.1622038482207545 0.6739673105899959 T T T
0.6060775706982875 0.8270541029980603 0.6702124399390914 T T T
0.8641685530012441 0.1110801159666229 0.6882182653551847 T T T
0.8587080984809362 0.7839337835640112 0.6882645473719707 T T T
0.4837938779097409 0.4357399126446910 0.7193452847549321 T T T
0.4446096904794785 0.4704849475244060 0.7621010813712707 T T T

CO/Cu(533) $E_{ads} = -1.03$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0467953869881879 0.2941571132913806 0.4658898599511858 T T T
0.0471280352483066 0.6275892388960751 0.4659944614454682 T T T
0.0470328843671051 0.9610053233232977 0.4658885558928079 T T T
0.3033864388726882 0.2468531252194128 0.4866924873474961 T T T
0.3027254602681418 0.5811884490645659 0.4868449294811922 T T T
0.3034771385415408 0.9138305078320769 0.4871374492666681 T T T
0.5583579109433274 0.2016013929067732 0.5066601925367543 T T T
0.5580859223273196 0.5347125547420043 0.5067071432562784 T T T
0.5582057960772225 0.8682363220069246 0.5068079646612695 T T T
0.8147754935644468 0.1544721282310989 0.5274745518696293 T T T
0.8149643949271735 0.4873799093356278 0.5274208661475436 T T T
0.8151235045661660 0.8206558800990913 0.5274426533164982 T T T
0.0717418626281345 0.1067722699611717 0.5480570720541315 T T T
0.0714552960386050 0.4402795428463493 0.5479768983979962 T T T
0.0699981056532928 0.7757504628469795 0.5483281604643022 T T T
0.3264318298844829 0.0629808336157106 0.5697381061268176 T T T
0.3263435715097921 0.3948383459118158 0.5690391762956003 T T T

0.3264381681229612	0.7263745552120668	0.5697258340915872	T	T	T
0.5821916453371381	0.0157828924568721	0.5885302371099234	T	T	T
0.5822255443129074	0.3477105766755013	0.5886710667957782	T	T	T
0.5826776792271369	0.6809917163048617	0.5883622570490568	T	T	T
0.8414936547562293	0.6319954678215581	0.6090676458389516	T	T	T
0.8424507548174973	0.2979154076824593	0.6091589203098872	T	T	T
0.8381952762802578	0.9684494316704040	0.6097195878680871	T	T	T
0.0955047692033741	0.5876283410916686	0.6314339901339145	T	T	T
0.0979390906216522	0.2518782322487104	0.6321686800763894	T	T	T
0.0973712588356828	0.9194065768624328	0.6322971899256631	T	T	T
0.3482817277223875	0.5448965470112597	0.6541367024130067	T	T	T
0.3485205490480224	0.2082255126319176	0.6540273768701937	T	T	T
0.3514327990548484	0.8737396967564646	0.6518736380293683	T	T	T
0.6071427252082358	0.4960920986772348	0.6710598639749087	T	T	T
0.6030983914440000	0.1642983535452243	0.6745252265395019	T	T	T
0.6067491750741236	0.8257173308486663	0.6709584103096972	T	T	T
0.8613926468260041	0.4490382920385805	0.6895063329935489	T	T	T
0.8593409778698853	0.1172367442518169	0.6895140946795945	T	T	T
0.8589593001160416	0.7841542297591252	0.6893726957837623	T	T	T
0.3908614506141505	0.3406604276157625	0.7129704836098600	T	T	T
0.3503000931184860	0.3743560298515072	0.7556007345107463	T	T	T

CO/Cu(533) $E_{ads} = -0.91$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 1
Selective dynamics
Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0465569672417936	0.2950573340615975	0.4660844848145770	T	T	T
0.0465262116924080	0.6279981710695425	0.4662630310802671	T	T	T

0.0463073453415954 0.9609965649478319 0.4660911405603467 T T T
0.3025065055184916 0.2470788634418254 0.4864509227076605 T T T
0.3026180944966289 0.5819880415706218 0.4864223860098831 T T T
0.3027886788971466 0.9143340832204643 0.4870294438160208 T T T
0.5582488533926514 0.2016316528213038 0.5065409323495308 T T T
0.5576096726574702 0.5353274012904299 0.5068326582007412 T T T
0.5578624508261396 0.8684626692040383 0.5067928788304186 T T T
0.8138898395007842 0.1548382782407223 0.5275596044295997 T T T
0.8143771312664621 0.4883609179650552 0.5273974769671597 T T T
0.8134986742079435 0.8219333862204730 0.5275351075956165 T T T
0.0702992472365289 0.1079968677291022 0.5477118332584194 T T T
0.0710100377896260 0.4421568118761845 0.5488846771844125 T T T
0.0711125522836278 0.7731570945236209 0.5487959383911752 T T T
0.3245693230847461 0.0640561231772314 0.5693370338116760 T T T
0.3251673100092018 0.3960463152712880 0.5677384478258043 T T T
0.3249231184859853 0.7280914003876408 0.5693494248510323 T T T
0.5796543561100387 0.0176372831098614 0.5887626163891534 T T T
0.5802200981628227 0.3492538940980011 0.5887921975627641 T T T
0.5816538609640802 0.6822533266809457 0.5885517281194119 T T T
0.8407283309366722 0.6333643173058632 0.6092971461262474 T T T
0.8400505314045006 0.3000322419268963 0.6089698907930472 T T T
0.8411920797907244 0.9650128267022471 0.6092799751512608 T T T
0.0951764900602074 0.5877892412343014 0.6355205918321936 T T T
0.0951711416256585 0.2520424363954758 0.6318298928013890 T T T
0.0952615142106629 0.9229721264673686 0.6317333747255394 T T T
0.3498663610411714 0.5445745831882323 0.6533175887486450 T T T
0.3497431829662380 0.2064999625868007 0.6534161024058375 T T T
0.3496611534761433 0.8752722253467846 0.6515813694760920 T T T
0.6035399581597477 0.4975002576033973 0.6716400296802363 T T T
0.6048814626454678 0.1636516985254239 0.6714943081923122 T T T
0.6019455946456861 0.8308525452867795 0.6715657847347610 T T T
0.8560001596093652 0.4531264763593484 0.6891746262041810 T T T
0.8575757808287421 0.1192460358820810 0.6892600425244151 T T T
0.8508662351592323 0.7905314791886432 0.6899662411148478 T T T
0.2413910024311482 0.4663083647893105 0.7010710638745681 T T T
0.2129890938253402 0.4899675866565455 0.7446958271113550 T T T

CO/Cu(533) $E_{ads} = -0.89$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F

0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0467713776318094	0.2942447446742747	0.4659090965811215	T	T	T
0.0467063030776685	0.6277847274319407	0.4660826317122213	T	T	T
0.0466908222170526	0.9613038946416822	0.4658848586706306	T	T	T
0.3029994421993910	0.2473287426635766	0.4866199701642972	T	T	T
0.3027794853241069	0.5811907563168937	0.4867719113088457	T	T	T
0.3030287154865893	0.9140346924756386	0.4867199248397422	T	T	T
0.5582690250280067	0.2024271751049558	0.5070688736079428	T	T	T
0.5579405575684686	0.5350668785455375	0.5069207106030026	T	T	T
0.5581933408342603	0.8672224765559065	0.5071179039810189	T	T	T
0.8141917666127951	0.1549254932910125	0.5274101401155021	T	T	T
0.8142119546648651	0.4879482397344540	0.5274250830037807	T	T	T
0.8141934213255104	0.8215598223999788	0.5275327996838299	T	T	T
0.0700103735368009	0.1083607167878555	0.5481835108191501	T	T	T
0.0702528650735969	0.4411975636115039	0.5481848836404813	T	T	T
0.0703042901893580	0.7752554511442920	0.5482222098754234	T	T	T
0.3253463721823262	0.0619694102721154	0.5687299231082679	T	T	T
0.3252881615592249	0.3956307996929447	0.5687306661146907	T	T	T
0.3257256064071296	0.7287357577880683	0.5689853951636852	T	T	T
0.5817450366382777	0.0152775092373454	0.5883323178550420	T	T	T
0.5824983996451193	0.3500531512618229	0.5897891783406186	T	T	T
0.5824973538077316	0.6793381302756724	0.5898010592479107	T	T	T
0.8405384332858483	0.6323128939919752	0.6091564016742333	T	T	T
0.8399276233516610	0.3000691391898205	0.6094736891412225	T	T	T
0.8405837328473545	0.9667810363938164	0.6091815361068429	T	T	T
0.0963998351241939	0.5863152141402027	0.6322446679297686	T	T	T
0.0968311794397362	0.2526962851422776	0.6320799713496766	T	T	T
0.0968869054238471	0.9196042247305437	0.6320477977861257	T	T	T
0.3486269542455122	0.5420472190542056	0.6512803692746573	T	T	T
0.3493839428391118	0.2088552097203633	0.6514159502956381	T	T	T
0.3488680711804889	0.8767815518919576	0.6513213151720895	T	T	T
0.6013761262087440	0.4989146682400932	0.6754121355438605	T	T	T
0.6036680624996920	0.1610459268290098	0.6711078400295006	T	T	T
0.6039276530067674	0.8327894771630033	0.6711068471812927	T	T	T
0.8627281133251340	0.4502102033652412	0.6892922982869417	T	T	T
0.8627297662105224	0.1121023563590320	0.6892706819379641	T	T	T
0.8590858385333668	0.7842726321790878	0.6893397158603556	T	T	T
0.6045398402189761	0.4962785409358053	0.7452935599109631	T	T	T
0.6004476638976209	0.4996782448048933	0.7888453374237534	T	T	T

CO/Cu(533) E_{ads} = −0.87 eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O
60 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0464852119953693 0.2945371153728722 0.4657869338434810 T T T
0.0464062331966626 0.6280850645373819 0.4660193198246095 T T T
0.0466030103239317 0.9613121109063691 0.4659802736960874 T T T
0.3029804483792454 0.2483645840064732 0.4868515762395215 T T T
0.3027918014321271 0.5809636554437739 0.4868061552305711 T T T
0.3029635382759734 0.9132349425413061 0.4869159376709075 T T T
0.5576157682731598 0.2020414058840984 0.5067438806230958 T T T
0.5576020516582112 0.5352988366596158 0.5067187716274247 T T T
0.5576600997081710 0.8686158804925049 0.5069118825076168 T T T
0.8137030141041097 0.1550371740702539 0.5275964147283910 T T T
0.8140859949544182 0.4879849611920263 0.5275290067367308 T T T
0.8140263002000917 0.8218396525626576 0.5275564847016160 T T T
0.0705732771334273 0.1079374909397971 0.5479104906647216 T T T
0.0707958561766884 0.4409941510178896 0.5479166944011115 T T T
0.0706803336946977 0.7746831524968593 0.5481476783759820 T T T
0.3250116504841641 0.0623800659119882 0.5684991721199428 T T T
0.3255539389050979 0.3973598543731461 0.5700389404758017 T T T
0.3257577233832932 0.7267341166430961 0.5699825249466129 T T T
0.5815821479060620 0.0158322690970696 0.5887049477802515 T T T
0.5807519667466736 0.3494687735451775 0.5888781431679662 T T T
0.5814884803561665 0.6816881751813094 0.5887180624244124 T T T
0.8408561947466358 0.6325105566256486 0.6091131645323247 T T T
0.8409050644902519 0.2993210553744119 0.6091854090961213 T T T
0.8407582423213484 0.9660683934912166 0.6092069981710474 T T T
0.0954621743279854 0.5865191189604718 0.6319416297667623 T T T
0.0964203789245511 0.2532525185447253 0.6320808253497382 T T T
0.0958152250186136 0.9213179014285302 0.6318342545200616 T T T
0.3482335934725947 0.5432330267676552 0.6552573965475593 T T T
0.3503976007169330 0.2052816156286051 0.6511671739996892 T T T
0.3503474277413691 0.8775554829143651 0.6512466066215180 T T T

0.6066436128150503 0.4969761263809800 0.6715458323613022 T T T
0.6065080875882100 0.1590799829097550 0.6714590507915904 T T T
0.6044526543488455 0.8295276610478620 0.6717830761497418 T T T
0.8597147834707022 0.4505954325065254 0.6895843359974192 T T T
0.8590326444976550 0.1174525066334107 0.6893730670608175 T T T
0.8588492280234857 0.7838726721742738 0.6895651076057995 T T T
0.3525171768886396 0.5396870995431913 0.7251809489947586 T T T
0.3480980780577284 0.5432805111945849 0.7687099116857991 T T T

CO/Cu(533) E_{ads} = −0.80 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0465743597892429 0.2955224088726056 0.4661321308661128 T T T
0.0465063853092952 0.6279666964656598 0.4663683287890929 T T T
0.0467850301523011 0.9602132154020576 0.4661587585302578 T T T
0.3020863315355272 0.2485077463675556 0.4869920987542991 T T T
0.3023774148375586 0.5808007094915083 0.4868814599414700 T T T
0.3029027957875609 0.9146169185219051 0.4864551028074559 T T T
0.5570808449081622 0.2023526928555220 0.5069800890772639 T T T
0.5576243872867833 0.5352473838693765 0.5064248577325432 T T T
0.5579671409732807 0.8685207938986271 0.5066525714872778 T T T
0.8144582136935856 0.1546340428962822 0.5271405203005202 T T T
0.8141860660856056 0.4881349188689318 0.5271857486164870 T T T
0.8144435133069294 0.8211730819383227 0.5272408623768096 T T T
0.0701115220812068 0.1088497024011148 0.5474966323475791 T T T
0.0703459927189922 0.4431400415362233 0.5496184927267660 T T T
0.0703466021768006 0.7728876312945713 0.5494622056410989 T T T

0.3255119492811572 0.0619147066593159 0.5687015634089101 T T T
0.3236772202580633 0.3970513609292489 0.5699076199604831 T T T
0.3244223266859729 0.7299716333329441 0.5683904989850931 T T T
0.5825321308590026 0.0144340590583582 0.5884116348554357 T T T
0.5819368269075632 0.3489650490650484 0.5882845269877508 T T T
0.5817432585817466 0.6814991932929060 0.5883329509974279 T T T
0.8400393340752651 0.6335398034620489 0.6087744094292733 T T T
0.8410931299361288 0.2992273279964441 0.6087821625051104 T T T
0.8402357629000964 0.9660235975646102 0.6086484077430321 T T T
0.1012920718962988 0.5826329774869441 0.6383192017732329 T T T
0.0972460944209658 0.2503961541075368 0.6317143497852334 T T T
0.0974700911586442 0.9210526942697672 0.6314286133116126 T T T
0.3543407021672980 0.5407484431400180 0.6510850208946032 T T T
0.3537339593701121 0.2025360724786207 0.6510395320126273 T T T
0.3514505751931294 0.8742736546141388 0.6512582186076574 T T T
0.6034858679717154 0.4975877444064472 0.6717133705235472 T T T
0.6056150125207662 0.1612741716243538 0.6713864313971587 T T T
0.6053166733486983 0.8295631874920648 0.6716555327072270 T T T
0.8566558192309569 0.4511578772771507 0.6889899804647405 T T T
0.8568623363088492 0.1211928697963060 0.6888467864280743 T T T
0.8560020593277683 0.7865663412413583 0.6916742801727426 T T T
0.0799566459841395 0.6004335119212520 0.7153547378707779 T T T
0.1512938351358354 0.5411196845339551 0.7534630086863958 T T T

CO/Cu(111) $E_{ads} = -1.11$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
3.8289832201000000 6.6319934786000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu C O
45 1 1
Selective dynamics
Direct
0.8888888887999968 0.2222222223999992 0.3170124957488483 F F F
0.2222222221000010 0.2222222223999992 0.3170124957488483 F F F
0.5555555553999980 0.2222222223999992 0.3170124957488483 F F F
0.8888888890000004 0.5555555553000033 0.3170124957488483 F F F
0.2222222222999974 0.5555555553000033 0.3170124957488483 F F F
0.5555555556000016 0.5555555553000033 0.3170124957488483 F F F
0.8888888891999969 0.8888888882000003 0.3170124957488483 F F F
0.2222222225000010 0.8888888882000003 0.3170124957488483 F F F
0.5555555557999980 0.8888888882000003 0.3170124957488483 F F F
0.0000000000000000 0.0000000000000000 0.3975777759823913 F F F
0.3333333332999970 0.0000000000000000 0.3975777759823913 F F F
0.6666666666000012 0.0000000000000000 0.3975777759823913 F F F
0.0000000002103135 0.3333333328999970 0.3975777759823913 F F F
0.3333333335000006 0.3333333328999970 0.3975777759823913 F F F
0.6666666668999994 0.3333333328999970 0.3975777759823913 F F F
0.9999999996666986 0.6666666672999995 0.3975777759823913 F F F
0.3333333329999988 0.6666666672999995 0.3975777759823913 F F F
0.6666666663000029 0.6666666672999995 0.3975777759823913 F F F
0.1111111113999996 0.1111111104999978 0.4771948603999974 F F F
0.4444444447999985 0.1111111104999978 0.4771948603999974 F F F
0.7777777781000026 0.1111111104999978 0.4771948603999974 F F F
0.1111111108999978 0.4444444449000002 0.4771948603999974 F F F
0.4444444442000020 0.4444444449000002 0.4771948603999974 F F F
0.7777777774999990 0.4444444449000002 0.4771948603999974 F F F

0.1111111111000014 0.7777777777999972 0.4771948603999974 F F F
0.4444444443999984 0.7777777777999972 0.4771948603999974 F F F
0.7777777777000026 0.7777777777999972 0.4771948603999974 F F F
0.8870258980062218 0.2231537177968832 0.5574931466075981 T T T
0.2231537174968850 0.2231537177968832 0.5574931466075981 T T T
0.5551927031354680 0.2229479269290664 0.5567059017021876 T T T
0.8892371814866777 0.5548589703266558 0.5567008128493214 T T T
0.2229479268290646 0.5551927030354733 0.5567059017021876 T T T
0.5551927033354715 0.5551927030354733 0.5567059017021876 T T T
0.8892371816866742 0.8892371806866777 0.5567008128493214 T T T
0.2231537178968850 0.8870258974062253 0.5574931466075981 T T T
0.5548589708266505 0.8892371806866777 0.5567008128493214 T T T
0.9998173143910591 0.9998173143910591 0.6376297616796833 T T T
0.3336987045178716 0.9998173143910591 0.6376297616796833 T T T
0.6678881966674908 0.9975569398650137 0.6369564603924118 T T T
0.9998173146013727 0.3336987041178716 0.6376297616796833 T T T
0.3326938163951567 0.3326938157951531 0.6398447543094079 T T T
0.6679457011096801 0.3326938157951531 0.6398447543094079 T T T
0.9975569395317123 0.6678881973674891 0.6369564603924118 T T T
0.3326938158951549 0.6679457015096801 0.6398447543094079 T T T
0.6678881963674925 0.6678881973674891 0.6369564603924118 T T T
0.4444444444444429 0.4444444444444429 0.6953350340513325 T T T
0.4444444444444429 0.4444444444444429 0.7415113112971099 T T T

CO/Cu(111) $E_{ads} = -1.10$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
3.8289832201000000 6.6319934786000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu C O
45 1 1
Selective dynamics
Direct
0.8888888887999968 0.2222222223999992 0.3170124957488483 F F F
0.2222222221000010 0.2222222223999992 0.3170124957488483 F F F
0.5555555553999980 0.2222222223999992 0.3170124957488483 F F F
0.8888888890000004 0.5555555553000033 0.3170124957488483 F F F
0.2222222222999974 0.5555555553000033 0.3170124957488483 F F F
0.5555555556000016 0.5555555553000033 0.3170124957488483 F F F
0.8888888891999969 0.8888888882000003 0.3170124957488483 F F F
0.2222222225000010 0.8888888882000003 0.3170124957488483 F F F
0.5555555557999980 0.8888888882000003 0.3170124957488483 F F F
0.0000000000000000 0.0000000000000000 0.3975777759823913 F F F
0.3333333332999970 0.0000000000000000 0.3975777759823913 F F F
0.6666666666000012 0.0000000000000000 0.3975777759823913 F F F
0.0000000002103135 0.3333333328999970 0.3975777759823913 F F F
0.3333333335000006 0.3333333328999970 0.3975777759823913 F F F
0.6666666668999994 0.3333333328999970 0.3975777759823913 F F F
0.9999999996666986 0.6666666672999995 0.3975777759823913 F F F
0.3333333329999988 0.6666666672999995 0.3975777759823913 F F F
0.6666666663000029 0.6666666672999995 0.3975777759823913 F F F
0.1111111113999996 0.1111111104999978 0.4771948603999974 F F F
0.4444444447999985 0.1111111104999978 0.4771948603999974 F F F
0.7777777781000026 0.1111111104999978 0.4771948603999974 F F F
0.1111111108999978 0.4444444449000002 0.4771948603999974 F F F
0.4444444442000020 0.4444444449000002 0.4771948603999974 F F F
0.7777777774999990 0.4444444449000002 0.4771948603999974 F F F

0.1111111111000014 0.7777777777999972 0.4771948603999974 F F F
0.4444444443999984 0.7777777777999972 0.4771948603999974 F F F
0.7777777777000026 0.7777777777999972 0.4771948603999974 F F F
0.8871761608489166 0.2234116708148264 0.5574627538837547 T T T
0.2222222221000010 0.2222222223999992 0.5566809782375515 T T T
0.5560788349362511 0.2234116708148264 0.5574627538837547 T T T
0.8871761610489202 0.5560788348362564 0.5574627538837547 T T T
0.2234116707148246 0.5560788348362564 0.5574627538837547 T T T
0.5555555556000016 0.5555555553000033 0.5556381134534192 T T T
0.8888888891999969 0.8888888882000003 0.5569838371554852 T T T
0.2234116709148282 0.8871761602489201 0.5574627538837547 T T T
0.5560788353362511 0.8871761602489201 0.5574627538837547 T T T
0.0000544849085813 0.0000544849085813 0.6378019649751181 T T T
0.3320415506314731 0.0025835653370407 0.6374572658988740 T T T
0.6665576967828315 0.0000544849085813 0.6378019649751181 T T T
0.0025835655473543 0.3320415502314731 0.6374572658988740 T T T
0.3320415508314767 0.3320415502314731 0.6374572658988740 T T T
0.6673725973583728 0.3319214719832502 0.6399482217801378 T T T
0.0000544845752799 0.6665576974828298 0.6378019649751181 T T T
0.3319214720832520 0.6673725977583729 0.6399482217801378 T T T
0.6673725967583763 0.6673725977583729 0.6399482217801378 T T T
0.5555555555555571 0.5555555555555571 0.6954670751186285 T T T
0.5555555555555571 0.5555555555555571 0.7416341755240907 T T T

CO/Cu(111) $E_{ads} = -1.07$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
3.8289832201000000 6.6319934786000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu C O
45 1 1
Selective dynamics
Direct
0.8888888887999968 0.2222222223999992 0.3170124957488483 F F F
0.2222222221000010 0.2222222223999992 0.3170124957488483 F F F
0.5555555553999980 0.2222222223999992 0.3170124957488483 F F F
0.8888888890000004 0.5555555553000033 0.3170124957488483 F F F
0.2222222222999974 0.5555555553000033 0.3170124957488483 F F F
0.5555555556000016 0.5555555553000033 0.3170124957488483 F F F
0.8888888891999969 0.8888888882000003 0.3170124957488483 F F F
0.2222222225000010 0.8888888882000003 0.3170124957488483 F F F
0.5555555557999980 0.8888888882000003 0.3170124957488483 F F F
0.0000000000000000 0.0000000000000000 0.3975777759823913 F F F
0.3333333332999970 0.0000000000000000 0.3975777759823913 F F F
0.6666666666000012 0.0000000000000000 0.3975777759823913 F F F
0.0000000002103135 0.3333333328999970 0.3975777759823913 F F F
0.3333333335000006 0.3333333328999970 0.3975777759823913 F F F
0.6666666668999994 0.3333333328999970 0.3975777759823913 F F F
0.9999999996666986 0.6666666672999995 0.3975777759823913 F F F
0.3333333329999988 0.6666666672999995 0.3975777759823913 F F F
0.6666666663000029 0.6666666672999995 0.3975777759823913 F F F
0.1111111113999996 0.1111111104999978 0.4771948603999974 F F F
0.4444444447999985 0.1111111104999978 0.4771948603999974 F F F
0.7777777781000026 0.1111111104999978 0.4771948603999974 F F F
0.1111111108999978 0.4444444449000002 0.4771948603999974 F F F
0.4444444442000020 0.4444444449000002 0.4771948603999974 F F F
0.7777777774999990 0.4444444449000002 0.4771948603999974 F F F

0.1111111111000014 0.7777777777999972 0.4771948603999974 F F F
0.4444444443999984 0.7777777777999972 0.4771948603999974 F F F
0.7777777777000026 0.7777777777999972 0.4771948603999974 F F F
0.8870854900150462 0.2230031535707653 0.5575099459823676 T T T
0.2232446897141855 0.2230031535707653 0.5575099459823676 T T T
0.5555384002230639 0.2222565327538746 0.5558509981933355 T T T
0.8890772801195581 0.5551787730608808 0.5569103137090821 T T T
0.2232825221487857 0.5544698920205775 0.5571837595378426 T T T
0.5555809190306462 0.5544698920205775 0.5571837595378426 T T T
0.8884278620723265 0.8896022795750369 0.5570579401519566 T T T
0.2224574938761990 0.8884183454476045 0.5569192503873026 T T T
0.5553031915526248 0.8896022795750369 0.5570579401519566 T T T
0.0007247860339845 0.9990931022148501 0.6376847546882232 T T T
0.3335154450511695 0.9990931022148501 0.6376847546882232 T T T
0.6692106951578580 0.9949119428842863 0.6375449587832875 T T T
0.0001638186030135 0.3330056961145971 0.6378350191908311 T T T
0.3324183758888637 0.3323275346107124 0.6394636701219909 T T T
0.6685874228004351 0.3323275346107124 0.6394636701219909 T T T
0.9999498975054166 0.6664232160775398 0.6375707843745602 T T T
0.3314205025574068 0.6704923281851976 0.6379110988044374 T T T
0.6669602196837445 0.6664232160775398 0.6375707843745602 T T T
0.4990057014796960 0.3353219270406100 0.6983513492419036 T T T
0.4993990858412474 0.3345351583175074 0.7442589918901987 T T T

CO/Cu(111) $E_{ads} = -0.99$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
3.8289832201000000 6.6319934786000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu C O
45 1 1
Selective dynamics
Direct
0.8888888887999968 0.2222222223999992 0.3170124957488483 F F F
0.2222222221000010 0.2222222223999992 0.3170124957488483 F F F
0.5555555553999980 0.2222222223999992 0.3170124957488483 F F F
0.8888888890000004 0.5555555553000033 0.3170124957488483 F F F
0.2222222222999974 0.5555555553000033 0.3170124957488483 F F F
0.5555555556000016 0.5555555553000033 0.3170124957488483 F F F
0.8888888891999969 0.8888888882000003 0.3170124957488483 F F F
0.2222222225000010 0.8888888882000003 0.3170124957488483 F F F
0.5555555557999980 0.8888888882000003 0.3170124957488483 F F F
0.0000000000000000 0.0000000000000000 0.3975777759823913 F F F
0.3333333332999970 0.0000000000000000 0.3975777759823913 F F F
0.6666666666000012 0.0000000000000000 0.3975777759823913 F F F
0.0000000002103135 0.3333333328999970 0.3975777759823913 F F F
0.3333333335000006 0.3333333328999970 0.3975777759823913 F F F
0.6666666668999994 0.3333333328999970 0.3975777759823913 F F F
0.9999999996666986 0.6666666672999995 0.3975777759823913 F F F
0.3333333329999988 0.6666666672999995 0.3975777759823913 F F F
0.6666666663000029 0.6666666672999995 0.3975777759823913 F F F
0.1111111113999996 0.1111111104999978 0.4771948603999974 F F F
0.4444444447999985 0.1111111104999978 0.4771948603999974 F F F
0.7777777781000026 0.1111111104999978 0.4771948603999974 F F F
0.1111111108999978 0.4444444449000002 0.4771948603999974 F F F
0.4444444442000020 0.4444444449000002 0.4771948603999974 F F F
0.7777777774999990 0.4444444449000002 0.4771948603999974 F F F

0.1111111111000014	0.7777777777999972	0.4771948603999974	F	F	F
0.4444444443999984	0.7777777777999972	0.4771948603999974	F	F	F
0.7777777777000026	0.7777777777999972	0.4771948603999974	F	F	F
0.8889727392727309	0.2220545214545311	0.5565109928925480	T	T	T
0.2233725188191897	0.2233725191191880	0.5575607298317209	T	T	T
0.5532549619616205	0.2233725191191880	0.5575607298317209	T	T	T
0.8895149415990105	0.5552425290004948	0.5568523026560186	T	T	T
0.2233725190191862	0.5532549618616258	0.5575607298317209	T	T	T
0.5552425293004930	0.5552425290004948	0.5568523026560186	T	T	T
0.8889727396727309	0.8889727386727344	0.5565109928925480	T	T	T
0.2220545215545329	0.8889727386727344	0.5565109928925480	T	T	T
0.5552425295004895	0.8895149407990104	0.5568523026560186	T	T	T
0.0000000000000000	0.0000000000000000	0.6373957062547717	T	T	T
0.3335455580066622	0.9970279833643261	0.6370596557402095	T	T	T
0.6694264585290099	0.9970279833643261	0.6370596557402095	T	T	T
0.9970279835746396	0.3335455576066622	0.6370596557402095	T	T	T
0.3333333335000006	0.3333333328999970	0.6412620483721980	T	T	T
0.6694264588290082	0.3335455576066622	0.6370596557402095	T	T	T
0.9970279830310247	0.6694264592290082	0.6370596557402095	T	T	T
0.3335455577066639	0.6694264592290082	0.6370596557402095	T	T	T
0.6666666663000029	0.6666666672999995	0.6376258235497190	T	T	T
0.3333333350000061	0.3333333328999970	0.7137656164547437	T	T	T
0.3333333350000061	0.3333333328999970	0.7589229414001153	T	T	T

CO/Cu(100) $E_{ads} = -1.08$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu C O
45 1 1
Selective dynamics
Direct

0.0000000000000000	0.0000000000000000	0.3173193249345303	F	F	F
0.3333333332999970	0.0000000000000000	0.3173193249345303	F	F	F
0.6666666666000012	0.0000000000000000	0.3173193249345303	F	F	F
0.0000000000000000	0.3333333332999970	0.3173193249345303	F	F	F
0.3333333332999970	0.3333333332999970	0.3173193249345303	F	F	F
0.6666666666000012	0.3333333332999970	0.3173193249345303	F	F	F
0.0000000000000000	0.6666666666000012	0.3173193249345303	F	F	F
0.3333333332999970	0.6666666666000012	0.3173193249345303	F	F	F
0.6666666666000012	0.6666666666000012	0.3173193249345303	F	F	F
0.1666666667000030	0.1666666667000030	0.3854655552433357	F	F	F
0.5000000000000000	0.1666666667000030	0.3854655552433357	F	F	F
0.8333333332999970	0.1666666667000030	0.3854655552433357	F	F	F
0.1666666667000030	0.5000000000000000	0.3854655552433357	F	F	F
0.5000000000000000	0.5000000000000000	0.3854655552433357	F	F	F
0.8333333332999970	0.5000000000000000	0.3854655552433357	F	F	F
0.1666666667000030	0.8333333332999970	0.3854655552433357	F	F	F
0.5000000000000000	0.8333333332999970	0.3854655552433357	F	F	F
0.8333333332999970	0.8333333332999970	0.3854655552433357	F	F	F
0.0000000000000000	0.0000000000000000	0.4552941175999976	F	F	F
0.3333333332999970	0.0000000000000000	0.4552941175999976	F	F	F
0.6666666666000012	0.0000000000000000	0.4552941175999976	F	F	F
0.0000000000000000	0.3333333332999970	0.4552941175999976	F	F	F
0.3333333332999970	0.3333333332999970	0.4552941175999976	F	F	F
0.6666666666000012	0.3333333332999970	0.4552941175999976	F	F	F

0.0000000000000000	0.6666666666000012	0.4552941175999976	F	F	F
0.3333333332999970	0.6666666666000012	0.4552941175999976	F	F	F
0.6666666666000012	0.6666666666000012	0.4552941175999976	F	F	F
0.1680965627013933	0.1687100608461307	0.5258202047512341	T	T	T
0.5000000000000000	0.1667291307506460	0.5240322941718674	T	T	T
0.8319034372986067	0.1687100608461307	0.5258202047512341	T	T	T
0.1680965627013933	0.4979566058538722	0.5258202047512341	T	T	T
0.5000000000000000	0.4999375359493570	0.5240322941718674	T	T	T
0.8319034372986067	0.4979566058538722	0.5258202047512341	T	T	T
0.1654762773706722	0.8333333332999970	0.5248570982119034	T	T	T
0.5000000000000000	0.8333333332999970	0.5248920801798747	T	T	T
0.8345237226293278	0.8333333332999970	0.5248570982119034	T	T	T
0.0000000000000000	0.0003761603130172	0.5934171081716784	T	T	T
0.3325838343389620	0.9980963938622907	0.5926015926034864	T	T	T
0.6674161655610362	0.9980963938622907	0.5926015926034864	T	T	T
0.0000000000000000	0.3333333332999970	0.5939179369702856	T	T	T
0.3345782245720130	0.3333333332999970	0.5969907060223036	T	T	T
0.6654217753279852	0.3333333332999970	0.5969907060223036	T	T	T
0.0000000000000000	0.6662905062869839	0.5934171081716784	T	T	T
0.3325838343389620	0.6685702727377105	0.5926015926034864	T	T	T
0.6674161655610362	0.6685702727377105	0.5926015926034864	T	T	T
0.5000000000000000	0.3333333332999970	0.6567152515209855	T	T	T
0.5000000000000000	0.3333333332999970	0.7024993080954829	T	T	T

CO/Cu(100) $E_{ads} = -1.07$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu C O
45 1 1
Selective dynamics
Direct

0.0000000000000000	0.0000000000000000	0.3173193249345303	F	F	F
0.3333333332999970	0.0000000000000000	0.3173193249345303	F	F	F
0.6666666666000012	0.0000000000000000	0.3173193249345303	F	F	F
0.0000000000000000	0.3333333332999970	0.3173193249345303	F	F	F
0.3333333332999970	0.3333333332999970	0.3173193249345303	F	F	F
0.6666666666000012	0.3333333332999970	0.3173193249345303	F	F	F
0.0000000000000000	0.6666666666000012	0.3173193249345303	F	F	F
0.3333333332999970	0.6666666666000012	0.3173193249345303	F	F	F
0.6666666666000012	0.6666666666000012	0.3173193249345303	F	F	F
0.1666666667000030	0.1666666667000030	0.3854655552433357	F	F	F
0.5000000000000000	0.1666666667000030	0.3854655552433357	F	F	F
0.8333333332999970	0.1666666667000030	0.3854655552433357	F	F	F
0.1666666667000030	0.5000000000000000	0.3854655552433357	F	F	F
0.5000000000000000	0.5000000000000000	0.3854655552433357	F	F	F
0.8333333332999970	0.5000000000000000	0.3854655552433357	F	F	F
0.1666666667000030	0.8333333332999970	0.3854655552433357	F	F	F
0.5000000000000000	0.8333333332999970	0.3854655552433357	F	F	F
0.8333333332999970	0.8333333332999970	0.3854655552433357	F	F	F
0.0000000000000000	0.0000000000000000	0.4552941175999976	F	F	F
0.3333333332999970	0.0000000000000000	0.4552941175999976	F	F	F
0.6666666666000012	0.0000000000000000	0.4552941175999976	F	F	F
0.0000000000000000	0.3333333332999970	0.4552941175999976	F	F	F
0.3333333332999970	0.3333333332999970	0.4552941175999976	F	F	F
0.6666666666000012	0.3333333332999970	0.4552941175999976	F	F	F

0.0000000000000000	0.6666666666000012	0.4552941175999976	F	F	F
0.3333333332999970	0.6666666666000012	0.4552941175999976	F	F	F
0.6666666666000012	0.6666666666000012	0.4552941175999976	F	F	F
0.1677389056515324	0.1677389056515324	0.5258228675243402	T	T	T
0.5000000000000000	0.1676393875570881	0.5252180945897962	T	T	T
0.8322610943484676	0.1677389056515324	0.5258228675243402	T	T	T
0.1676393875570881	0.5000000000000000	0.5252180945897962	T	T	T
0.5000000000000000	0.5000000000000000	0.5217554082650864	T	T	T
0.8323606124429119	0.5000000000000000	0.5252180945897962	T	T	T
0.1677389056515324	0.8322610943484676	0.5258228675243402	T	T	T
0.5000000000000000	0.8323606124429119	0.5252180945897962	T	T	T
0.8322610943484676	0.8322610943484676	0.5258228675243402	T	T	T
0.0000000000000000	0.0000000000000000	0.5937896536044036	T	T	T
0.3339769971459887	0.0000000000000000	0.5932975743048132	T	T	T
0.6660230027540095	0.0000000000000000	0.5932975743048132	T	T	T
0.0000000000000000	0.3339769971459887	0.5932975743048132	T	T	T
0.3346058211030396	0.3346058211030396	0.5952645035544819	T	T	T
0.6653941787969586	0.3346058211030396	0.5952645035544819	T	T	T
0.0000000000000000	0.6660230027540095	0.5932975743048132	T	T	T
0.3346058211030396	0.6653941787969586	0.5952645035544819	T	T	T
0.6653941787969586	0.6653941787969586	0.5952645035544819	T	T	T
0.5000000000000000	0.5000000000000000	0.6413290458967609	T	T	T
0.5000000000000000	0.5000000000000000	0.6881122943317308	T	T	T

CO/Cu(100) $E_{ads} = -1.05$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu C O
45 1 1
Selective dynamics
Direct

0.0000000000000000	0.0000000000000000	0.3173193249345303	F	F	F
0.3333333332999970	0.0000000000000000	0.3173193249345303	F	F	F
0.6666666666000012	0.0000000000000000	0.3173193249345303	F	F	F
0.0000000000000000	0.3333333332999970	0.3173193249345303	F	F	F
0.3333333332999970	0.3333333332999970	0.3173193249345303	F	F	F
0.6666666666000012	0.3333333332999970	0.3173193249345303	F	F	F
0.0000000000000000	0.6666666666000012	0.3173193249345303	F	F	F
0.3333333332999970	0.6666666666000012	0.3173193249345303	F	F	F
0.6666666666000012	0.6666666666000012	0.3173193249345303	F	F	F
0.1666666667000030	0.1666666667000030	0.3854655552433357	F	F	F
0.5000000000000000	0.1666666667000030	0.3854655552433357	F	F	F
0.8333333332999970	0.1666666667000030	0.3854655552433357	F	F	F
0.1666666667000030	0.5000000000000000	0.3854655552433357	F	F	F
0.5000000000000000	0.5000000000000000	0.3854655552433357	F	F	F
0.8333333332999970	0.5000000000000000	0.3854655552433357	F	F	F
0.1666666667000030	0.8333333332999970	0.3854655552433357	F	F	F
0.5000000000000000	0.8333333332999970	0.3854655552433357	F	F	F
0.8333333332999970	0.8333333332999970	0.3854655552433357	F	F	F
0.0000000000000000	0.0000000000000000	0.4552941175999976	F	F	F
0.3333333332999970	0.0000000000000000	0.4552941175999976	F	F	F
0.6666666666000012	0.0000000000000000	0.4552941175999976	F	F	F
0.0000000000000000	0.3333333332999970	0.4552941175999976	F	F	F
0.3333333332999970	0.3333333332999970	0.4552941175999976	F	F	F
0.6666666666000012	0.3333333332999970	0.4552941175999976	F	F	F

0.0000000000000000	0.6666666666000012	0.4552941175999976	F	F	F
0.3333333332999970	0.6666666666000012	0.4552941175999976	F	F	F
0.6666666666000012	0.6666666666000012	0.4552941175999976	F	F	F
0.1684006054732237	0.1684006054732237	0.5254424956560939	T	T	T
0.4982660612267793	0.1684006054732237	0.5254424956560939	T	T	T
0.8333333332999970	0.1666703547745811	0.5248668548577271	T	T	T
0.1684006054732237	0.4982660612267793	0.5254424956560939	T	T	T
0.4982660612267793	0.4982660612267793	0.5254424956560939	T	T	T
0.8333333332999970	0.4999963119254218	0.5248668548577271	T	T	T
0.1666703547745811	0.8333333332999970	0.5248668548577271	T	T	T
0.4999963119254218	0.8333333332999970	0.5248668548577271	T	T	T
0.8333333332999970	0.8333333332999970	0.5247519695274860	T	T	T
0.9999430374543152	0.9999430374543152	0.5927557975816455	T	T	T
0.3333333332999970	0.9970460625930357	0.5930215042855878	T	T	T
0.6667236291456859	0.9999430374543152	0.5927557975816455	T	T	T
0.9970460625930357	0.3333333332999970	0.5930215042855878	T	T	T
0.3333333332999970	0.3333333332999970	0.5982256126482071	T	T	T
0.6696206040069654	0.3333333332999970	0.5930215042855878	T	T	T
0.9999430374543152	0.6667236291456859	0.5927557975816455	T	T	T
0.3333333332999970	0.6696206040069654	0.5930215042855878	T	T	T
0.6667236291456859	0.6667236291456859	0.5927557975816455	T	T	T
0.3333333332999970	0.3333333332999970	0.6705638694502909	T	T	T
0.3333333332999970	0.3333333332999970	0.7157296787066940	T	T	T

CO/Cu(211) $E_{ads} = -1.12$ eV
1.00000000000000
6.2527034153000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.3164343000000009
Cu C O
45 1 1
Selective dynamics
Direct

0.0061862950247047	0.1666666667000030	0.3120745335338029	F	F	F
0.0061862950247047	0.5000000000000000	0.3120745335338029	F	F	F
0.0061862950247047	0.8333333332999970	0.3120745335338029	F	F	F
0.3355456677560653	0.0000000000000000	0.3354619372229379	F	F	F
0.3355456677560653	0.3333333332999970	0.3354619372229379	F	F	F
0.3355456677560653	0.6666666666000012	0.3354619372229379	F	F	F
0.6630854692850079	0.1666666667000030	0.3607350091654666	F	F	F
0.6630854692850079	0.5000000000000000	0.3607350091654666	F	F	F
0.6630854692850079	0.8333333332999970	0.3607350091654666	F	F	F
0.9944057463905267	0.0000000000000000	0.3915351276171819	F	F	F
0.9944057463905267	0.3333333332999970	0.3915351276171819	F	F	F
0.9944057463905267	0.6666666666000012	0.3915351276171819	F	F	F
0.3330656692422309	0.1666666667000030	0.4179888222780335	F	F	F
0.3330656692422309	0.5000000000000000	0.4179888222780335	F	F	F
0.3330656692422309	0.8333333332999970	0.4179888222780335	F	F	F
0.6656564241704075	0.0000000000000000	0.4448469552356400	F	F	F
0.6656564241704075	0.3333333332999970	0.4448469552356400	F	F	F
0.6656564241704075	0.6666666666000012	0.4448469552356400	F	F	F
0.0003515212697778	0.1666666667000030	0.4732099031121066	F	F	F
0.0003515212697778	0.5000000000000000	0.4732099031121066	F	F	F
0.0003515212697778	0.8333333332999970	0.4732099031121066	F	F	F
0.3333333329999988	0.0000000000000000	0.5000000000000000	F	F	F
0.3333333329999988	0.3333333332999970	0.5000000000000000	F	F	F
0.3333333329999988	0.6666666666000012	0.5000000000000000	F	F	F

0.6663151448302216 0.1666666667000030 0.5267900968878934 F F F
0.6663151448302216 0.5000000000000000 0.5267900968878934 F F F
0.6663151448302216 0.8333333332999970 0.5267900968878934 F F F
0.9983244433132867 0.0000000000000000 0.5551738321969282 T T T
0.9981471708257814 0.3333222485748806 0.5550073750148670 T T T
0.9981471708257814 0.6666777513251176 0.5550073750148670 T T T
0.3301666679875126 0.1666603970111424 0.5816250868696002 T T T
0.3312349264582366 0.5000000000000000 0.5818142561619624 T T T
0.3301666679875126 0.8333396029888576 0.5816250868696002 T T T
0.6670302888740878 0.0000000000000000 0.6082063548109602 T T T
0.6675752058449902 0.3359748920962460 0.6093187787337726 T T T
0.6675752058449902 0.6640251078037522 0.6093187787337726 T T T
0.9969084561694572 0.1666937804113857 0.6389498026132543 T T T
0.9985386934271290 0.5000000000000000 0.6386109226182199 T T T
0.9969084561694572 0.8333062195886143 0.6389498026132543 T T T
0.3243883333514432 0.0000000000000000 0.6640718389521183 T T T
0.3250537927911381 0.3331314010788091 0.6636841200563595 T T T
0.3250537927911381 0.6668685988211891 0.6636841200563595 T T T
0.6539362842350513 0.1643683383466055 0.6877925113191665 T T T
0.6602150913003371 0.5000000000000000 0.6914510809111931 T T T
0.6539362842350513 0.8356316616533945 0.6877925113191665 T T T
0.6768396591975048 0.5000000000000000 0.7611394396284012 T T T
0.6773248574130619 0.5000000000000000 0.8048687742368728 T T T

CO/Cu(211) $E_{ads} = -1.11$ eV
1.00000000000000
6.2527034153000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.3164343000000009
Cu C O
45 1 1
Selective dynamics
Direct
0.0061862950247047 0.1666666667000030 0.3120745335338029 F F F
0.0061862950247047 0.5000000000000000 0.3120745335338029 F F F
0.0061862950247047 0.8333333332999970 0.3120745335338029 F F F
0.3355456677560653 0.0000000000000000 0.3354619372229379 F F F
0.3355456677560653 0.3333333332999970 0.3354619372229379 F F F
0.3355456677560653 0.6666666666000012 0.3354619372229379 F F F
0.6630854692850079 0.1666666667000030 0.3607350091654666 F F F
0.6630854692850079 0.5000000000000000 0.3607350091654666 F F F
0.6630854692850079 0.8333333332999970 0.3607350091654666 F F F
0.9944057463905267 0.0000000000000000 0.3915351276171819 F F F
0.9944057463905267 0.3333333332999970 0.3915351276171819 F F F
0.9944057463905267 0.6666666666000012 0.3915351276171819 F F F
0.3330656692422309 0.1666666667000030 0.4179888222780335 F F F
0.3330656692422309 0.5000000000000000 0.4179888222780335 F F F
0.3330656692422309 0.8333333332999970 0.4179888222780335 F F F
0.6656564241704075 0.0000000000000000 0.4448469552356400 F F F
0.6656564241704075 0.3333333332999970 0.4448469552356400 F F F
0.6656564241704075 0.6666666666000012 0.4448469552356400 F F F
0.0003515212697778 0.1666666667000030 0.4732099031121066 F F F
0.0003515212697778 0.5000000000000000 0.4732099031121066 F F F
0.0003515212697778 0.8333333332999970 0.4732099031121066 F F F
0.3333333329999988 0.0000000000000000 0.5000000000000000 F F F
0.3333333329999988 0.3333333332999970 0.5000000000000000 F F F
0.3333333329999988 0.6666666666000012 0.5000000000000000 F F F

0.6663151448302216	0.1666666667000030	0.5267900968878934	F	F	F
0.6663151448302216	0.5000000000000000	0.5267900968878934	F	F	F
0.6663151448302216	0.8333333332999970	0.5267900968878934	F	F	F
0.9990763593678835	0.9993273264483875	0.5552212237871359	T	T	T
0.0006999262498013	0.3333333332999970	0.5551404270702278	T	T	T
0.9990763593678835	0.6673393401516137	0.5552212237871359	T	T	T
0.3330176818170187	0.1662359686771993	0.5820412042881813	T	T	T
0.3330176818170187	0.5004306980228037	0.5820412042881813	T	T	T
0.3327872841173303	0.8333333332999970	0.5818870018589877	T	T	T
0.6698626438596662	0.0020312844577148	0.6097527136025818	T	T	T
0.6695878326514730	0.3333333332999970	0.6076512277146549	T	T	T
0.6698626438596662	0.6646353821422863	0.6097527136025818	T	T	T
0.9992217519480988	0.1650946583736896	0.6387229660356581	T	T	T
0.9992217519480988	0.5015720083263133	0.6387229660356581	T	T	T
0.0022487065381611	0.8333333332999970	0.6395960592232655	T	T	T
0.3309099941036564	0.0006935018310656	0.6645878871833730	T	T	T
0.3221014931280450	0.3333333332999970	0.6630718906117252	T	T	T
0.3309099941036564	0.6659731647689355	0.6645878871833730	T	T	T
0.6605261505644933	0.1699896580492748	0.6909258838088448	T	T	T
0.6605261505644933	0.4966770086507282	0.6909258838088448	T	T	T
0.6595227975368374	0.8333333332999970	0.6890412620180655	T	T	T
0.6655414458143980	0.3333333333333357	0.7487632081239397	T	T	T
0.6639098057751838	0.3333333333333357	0.7930506072478991	T	T	T

CO/Cu_{13} $E_{ads} = -1.62$ eV
1.00000000000000
30.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 30.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.0000000000000000
Cu C O
13 1 1
Direct
0.5726061652909051 0.4714412311841693 0.4791856591004285
0.5247459741781701 0.4355621281596749 0.5379448647769104
0.4441677719605326 0.4449015162604924 0.5153653438893061
0.5012099544684545 0.5010387400382803 0.4980824318731749
0.4785043040296713 0.4953344632729754 0.5736843701911185
0.5590331273239907 0.5116781632451742 0.5511730847036418
0.5026567662219549 0.4290104387680007 0.4577994225360528
0.5557991312694147 0.5541851721761532 0.4781775664618280
0.4968087435973478 0.5698216779633708 0.5371318860553826
0.5211576717979864 0.5032991245069004 0.4208703984471322
0.4747997376855815 0.5634569398710317 0.4566159905527248
0.4405610255650829 0.4874688317173829 0.4438281555287061
0.4272802347653667 0.5271680191416067 0.5156644100111923
0.4359892457012692 0.4207664224612080 0.4523583237691794
0.4129991554134261 0.3926206215062810 0.4364509937648646

CO/Cu_{13} $E_{ads} = -1.47$ eV
1.00000000000000
30.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 30.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.0000000000000000
Cu C O
13 1 1
Direct

0.5743514443000266 0.4723099671473785 0.4819505165073713
0.5322533770013825 0.4393852490393069 0.5448306427981078
0.4499861076858060 0.4431558291546231 0.5282463447873118
0.5004411725622884 0.4986289442271477 0.5006425163367193
0.4831184032599191 0.5008446166433248 0.5789270007430347
0.5597405716447975 0.5171017223406174 0.5496415445299901
0.5045778980468378 0.4264042014881839 0.4655038119718992
0.5516758895157831 0.5540352802293966 0.4745753829727616
0.4977028416993347 0.5707634613646119 0.5364808737370094
0.5189604661713644 0.4966471391103117 0.4227558632433543
0.4691153298151748 0.5577433876182892 0.4566585580688193
0.4407485067358705 0.4794499460930635 0.4512725394952545
0.4271065162517023 0.5250166931644407 0.5198137654620854
0.3991884490093753 0.4548618555619122 0.4159638455945381
0.3726808318435875 0.4380718637567574 0.3937365286935641

CO/Cu_{55} $E_{ads} = -1.32$ eV
1.00000000000000
26.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 26.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.0000000000000000
Cu C O
55 1 1
Direct
0.4998759969431604 0.5001006453605138 0.5000348491373443
0.5000089563868647 0.4999525235743072 0.5927044394315480
0.4999129218852641 0.4999857944879514 0.6831912154872899
0.5681106827520269 0.4504953213813810 0.6373683448694197
0.5667481634200306 0.4514485282461813 0.5414122718225377
0.5667293280665154 0.5489663752909856 0.5415371253055318
0.4742629823628821 0.5788234507943278 0.5413833268586621
0.4170895205286185 0.5000946303767302 0.5413864431268466
0.4740403868895033 0.4213760717175516 0.5415000325316958
0.5254846581208482 0.4214215759388865 0.4587182489051798
0.5826122764869917 0.5000399972011410 0.4587249300953933
0.5257202505501123 0.5788509267186619 0.4585507705667676
0.4329409335912840 0.5487881092836931 0.4586435552409517
0.4329881869732632 0.4511964352588241 0.4585158075490823
0.4997258711203426 0.5002455138296954 0.4074134855190232
0.6318101817480440 0.4040799727908232 0.5834381909003887
0.6323742320057359 0.5965253737041979 0.5820942690264037
0.4494309038468284 0.6558484272364390 0.5819625149070334
0.3361358233339033 0.4999181871203477 0.5819074058363001
0.4491343996760889 0.3441849787531478 0.5820254551903203
0.5490509455117785 0.3439209533199206 0.4176863411577360
0.6635995089006915 0.5015342022248417 0.4177170741191901
0.5506714634131552 0.6558698363399391 0.4180483223716962
0.3675532635508265 0.5963509145027647 0.4179595643206315
0.3675058723761609 0.4036468116337799 0.4179934739410883
0.4999051366803133 0.5001404705525243 0.3167859857380078
0.5685407000657181 0.5493607107996462 0.6368821269591447
0.4743065877048415 0.5803302692674103 0.6363888361817899
0.4156521641216824 0.4995444500014077 0.6363790487210321
0.4741557348366825 0.4194557903718645 0.6368570713429762
0.6359954637514826 0.4997967844627376 0.5842023037471248
0.5421375885969338 0.3706210157523622 0.5842183947490129
0.5952818589673342 0.3677844622929672 0.5004260860275155

0.6550604873879133 0.4501130546417914 0.5003952465258458
0.5423526477521936 0.6298611232577030 0.5843098484213965
0.6521330272918971 0.5494670827605220 0.4998177380180015
0.5948126827642489 0.6300523106017429 0.4998118834806048
0.3897618517624631 0.5800886921642314 0.5852471210633334
0.5003774978950042 0.6604121390638859 0.5002328461554236
0.4061820516996859 0.6306400125023695 0.4994607823851646
0.3896291626038305 0.4195312538196984 0.5842741562511613
0.3468923172161423 0.5488750968715125 0.4994434020467718
0.3476257117199575 0.4501003481523291 0.5001806706645454
0.4056298815419932 0.3696286479303448 0.4997541547608653
0.4999121386268942 0.3399684387428507 0.4997587523939770
0.6119737423258498 0.4185899138520204 0.4141351003360936
0.4571798910762081 0.3697706976889627 0.4153641156090238
0.5260090532345769 0.4198024378455094 0.3640616037907349
0.6105948965922899 0.5810069392600878 0.4154260121699356
0.5843105527646093 0.5001184235629591 0.3640719617374643
0.4579571389709647 0.6295947229920786 0.4153788856250558
0.5265714909382114 0.5803726237414963 0.3631976581287944
0.3638593832784652 0.5000283855791762 0.4153566661747887
0.4319288829361290 0.5495095047426309 0.3633268969950257
0.4318393143593888 0.4500086929224948 0.3631801768292064
0.6625354412861654 0.3817275904744420 0.4621108890812180
0.6987569733698639 0.3553516561063108 0.4537172535698109

CO/Cu_{55} E_{ads} = −1.22 eV
1.00000000000000
26.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 26.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.0000000000000000
Cu C O
55 1 1
Direct
0.4997378068616546 0.5000063327028227 0.4999143939480262
0.4979452574963557 0.5000130495298060 0.5915113629979414
0.4998753876521292 0.5000223896987874 0.6827970156625305
0.5695419166960592 0.4486036690327467 0.6388384655415487
0.5665049566517129 0.4516771778779171 0.5427118738169098
0.5665075917365249 0.5483623225562030 0.5427250389025604
0.4738985350412880 0.5789894711913752 0.5412146348643193
0.4161551631593513 0.4999932445499377 0.5406579076315291
0.4738849170099169 0.4210237404465073 0.5411993456057189
0.5257595802271138 0.4211351880318333 0.4593194433917444
0.5827517690129436 0.5000180374935614 0.4591952011641032
0.5257734921838095 0.5788795908245218 0.4593335694284032
0.4328172164480169 0.5487225556787987 0.4584734513074066
0.4328134886893699 0.4512654199595005 0.4584633551074969
0.5000024859998996 0.4999973006803543 0.4076544699018583
0.6323905234231690 0.4034144672588835 0.5823349061058632
0.6323957219317294 0.5966324827451919 0.5823487019412892
0.4487688088979194 0.6559121812153661 0.5821260979455886
0.3355065519746434 0.4999858653030441 0.5812159766397511
0.4487719863163475 0.3440999443332675 0.5821179287612335
0.5506407773484965 0.3439218545940417 0.4191147212512012
0.6638258351125816 0.5000158825813493 0.4188085729112814
0.5506452652959775 0.6560946542327211 0.4191270724796140
0.3676879182951774 0.5963830158449700 0.4175085453456935

0.3676827402706234 0.4035980272733713 0.4174900746974922
0.5009688325090147 0.5000017256163353 0.3170446953745826
0.5695470877400970 0.5514508244582760 0.6388576716673210
0.4728844180525575 0.5798382068238278 0.6364380429696618
0.4145386832543203 0.5000025511232462 0.6369257740447738
0.4728767922655556 0.4201969432385945 0.6364266108876512
0.6376495400616992 0.5000249915870246 0.5837952962780451
0.5417619198105174 0.3706400711413209 0.5850553739806417
0.5939234737637451 0.3697928829850857 0.5010084634326147
0.6520439438297260 0.4496639233279015 0.5001504646798038
0.5417707005062579 0.6294078123206608 0.5850657172972170
0.6520463640028278 0.5503815307012070 0.5001531088777353
0.5939440586286342 0.6302469744791921 0.5010155571239002
0.3889381342235753 0.5799372810409923 0.5843683138231068
0.4998708147035223 0.6611035559643330 0.5006138879701129
0.4060198628713876 0.6302354162991500 0.4996136243923415
0.3889274897566362 0.4200451831100715 0.5843599139052399
0.3468073006428660 0.5495866290019714 0.4993289427452655
0.3468096381553031 0.4503760860107772 0.4993241609014202
0.4060114743851370 0.3697439074950141 0.4995939877260857
0.4998552660831501 0.3389076719703598 0.5005968782025172
0.6108616059641570 0.4194839061208133 0.4164432938994889
0.4580339913039019 0.3696368898086760 0.4163775276227001
0.5260733985983188 0.4196519647562326 0.3642872112840316
0.6108807395100061 0.5805502091984291 0.4164519387828784
0.5847561345563567 0.5000091492965949 0.3644968211746991
0.4580394185973119 0.6303514430446820 0.4163960496526967
0.5260877495553463 0.5803433787960046 0.3643099824779941
0.3632607128343199 0.4999909141532783 0.4149188452393558
0.4323095040788286 0.5505309965220578 0.3634806240742495
0.4323065114257794 0.4494583339152962 0.3634694937249087
0.5796975749011989 0.5000201016057336 0.6950308999727363
0.5990041543099539 0.4999959073075931 0.7364245111516325

CO/Cu_{55} E_{ads} = −1.17 eV
1.00000000000000
26.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 26.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.0000000000000000
Cu C O
55 1 1
Direct
0.5000434155859058 0.4999651150308369 0.5001096336306833
0.5009059303885135 0.4993036059515668 0.5931197686137226
0.4987603307639665 0.5008344446048657 0.6836545182109730
0.5698964274690714 0.4491592815793516 0.6398900649106323
0.5669370578967876 0.4513376764719643 0.5426716125102583
0.5671609983966822 0.5483035262879312 0.5420300138356672
0.4747352232221821 0.5786101589708968 0.5415045092912764
0.4174156231196057 0.4997160883523865 0.5414833788759893
0.4748028551765060 0.4211855215950366 0.5419762004067952
0.5255023212958271 0.4212240258136157 0.4589621819995206
0.5828143398593283 0.5001199093955159 0.4589848323044607
0.5254412768035313 0.5786011859725072 0.4585648387658562
0.4329723852401040 0.5487325645046320 0.4587597625015452
0.4331224926997085 0.4515276896153117 0.4585103766229742
0.5001774896622542 0.4999007871631768 0.4074559225351352

0.6334037491527822 0.4030203774163312 0.5808193703049640
0.6327076136445556 0.5960865103613358 0.5824925520863181
0.4498781595568197 0.6558464700665567 0.5816972345282351
0.3362469136212859 0.4995057272239526 0.5816360183128970
0.4496633197284895 0.3440373986850341 0.5823934778769456
0.5501156329930863 0.3441640922727565 0.4182800487101676
0.6637448154320421 0.5005080482470177 0.4183523870615475
0.5504046756573768 0.6556557466622064 0.4179482929358511
0.3672520172059178 0.5965453944934481 0.4183602967029995
0.3675998265270902 0.4039302257007485 0.4178607538024869
0.5004215923329293 0.4997651237740502 0.3167202914896591
0.5684943620867809 0.5499871503775416 0.6368914618345762
0.4739925473413197 0.5801278162856359 0.6366829491588137
0.4157630704274108 0.4999208477315628 0.6366551747537867
0.4735151740738927 0.4193086261356458 0.6368410816072239
0.6370806887651758 0.5002255407872375 0.5844606775888278
0.5421085173243674 0.3694532769730028 0.5843564607509307
0.5944239650458212 0.3701008762501062 0.5002205230317229
0.6526686451512622 0.4503909293335344 0.5002714845616403
0.5422064538795915 0.6302482179115519 0.5845153310345308
0.6530113962978812 0.5496817215916719 0.4999864574186627
0.5937827472228194 0.6290156616301706 0.5001309773337330
0.3903764096712051 0.5796291256940505 0.5842024069560852
0.4997490119232515 0.6607548140294437 0.5001708235906313
0.4059105216326271 0.6300143251670935 0.4997425975532141
0.3891748827565984 0.4195633883234728 0.5844116760843973
0.3473288362200388 0.5492966255449885 0.4997116066845262
0.3470469475385999 0.4505919664017577 0.5000843290351905
0.4062980159015889 0.3709221293796032 0.5000270947337858
0.4999869456085434 0.3390995868010157 0.4998719103678024
0.6100648920487500 0.4200554693157638 0.4166642054902333
0.4580518863217158 0.3698994315304453 0.4153940748625832
0.5257600981913337 0.4197084894132710 0.3634757534782747
0.6107529835639857 0.5801465280892562 0.4155020032461491
0.5843295376401372 0.5003767745960677 0.3635259303309528
0.4580075853915394 0.6300939549056639 0.4153251423184753
0.5259917746973400 0.5806731397854388 0.3633559088853101
0.3633504646758935 0.4998013802951237 0.4152944153474258
0.4320629884748381 0.5493613737967841 0.3640523651713619
0.4313635101851631 0.4504567359020108 0.3633072699321994
0.5997098315241458 0.4269961584356480 0.6996341592926165
0.6184782673409877 0.4130254627989323 0.7373115774531194

CO/Cu$_{55}$ E$_{ads}$ = −1.15 eV
1.00000000000000
26.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 26.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.0000000000000000
Cu C O
55 1 1
Direct
0.4999947226838301 0.5000021634944378 0.5006866275562148
0.4999618803986797 0.4999844660393162 0.5946220806615523
0.4999406472754096 0.4999767558204445 0.6871631393481197
0.5681609350860223 0.4504443045508545 0.6367320730932834
0.5668975470386162 0.4513305143143059 0.5415732537424360
0.5668904734362206 0.5486394407813867 0.5415750293072163

0.4743933356959640	0.5786981214201301	0.5415130224961983
0.4172670515999060	0.5000067952920444	0.5415281305194984
0.4744184783155186	0.4213050995581798	0.5415258202802294
0.5255979812961907	0.4213299260788979	0.4587902476726723
0.5827186579183875	0.4999944896908639	0.4587953754640738
0.5255760075504404	0.5786818856560608	0.4587872773162324
0.4331106004021533	0.5486624502059798	0.4587484371491037
0.4331211247390865	0.4513766421313250	0.4587499283129586
0.5000301679893402	0.5000205915551637	0.4077780965293027
0.6324119491349941	0.4036751780022725	0.5822725490649002
0.6324004907363433	0.5962874707678361	0.5822682758277110
0.4493721517626983	0.6557518435953877	0.5822105745675744
0.3362144428674765	0.4999999241292090	0.5821669157073626
0.4493881121952704	0.3442434586021783	0.5822089911788858
0.5506183200042609	0.3442900123679790	0.4180015447947639
0.6637483983848438	0.4999938067706242	0.4180618405047495
0.5506095879755247	0.6557249709930900	0.4180122556168839
0.3676167353260397	0.5963003716968373	0.4179519052316040
0.3676380642826870	0.4037353052428770	0.4179498901614139
0.5000674774365301	0.5000291417021370	0.3172110946147867
0.5681624107426395	0.5495037353337838	0.6367291146266505
0.4738677417090078	0.5801793090028823	0.6366561564203028
0.4156747161765635	0.4999877075856734	0.6366805998616922
0.4738997865038442	0.4197784387644216	0.6366805322914607
0.6368177311879475	0.4999807568405759	0.5841402711332986
0.5422559846414571	0.3697676893563765	0.5841169441508721
0.5944445220806884	0.3701785249043097	0.5000191081543419
0.6525265649869536	0.4502974314398174	0.5000504539548805
0.5422386642009370	0.6301999739995087	0.5841029754841844
0.6525287485209113	0.5496419251234103	0.5000653863063156
0.5944259833123484	0.6297780489007450	0.5000159121230614
0.3892378565929344	0.5804815050717631	0.5840350719843851
0.4998657842035551	0.6604908819916032	0.4999819833488353
0.4057458265752273	0.6299753939187596	0.4999454719924062
0.3892649158278350	0.4195291971568806	0.5840432649050140
0.3473935799291153	0.5494635113459353	0.4999302529125969
0.3474010282199400	0.4505645719140438	0.4999223988275166
0.4057845282541024	0.3700644366419727	0.4999438495749972
0.4999098467435011	0.3395150813640335	0.4999923739456885
0.6107259489405438	0.4195408336162432	0.4160067552867470
0.4577805303525045	0.3698417412138630	0.4159390828598042
0.5261391900919981	0.4197740301564259	0.3636033475471922
0.6107055794280043	0.5804441707017803	0.4160041083368554
0.5843772768100647	0.5000152991821464	0.3636295940612121
0.4577597610112013	0.6302068980715713	0.4159382367651875
0.5261181163132294	0.5802767304569559	0.3635994901182051
0.3632182719287352	0.5000177644613273	0.4159130791566790
0.4317967075711081	0.5496021415403536	0.3635650164751815
0.4317945235021170	0.4504713687600927	0.3635663640599240
0.5000087965224633	0.5000453134383923	0.7576050568777898
0.5000838004043990	0.5001405932742388	0.8018624805794484

CO/Cu_{55} E_{ads} = −1.10 eV

1.00000000000000

26.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	26.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.0000000000000000

Cu C O
55 1 1
Direct
0.4996789562868769 0.5002242114257357 0.4997460263563164
0.4991868203482929 0.5005227881370740 0.5919356710892985
0.5009937796329283 0.4993850741127470 0.6833216801123644
0.5699915385430279 0.4493276510681162 0.6387788103876656
0.5664333909224301 0.4517392598211178 0.5430045137375239
0.5666123658652301 0.5487083783893926 0.5419344818206205
0.4740591710022185 0.5792521597592685 0.5406906049756320
0.4165788867026588 0.5000651272150364 0.5407348632625730
0.4741624640482278 0.4215816715585278 0.5417796456636524
0.5255147847213807 0.4212917584564373 0.4592198674648972
0.5827564788649960 0.5001110327771369 0.4591711775470403
0.5254392329306475 0.5787545357918029 0.4583019146005699
0.4326057435294284 0.5489365631372833 0.4582840802424412
0.4329294909318838 0.4515083414767942 0.4581905856323198
0.4999594466957296 0.5000740953379557 0.4072982762712561
0.6325557659996836 0.4036617453340484 0.5821228761699714
0.6322613524996316 0.5968739509701942 0.5821268247633700
0.4492020708668080 0.6560822014878798 0.5812757288814004
0.3357981234202597 0.4999451639992850 0.5812548435367868
0.4487762177478260 0.3443020832968726 0.5820995550536906
0.5501641490536928 0.3440288564496078 0.4189545111984264
0.6638859273804650 0.5004700867821528 0.4188821639345640
0.5505703623143360 0.6555997663893832 0.4175782894076118
0.3671699124651334 0.5965344733466765 0.4173947629117714
0.3676954138483238 0.4037900309727524 0.4174234367911038
0.5007389948405103 0.4995839216708908 0.3165937690872810
0.5676448605840095 0.5525471632632727 0.6363944699217576
0.4734516660018582 0.5799701483222780 0.6365996711617843
0.4156578646254167 0.5003700567777135 0.6366917135293356
0.4712111500245706 0.4195567603973335 0.6363277024976917
0.6360729743407751 0.5006247501901777 0.5851790281593864
0.5413886743323902 0.3706895067234584 0.5852963953281340
0.5944365827913167 0.3703094082752816 0.5007623103252581
0.6524090122468135 0.4502410231750489 0.5007179583304839
0.5417081467122606 0.6308933657409469 0.5840877024393587
0.6524344951199945 0.5499617581996264 0.5000386117927333
0.5935366404749738 0.6294712532231257 0.4998152116742296
0.3902286123996065 0.5796299091976389 0.5845695391361332
0.4993531810293639 0.6610892083635210 0.4996213945069803
0.4054995562395714 0.6304410924932489 0.4990191951098036
0.3884385656469356 0.4198390770530265 0.5841948969979222
0.3468144956005025 0.5495468352278989 0.4990138196359957
0.3466605767066052 0.4507683521000482 0.4995459754087457
0.4058421243741019 0.3709427063069075 0.4997137165791458
0.4997152400872618 0.3395004748815651 0.5001004883012837
0.6100761849221407 0.4200444164755164 0.4165575480790539
0.4578944562508304 0.3698456979042460 0.4152244304144987
0.5258208756934611 0.4196871564650314 0.3641447753563290
0.6107828871056573 0.5803274600831202 0.4151940989271370
0.5844185146593917 0.5003355649913868 0.3641362535802208
0.4579641292196410 0.6298483410999515 0.4147431061143233
0.5265005038230939 0.5806112522472346 0.3630813445520675
0.3634849115454098 0.4998772781022228 0.4145930539778429
0.4320513310113663 0.5495062559955688 0.3634779060329095
0.4315909368933505 0.4499366501637097 0.3630183846997935

0.5675703492165679 0.4564612808906764 0.7101232082504806
0.5756115559907946 0.4548670987895832 0.7542868778450420

CO/Cu_{147} E_{ads} = −1.00 eV
1.00000000000000
31.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 31.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 31.0000000000000000
Cu C O
147 1 1
Direct
0.4152715072505168 0.3865827665229087 0.4363565098847402
0.6034163483799710 0.4656108649013879 0.4232191871843636
0.4180238472313590 0.5367064949714075 0.3735716255879916
0.4236921312215957 0.5862953457616992 0.7018705100902547
0.3967413875589507 0.6628523118253367 0.4315579666977564
0.5876424415502496 0.3264922569964538 0.4353097258880566
0.6298494871473670 0.4365171505182735 0.3549940013215709
0.5303878445479355 0.4289612615679942 0.5019659873685303
0.7303480459403746 0.4845146488226732 0.4741183180668351
0.6272569171731672 0.5958104764344002 0.6287018502315478
0.6611275857244986 0.4574610335551925 0.6190772219182216
0.5912592493315522 0.2864337368020380 0.5059404237122808
0.6190516028657364 0.4760843618722479 0.5552126220607897
0.4241054486611148 0.3919968402627821 0.5172101058617853
0.4879625574139501 0.3705810698507396 0.4700150079575464
0.4079011202041110 0.4282252700987701 0.6674938062514555
0.4695356477857939 0.5709570850970798 0.4981566979893187
0.6971401459666400 0.4707293170703535 0.5470107941453710
0.3423850163110849 0.3944843994586151 0.5267430604964050
0.4158009774100040 0.4612575548863696 0.4040944605088138
0.5097871590747066 0.4604994424355650 0.2993372625225076
0.3906849670635301 0.3407023163548187 0.5660918821596606
0.3700404385662027 0.5634723468161116 0.6451567268747559
0.3726393881712997 0.4041231944014165 0.3713393318798244
0.3808718605933641 0.5237430411802302 0.4448917947592646
0.6986308488410644 0.5473529695442054 0.5148614755453115
0.6446594061497660 0.5961783362229305 0.3923867218379333
0.4578025750278234 0.4434901269636508 0.4683581726308374
0.4403509942318679 0.3559565374512241 0.3671942924591668
0.6108482271219178 0.5453715057531057 0.4419401423151186
0.4829163209793468 0.4135073126534939 0.3998969033816467
0.5349898494842670 0.6741972439320010 0.3991900534137713
0.4537974959848146 0.3153133462182347 0.5197606402168311
0.4758558865592232 0.3799069161433687 0.6633034450696795
0.6534293002627527 0.4017692940939702 0.5586459504563495
0.4151436947756157 0.5070558182987726 0.6861607456304691
0.6373558914547582 0.3911619353309255 0.4234401976953753
0.3109293555684775 0.4592168271483341 0.5673151964352676
0.6093238092694193 0.6593673754874526 0.4336041038542334
0.5596433572990394 0.6438956796629427 0.6328546533462512
0.6137342291470658 0.3900330887849762 0.6300450909725794
0.5082785479378394 0.3839219234329048 0.3314740956396616
0.6889914906978580 0.5408285098991545 0.4326684151608919
0.5921219889638175 0.5719848763597002 0.3324603041731262
0.5242930872923485 0.6202031341288591 0.3366529287952030
0.5766205562650601 0.4947383774365054 0.4914965745405337

0.3964836165223697	0.5342214237663784	0.5769512909442319
0.3891219048084992	0.4546014860475437	0.5581052121712852
0.4389325012596765	0.6425202688784697	0.4961896528820666
0.5283023157488281	0.3045215240033102	0.5538609093228737
0.4491087072405681	0.5577858933616547	0.6348312139699855
0.6639997947056189	0.6093948560679272	0.5553034807888935
0.4402092005531227	0.4305708307278527	0.3321605824163281
0.3465841312693296	0.5980739010597209	0.4414825334062014
0.5825408928480148	0.3690977198702530	0.3658228458784403
0.6033011378799666	0.3370047851411447	0.5685494809105290
0.4088243612100860	0.7135048235978083	0.4940483379250988
0.3914329674278142	0.5772093324670200	0.5068101017983924
0.5758751503283464	0.6079668722779469	0.4828315694012995
0.5846621613358457	0.6133113495808631	0.5636846065046501
0.4340630226974685	0.3988745930332721	0.5984938798635180
0.4434073698991786	0.6010889863821941	0.5661468621550724
0.4454715057644039	0.3126192178490524	0.4378198306804318
0.3809883610267497	0.3340390649603986	0.4856530826555812
0.3389032045454206	0.5424339906282343	0.3809914659710931
0.5184663368226986	0.2979756960220057	0.4716017278990633
0.5653106819496483	0.6001931503925358	0.4024282302965137
0.3741345904568713	0.4794226961914335	0.3398340094566823
0.3358676763505160	0.3904941065040440	0.4447304164433082
0.3599620092093391	0.6493262252940454	0.5048639428997983
0.3731854683479559	0.3300760541751707	0.4049576191329252
0.6573639204693171	0.6053860458642558	0.4732813091762086
0.5841017385317006	0.5386271847237403	0.5960543850935452
0.6267818966032022	0.6698700046716939	0.5949854072263763
0.4431978795787516	0.5078363400253236	0.3035166846616219
0.4173793458912344	0.6308805780561019	0.6342772012300161
0.5819782172250517	0.4632039121610070	0.6265496460618574
0.5119405525426809	0.6292581158887670	0.5301534328146575
0.4506413348173565	0.5884510966852751	0.3221624231965181
0.6189864090751869	0.6659274670275692	0.5142972668252730
0.6538384353101070	0.4895165955570998	0.4827987783900050
0.4651852045455249	0.3258266116413215	0.6006345064231747
0.3012155286661827	0.4525940384498386	0.4851797083226393
0.5567996547417466	0.4920906891588386	0.6966489461764378
0.6205030565912111	0.5520170753208596	0.5234123795769341
0.4591229031310475	0.5182343451991879	0.4370516312771954
0.3625407817276841	0.6087845746376205	0.5767097660785125
0.5421538890345940	0.5564193819619614	0.5317782389649502
0.5084071235087586	0.4306997181177632	0.6133210436989183
0.4746299417685467	0.5287285386716134	0.5671420578848345
0.4278018167530640	0.5905573120096330	0.4341767046820946
0.5720913666029779	0.4092724833731672	0.5659981144327280
0.3552456535331524	0.4040345645517482	0.6074136583885107
0.3460617825083170	0.5104475121487154	0.5172675346472527
0.3774385156605778	0.5551344413329210	0.3105513363096594
0.2695667107596900	0.5155665361623422	0.5258609271268228
0.5587536819505843	0.5214350101727007	0.3825530058669333
0.4999468998520970	0.4999084689284025	0.5000937414541328
0.5401295093275315	0.3549844332460132	0.6183196555703361
0.4233413612942685	0.5051475064397200	0.5086178434793066
0.5324650082503900	0.5497979897887910	0.4515096908377990
0.4917330470126744	0.6160185513230065	0.6686581032142964
0.5021163803465941	0.6227549211214781	0.4487073312998512
0.5508324286111497	0.4421696172926673	0.3652973187404377

0.4978650974715885 0.3772002679507985 0.5513370553618836
0.5178328761180433 0.5411876424813440 0.3142251976221241
0.6399196480737347 0.5168270695266867 0.3706834893930518
0.3184561859230877 0.5397936229147536 0.5862289412997445
0.5140696677026446 0.3377605921602067 0.3995388393707341
0.6258499855683399 0.5205420148420955 0.6602905613276538
0.5610791279160305 0.3573636654726011 0.5038804229676026
0.5763002325118464 0.4137603088153446 0.2982095725839392
0.3598510164329554 0.4831636094374869 0.6295094715313873
0.6814101414407969 0.4601971487543823 0.4138777840603683
0.3863164388088340 0.6098364924206635 0.3700888982496872
0.4815342554760147 0.7018652204288478 0.5284429151177974
0.3027709611634447 0.5292109576810026 0.4530008162462597
0.6085161265689975 0.4226865619674776 0.4933501878884232
0.6400887103730829 0.3505986499524415 0.4952272678277271
0.3134113189687897 0.5831423474165051 0.5155550338989122
0.3341974953472398 0.4656190897000682 0.4107517628151305
0.5848325102584914 0.4929634447208757 0.3139000041802385
0.5564968737862231 0.3987816648277386 0.4339715866764090
0.5597592119187516 0.5693309815108976 0.6680339943653120
0.6226445731128241 0.4448519222451786 0.6895137477337475
0.5493923863942918 0.4115188317371785 0.6778890314986302
0.4599346463009349 0.6447955303963833 0.3818654112488159
0.4412128367569671 0.4785162750786783 0.6175098906319502
0.5544749379549152 0.6872051324156501 0.5622211714006741
0.4915639581978714 0.5692433622399811 0.3867371264567136
0.3793960316217740 0.4478202786546336 0.4767687774407217
0.4858840618390044 0.6620568055233165 0.6005384157826347
0.5407882267700308 0.4816542388357813 0.5630407509322067
0.6656615566285772 0.5342528432961831 0.5893220980923591
0.4843121951390178 0.4893929289006467 0.3680806071590734
0.5170374367836962 0.5863300845496845 0.6002445780577006
0.4010632104150921 0.3482820141677996 0.6477132715631423
0.4901798709597753 0.5394490195137431 0.7008368861784385
0.6865292439915051 0.4168715117003979 0.4845464996355207
0.4821259401345901 0.4587202497544918 0.6860606148938755
0.5461465044225411 0.6844143421932405 0.4802739438292678
0.5977171359002917 0.6499866546891901 0.3537853217842849
0.4672997071184192 0.4498347015016056 0.5488606567813186
0.4123407438319671 0.6733874563766563 0.5647122003653837
0.4717454808594206 0.6954261392504179 0.4461402938272903
0.5155730795852430 0.5104192050909659 0.6320879392046420
0.5253114447158342 0.4711353549304788 0.4329504993471727
0.3759333936017534 0.3097981628921770 0.6851970255972585
0.3603036871346044 0.2857848243151924 0.7086808304506618

CO/Cu_{147} $E_{ads} = -0.99$ eV
1.00000000000000
31.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 31.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 31.0000000000000000
Cu C O
147 1 1
Direct
0.4151637511646681 0.3867536058109189 0.4364284432443489
0.6034877893858869 0.4657844728883493 0.4233013945397814
0.4182366861654404 0.5368543772877989 0.3733422312567411

0.4234104773968492	0.5862138292092502	0.7014807968465395
0.3969412279713253	0.6627959697828928	0.4312337740714870
0.5875042450446507	0.3266507478155103	0.4353793897900559
0.6300387992643929	0.4365847894016148	0.3551500051904288
0.5300619592921094	0.4289097771708074	0.5021966693023782
0.7301502091654016	0.4844394525657026	0.4744638330202524
0.6269437782301945	0.5956229246718058	0.6287388694622470
0.6606884700945245	0.4574431369115987	0.6191599733962363
0.5909887731155077	0.2865786017872202	0.5059954971042652
0.6186041346966997	0.4760217128683865	0.5553677098073286
0.4239901953568626	0.3920204669906194	0.5174991396736061
0.4878052442530360	0.3706555581175295	0.4699627418887181
0.4068517383745567	0.4280780832170391	0.6674228174618113
0.4696261944220496	0.5708582300690970	0.4979669966306646
0.6967956957463987	0.4706973117456610	0.5472387688222148
0.3426647927160255	0.3946563757506035	0.5265701869245429
0.4157721096344179	0.4614288019858535	0.4037592594398448
0.5099472006810255	0.4606958064324159	0.2993561834768044
0.3905058965268458	0.3407618096531490	0.5665829395726095
0.3697610775330030	0.5635733195160376	0.6446719274283488
0.3726516129744244	0.4043210035946770	0.3710148468716406
0.3808559344865775	0.5238662970449107	0.4444693587738598
0.6986118328255216	0.5473198732491734	0.5151822127973515
0.6451255406859819	0.5963763158751682	0.3925597420286293
0.4577062716386456	0.4435302908156440	0.4682849611280689
0.4402587019699574	0.3561861768613119	0.3670077108852894
0.6109214034673088	0.5455020742216417	0.4419336101026614
0.4828802888703526	0.4137251301124886	0.3997817196738652
0.5355325890796895	0.6743026691876934	0.3990846506700705
0.4535280955791176	0.3154949355869031	0.5195546628312860
0.4752864146502978	0.3768743162314610	0.6674793225189717
0.6532121690915795	0.4017244470642983	0.5587106076928580
0.4145853517966343	0.5069965042477185	0.6859266146676700
0.6373751130508569	0.3912261224137453	0.4234831663235157
0.3110865397615440	0.4590259610501877	0.5670787006209475
0.6098183903086735	0.6594752735721622	0.4336232626895020
0.5593819132890384	0.6438421193571076	0.6327434427142855
0.6134560594924114	0.3899879048418203	0.6300126121582003
0.5083028210967124	0.3841398662023582	0.3314820826179565
0.6891376222304714	0.5409038157829197	0.4328977112364791
0.5926916066244976	0.5722531064382432	0.3325799772449701
0.5249313790805041	0.6203413618686444	0.3367839520617906
0.5764153890794101	0.4947400159766980	0.4916582680599263
0.3963132690166880	0.5341561847510254	0.5766483543857340
0.3891667772752265	0.4542713515229288	0.5581101128312954
0.4391517989040961	0.6424609667535878	0.4959124507771305
0.5279067813687580	0.3044161157024678	0.5537925618300434
0.4488342025252359	0.5575279473498884	0.6346064679769596
0.6639746181240338	0.6093208179027532	0.5555352576681671
0.4402144688255213	0.4308032434954124	0.3319268640093185
0.3466048796353403	0.5981001379229123	0.4409907892500380
0.5825312504323638	0.3692273068304546	0.3659613240764422
0.6030483633506333	0.3370320580246209	0.5685764045750707
0.4090130054879300	0.7133094201463241	0.4937602028982602
0.3914388690330735	0.5771911194661289	0.5063988682466474
0.5759616093870964	0.6080255598164506	0.4827134819670167
0.5845636121948392	0.6132042553720259	0.5635784629908316
0.4350657834189703	0.3991909405520316	0.5989542653304331

0.4433556921798337	0.6009541152911174	0.5658707833659185
0.4453747619132140	0.3128024020245636	0.4375785847253857
0.3810034009242280	0.3342304012901625	0.4858076550735976
0.3388907004387159	0.5425820245731447	0.3805223971470575
0.5182884801709549	0.2980869863936730	0.4714091795239009
0.5658092427403603	0.6005056888132911	0.4022746069672369
0.3741596403111535	0.4795707009973517	0.3394080888262362
0.3359551720960905	0.3907038674952050	0.4444639109173510
0.3600155659994907	0.6492467754560061	0.5044842905152972
0.3732066509399462	0.3304062314636420	0.4049098200704351
0.6575965006745458	0.6054507057886743	0.4734685030579193
0.5837400241339749	0.5383647609908923	0.5960341498242756
0.6265548785371581	0.6696578735984503	0.5950885750779975
0.4434537390772800	0.5079919018893119	0.3033647078433371
0.4172334198327718	0.6308200652621589	0.6338987572687509
0.5812391752335356	0.4628651930069316	0.6266877442600207
0.5120378614109152	0.6292459952133427	0.5299748931012358
0.4510270248449382	0.5885680513808257	0.3220789419100807
0.6190985345356749	0.6659331656556029	0.5143393939676676
0.6536796255706100	0.4896211363625196	0.4829370923895021
0.4644337121430241	0.3253564842074412	0.6004670602916483
0.3013362420428934	0.4526399239663321	0.4847605172377704
0.5563289997674778	0.4921238168259496	0.6966013530775474
0.6204117309514589	0.5520345887128700	0.5234377531479932
0.4591575301652483	0.5182537446089820	0.4369499327286415
0.3624141669521179	0.6088010890181139	0.5762708373553368
0.5420304288440498	0.5562155597693462	0.5317548633460487
0.5072815481946379	0.4293181549122205	0.6146002080332039
0.4744035724915100	0.5284123708436349	0.5670999178171653
0.4280206442240385	0.5905597232616732	0.4339149729323116
0.5718486650750138	0.4093135510135461	0.5660463459449353
0.3553126348984801	0.4035887621425101	0.6074736206795407
0.3461115138224519	0.5101991705180245	0.5169718763775973
0.3779398997117017	0.5553943546082574	0.3103091098620280
0.2697150484873339	0.5154073387496246	0.5253873196284538
0.5590590154551073	0.5217251737452934	0.3825715634560707
0.4999492790247593	0.5000250382285631	0.4999175065457203
0.5397446937201063	0.3550378049492501	0.6179340791549728
0.4232692397928620	0.5050960367691926	0.5084323785315337
0.5326554471086894	0.5500328154146497	0.4512707409721545
0.4914103813812598	0.6159939072602384	0.6684223028725926
0.5024887018934396	0.6228375373012599	0.4485025337840837
0.5509833807732232	0.4424271929827212	0.3654080023862316
0.4974756028660709	0.3770192653517030	0.5517118588790599
0.5182537030728531	0.5413767002812562	0.3142782600013774
0.6402692673906970	0.5169553449563347	0.3707603203294159
0.3183023324950343	0.5398386465049984	0.5857106127756428
0.5140031625345245	0.3379113535246077	0.3994330338344962
0.6254237600954951	0.5204348396465693	0.6602847818067856
0.5607451692365494	0.3574174134157056	0.5040534513276745
0.5763887053708808	0.4140102361959462	0.2984356776531950
0.3595823753533046	0.4831741477329410	0.6289930250530756
0.6815031937524061	0.4602264447332086	0.4140205720784944
0.3865143800029700	0.6099402000312418	0.3697972998476499
0.4816392803534709	0.7018701325426794	0.5283172641576391
0.3027804876351886	0.5292644405490237	0.4525133840894822
0.6083221834297574	0.4226939002440079	0.4933828480370402
0.6398986692659364	0.3506294478131228	0.4952435427148309

0.3133556990440598 0.5830664777776479 0.5150201074259115
0.3340859337831760 0.4657644536039930 0.4102156658922981
0.5851043604463411 0.4931787251573116 0.3139314149030125
0.5563832886724359 0.3989306630827835 0.4340698876794546
0.5594066551516065 0.5693165866287248 0.6679857446890668
0.6222445030059727 0.4448735365789049 0.6895174159532311
0.5493714555632383 0.4115225679594313 0.6780903722413878
0.4603508753666626 0.6448649528724324 0.3817394457189426
0.4409084208744806 0.4780895973498397 0.6176206520699614
0.5544499380219396 0.6872503149020560 0.5621508714431541
0.4919278580415508 0.5694007685653657 0.3866487798833217
0.3793870767661884 0.4480370233855510 0.4763114500380070
0.4857805386178033 0.6620994468378887 0.6003410879667866
0.5400534022263579 0.4810731436983198 0.5634211520831323
0.6654327284228355 0.5341918657849659 0.5894755126603187
0.4844717043153854 0.4895950867624152 0.3680549301822579
0.5168192002323940 0.5862799773452482 0.6001057113223091
0.4008237273210324 0.3493414968834797 0.6462040486225126
0.4898101207046094 0.5394196481318638 0.7006669087187612
0.6863242554860518 0.4168843858729921 0.4846642590166284
0.4815851934589382 0.4588734491728715 0.6856357925923559
0.5464043049748395 0.6845529100038615 0.4801656339321673
0.5986698839577360 0.6503899194534372 0.3537360764297635
0.4672348951183043 0.4498375620968136 0.5488258560265930
0.4123385275043020 0.6732811662960475 0.5644237864112400
0.4719969321601206 0.6954628816896667 0.4458927776363180
0.5153064724807579 0.5103553460573022 0.6319647057425408
0.5253104280659537 0.4713003127658219 0.4330230325713798
0.4721434190294057 0.3431759375216191 0.7164916423427655
0.4702085443349200 0.3221398435283681 0.7470498472198017

CO/Cu_{147} $E_{ads} = -0.96$ eV
1.00000000000000
31.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 31.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 31.0000000000000000
Cu C O
147 1 1
Direct
0.4152290537459859 0.3866372442617368 0.4367840499125399
0.6034681296191038 0.4659463730856257 0.4230555568604630
0.4179909673924024 0.5367319481423268 0.3735269378241859
0.4236492906898308 0.5863699395677830 0.7015963415925613
0.3968483273608069 0.6627090586930364 0.4313670795540018
0.5875314630941182 0.3268083986698345 0.4353339373971929
0.6299212218345377 0.4367019963417167 0.3549199121950735
0.5302739149134791 0.4290390863225764 0.5021446900543577
0.7301050419236129 0.4844980684188616 0.4741762762488475
0.6273391167487695 0.5955522121511525 0.6286628938036213
0.6606080395259253 0.4573998505982220 0.6192221915885743
0.5911786054862946 0.2865809242509606 0.5057395464371284
0.6188033917452043 0.4759932544259248 0.5553731540147618
0.4241981574169200 0.3918257655694977 0.5178514030282435
0.4879636974509017 0.3706438971351312 0.4700248303759821
0.4080149492519201 0.4278874357529038 0.6678381573640126
0.4696961701575132 0.5709989278317276 0.4979737637313241
0.6970177124077604 0.4708407271163111 0.5471879269530888

0.3427004650749439	0.3943742203579790	0.5271990155574233
0.4157224087298034	0.4612511208823029	0.4040110233485296
0.5096438371378073	0.4607200945239541	0.2993819145192673
0.3908335058615545	0.3405922827657017	0.5671684590153010
0.3699650741960010	0.5636862345327600	0.6448691051992254
0.3726779440402670	0.4042234961476808	0.3712965788087402
0.3807794449669059	0.5237638508812210	0.4448377174268477
0.6985322927998462	0.5473823296038272	0.5148245808808050
0.6452502463160179	0.5968081314523610	0.3920635540987031
0.4578961437813973	0.4435413226645951	0.4682496046196086
0.4402407371608251	0.3561578525894511	0.3671484221172694
0.6110679164507273	0.5457556105272443	0.4416712507380012
0.4828107416742587	0.4137419765252809	0.3997975874779532
0.5355650550015824	0.6743935490666380	0.3989374774966153
0.4535530572568119	0.3153635231177734	0.5199330481257916
0.4763178671286533	0.3783528774130483	0.6659975395682851
0.6536585994346363	0.4019094595967030	0.5586052897756982
0.4144350684586634	0.5072993078739565	0.6860806538456073
0.6373332227269127	0.3914190000800485	0.4233049331317770
0.3111560556393441	0.4588366888827729	0.5675116388234595
0.6100485424391280	0.6598325218460036	0.4331546613027433
0.5597105338563427	0.6438915001420158	0.6327257162580827
0.6133684617346987	0.3898354574179111	0.6297558065296278
0.5081677578714516	0.3840628671691115	0.3313991183566768
0.6889800893626555	0.5410311026333808	0.4324459567528416
0.5925216505016377	0.5725002485005402	0.3324022873121300
0.5245937670142651	0.6204054105800125	0.3366228171189343
0.5765742855552608	0.4948947031443754	0.4911385441211874
0.3965513542651291	0.5342155377137714	0.5768971391322223
0.3893565390563155	0.4541952144381476	0.5585912660042737
0.4391869195647978	0.6424753153863322	0.4959193589211024
0.5279954985374978	0.3040995780883898	0.5533586547758546
0.4490912067406829	0.5576134615155786	0.6347202377686951
0.6639630604541807	0.6093330459797404	0.5552253712344039
0.4399717549649757	0.4305912998072549	0.3318783044482997
0.3463168866325284	0.5981533285050594	0.4412750035940955
0.5824479143122120	0.3693348629080396	0.3659177466859880
0.6039865393297338	0.3369835306648756	0.5679772039586615
0.4089861535620609	0.7133036129764077	0.4938570622081460
0.3914820474640476	0.5772086698681843	0.5065558460177366
0.5761568598901955	0.6082603625867109	0.4824939502617311
0.5847871253469819	0.6132001623223483	0.5634734871530980
0.4356817336368559	0.3993169736259040	0.5991845211651271
0.4435838736515685	0.6010123620477369	0.5658589839737282
0.4454325522634676	0.3127754795908486	0.4378987913723781
0.3809228580706098	0.3341001938656717	0.4861799999805506
0.3384494676582224	0.5423283928616817	0.3807912019661969
0.5184012813863903	0.2980779837307533	0.4712983362654029
0.5658654670480034	0.6007328403864099	0.4020427382386224
0.3736676287454518	0.4793318312024747	0.3396555478111106
0.3360427875300819	0.3906132323139788	0.4448680134342261
0.3599528921606901	0.6493147805152981	0.5046971506799496
0.3733568913947625	0.3302258962702874	0.4052345223339817
0.6575186119474087	0.6055229701939432	0.4731300321794403
0.5839604297537301	0.5383447697156333	0.5961098201006789
0.6266603670396258	0.6696492046127749	0.5949405434508880
0.4429476129796843	0.5077855455202667	0.3035327959788820
0.4175288797456703	0.6307631633624611	0.6339950938552036

0.5805570586853996	0.4620358683584604	0.6271303219051138
0.5121380031503868	0.6293772959446526	0.5298525905724530
0.4508193113859280	0.5884626671568791	0.3223219564375417
0.6190620128545792	0.6660230998713284	0.5139917786890625
0.6537367670154046	0.4897661185502888	0.4828156989959733
0.4651395398677049	0.3256520332594618	0.6011142274855821
0.3014643804303406	0.4525841116839759	0.4852483324817710
0.5562689242510371	0.4920688238569690	0.6964915878659818
0.6204650904193911	0.5520241656322733	0.5233689994051650
0.4591926046011599	0.5183333727854185	0.4369740929890983
0.3626485419540557	0.6087657772827881	0.5764156303103189
0.5420844057190477	0.5566390662575517	0.5314689034729719
0.5081099935196762	0.4308013943499817	0.6128622170822289
0.4746956748694384	0.5285264431950202	0.5671233649255266
0.4278625948684267	0.5904781596019126	0.4340114209704485
0.5721537264342955	0.4094483245831296	0.5658663269651121
0.3557050771258980	0.4033448445414423	0.6080812652208194
0.3462702497663345	0.5101044743343521	0.5174124280194113
0.3773534082331251	0.5550339566928549	0.3106537603961231
0.2699016761688537	0.5154295763603810	0.5259889369476741
0.5589457843370278	0.5219248177203983	0.3825065765698803
0.4999951381253248	0.5000245303478846	0.4999614775824341
0.5405716760793409	0.3545838297562309	0.6160055350043775
0.4233941325530954	0.5052980231927504	0.5085632227587881
0.5327628059395977	0.5501881284298018	0.4511765663722692
0.4916917652105226	0.6162990088968920	0.6684048754534891
0.5025550294619495	0.6228515706773075	0.4484033296474256
0.5508241964859257	0.4425383497387262	0.3653112294588530
0.4975183551908567	0.3771218698441541	0.5514796192977425
0.5178531258500817	0.5414582038474824	0.3144064666235046
0.6401980206504548	0.5171939664056847	0.3704621333658601
0.3185775436733365	0.5397209451424253	0.5861325898498816
0.5139846743814042	0.3380399618754567	0.3994642850143099
0.6255450777321213	0.5200713577625540	0.6602100416684034
0.5608974548229217	0.3574403217178465	0.5039602047083543
0.5761588926797739	0.4140757232166039	0.2983244959533174
0.3598413386321162	0.4829035441577110	0.6294288984577190
0.6814471314031622	0.4604050631610816	0.4137342550044961
0.3861307048990634	0.6096913123222835	0.3700537618201061
0.4817018947927749	0.7019487335811689	0.5283045053167869
0.3028314718450386	0.5292655879422372	0.4529338858800978
0.6084897552615536	0.4227770988043658	0.4932970988507823
0.6401319456863732	0.3507201742039122	0.4948580616737761
0.3134484627191051	0.5830828640363998	0.5153546437917812
0.3341654563835266	0.4656178009986763	0.4107549332705090
0.5848200250514626	0.4933196061630803	0.3139730844937662
0.5564094658895663	0.3991051432375885	0.4339632036527743
0.5599515773816902	0.5694355906247416	0.6680167207853984
0.6213272242776364	0.4441208287298137	0.6895530036272469
0.5485798911712926	0.4097235518316533	0.6799382371492153
0.4601942967961518	0.6446399904077127	0.3817689478373212
0.4410404876410975	0.4782144132447486	0.6174893092412189
0.5546123612480639	0.6873153135837771	0.5619851973075760
0.4918391926906315	0.5694833416613260	0.3866142449749269
0.3795481517014020	0.4478159607896213	0.4768964440977984
0.4860059160072695	0.6621136186102802	0.6002799414352822
0.5408836258023478	0.4818885697757916	0.5627499247604921
0.6656543488262900	0.5341291917108596	0.5894913869667303

0.4842209674015349 0.4895785898800291 0.3680837350344139
0.5170773939469615 0.5863460002827814 0.6001517197148041
0.4029586928168184 0.3495590943255840 0.6474470683089260
0.4902938364771212 0.5401831460666442 0.7008213537747489
0.6865055344220955 0.4170040830530728 0.4844842840184262
0.4812248606937150 0.4607123741461999 0.6853409374784973
0.5465059484625709 0.6846929702520841 0.4799666465995603
0.5983926207447806 0.6506645975732568 0.3532310922417640
0.4670776546709490 0.4499534364219235 0.5484938598504978
0.4124974249105788 0.6732382173803819 0.5645497447152650
0.4720153081399821 0.6953260286846941 0.4459205218346926
0.5156753331658498 0.5105129062815682 0.6318901917936782
0.5253412647432650 0.4713675734889900 0.4328989431983039
0.5154473308940187 0.3682152787870179 0.7151898009141002
0.5178368854556220 0.3487341443283047 0.7473243054486230

CO/Cu_{147} $E_{ads} = -0.93$ eV
1.00000000000000
31.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 31.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 31.0000000000000000
Cu C O
147 1 1
Direct
0.4150573229486022 0.3868019955345329 0.4361749507039466
0.6033870315373329 0.4657661796244922 0.4233060892388252
0.4180644647671364 0.5368630867712807 0.3733456843312444
0.4235462236525742 0.5862595032931588 0.7016211063120046
0.3968408050326080 0.6627971232323169 0.4313988574552232
0.5875371900833390 0.3266796310248622 0.4353240404678319
0.6298971953997943 0.4366099514022725 0.3551385852449285
0.5300824633702820 0.4288711377481206 0.5021775507040303
0.7300536903585320 0.4844452869718442 0.4744164318498980
0.6269665586468469 0.5953762824263484 0.6287530264023642
0.6606033563925316 0.4572797588848501 0.6192859650485931
0.5911293028342633 0.2865467238962775 0.5058821170383492
0.6185445412755509 0.4758649146463594 0.5554610963839366
0.4238503766588398 0.3919560669659083 0.5170710499559765
0.4877610152966778 0.3706651628414979 0.4699391145320896
0.4064522972281522 0.4290306979324519 0.6672920257324314
0.4695271058698633 0.5708337630873676 0.4980459808325577
0.6967060438628112 0.4706132070701148 0.5472708231098534
0.3427844178281123 0.3946997503544913 0.5266485598333133
0.4156411703281717 0.4614359969986534 0.4036860261579299
0.5097836734304387 0.4606687989871727 0.2993426969419256
0.3907366569019579 0.3408815068661842 0.5673014522840190
0.3698389196446912 0.5636558565919793 0.6447513506644873
0.3723636747647887 0.4043177905055296 0.3709079061533110
0.3807163496309304 0.5239139672003876 0.4444659506765588
0.6985394633846860 0.5472355239026616 0.5151348295483519
0.6448752913657685 0.5961886803575897 0.3925492105793950
0.4576430980909146 0.4435216177320758 0.4681959187324326
0.4401256805532620 0.3561702013320886 0.3668781151144988
0.6107874572043279 0.5453927613508627 0.4420114548096045
0.4827849142539625 0.4136841435559235 0.3997098735845331
0.5352228679458064 0.6741823036978756 0.3991856455388622
0.4535327177355805 0.3153789198484386 0.5193070737640170

0.4762694524444779	0.3772811213889977	0.6674014285615416
0.6532269270068727	0.4016182353460209	0.5588064942669853
0.4147264811318466	0.5071969131732058	0.6860217518257782
0.6373406731707746	0.3912747647243566	0.4235307717226670
0.3111829233092097	0.4589505602347666	0.5672604294909204
0.6095328271160887	0.6593623290224004	0.4337295135319544
0.5595374827955569	0.6436550836537626	0.6328678962023688
0.6134285183889649	0.3897642827265042	0.6301434946733531
0.5082287124762289	0.3841258224936733	0.3314242329872014
0.6890748429860456	0.5409161271072692	0.4328615986208751
0.5923200087681973	0.5721214024014439	0.3325642767423120
0.5246086928703604	0.6202270010143581	0.3368672897184303
0.5763346665170149	0.4945660020363905	0.4917598511129798
0.3963243258020147	0.5341227933653468	0.5767190816125558
0.3888779624182241	0.4545053261076364	0.5579153770277203
0.4390735908038081	0.6424297058236281	0.4960821599406706
0.5281583431922412	0.3043618006259812	0.5535745586863394
0.4489456776100652	0.5575635452436073	0.6347180343676618
0.6639569575689462	0.6091895774707363	0.5554942381980070
0.4400583625821383	0.4308336493857123	0.3318463639635899
0.3465127011587626	0.5981461239628930	0.4410409002795114
0.5825218824983323	0.3692885720203635	0.3659108095034275
0.6030304880754245	0.3369390253265246	0.5686256724139905
0.4090151630382554	0.7133455761059726	0.4939059309575726
0.3913572890364841	0.5772355219199634	0.5065120482626436
0.5758812883764974	0.6078540036681505	0.4828072961446817
0.5845684435915224	0.6130261619264210	0.5636797241541790
0.4347881594290309	0.3996864495322273	0.5978200417593189
0.4433915738799859	0.6009321859946392	0.5659984200403865
0.4452822102403484	0.3128667055133439	0.4374783226323310
0.3810119086288274	0.3342140512583196	0.4859564224889850
0.3387710074186468	0.5426761368634828	0.3805523560958777
0.5183446911322269	0.2981021079928459	0.4712617981003697
0.5654779179743634	0.6002965863294759	0.4023755182431170
0.3740326005791845	0.4796234234187284	0.3393616459378463
0.3358977421017769	0.3907298506423508	0.4445247159129253
0.3599855771165467	0.6492866630635316	0.5046407988362328
0.3730229868907989	0.3304970373207275	0.4048777736111441
0.6575410587114164	0.6054095437402097	0.4734025492351147
0.5837093746956324	0.5381625717180021	0.5961561574342930
0.6266308090973597	0.6694514300497163	0.5950629172327633
0.4432788655056435	0.5080613905127068	0.3033427028472589
0.4173752938866772	0.6308096660453626	0.6340440853093382
0.5811363724360158	0.4625636658773438	0.6268761491135058
0.5120404239765889	0.6291502189151459	0.5300503016037713
0.4507191941469313	0.5886106769322188	0.3219543418321918
0.6191383798125075	0.6658365478250684	0.5143381969518652
0.6536096371728269	0.4895125882075196	0.4829956890766904
0.4648019256665922	0.3249156737603935	0.5993715274891971
0.3013102571888832	0.4526590979410843	0.4848651417592362
0.5563576847242709	0.4918321826332971	0.6967745830363541
0.6203449917967825	0.5519387417238190	0.5234194709954300
0.4589918509652003	0.5182092216671732	0.4369566626577573
0.3624530298383390	0.6088006762607885	0.5763551182873893
0.5419550982637631	0.5560627887983776	0.5319207420074109
0.5072601680143112	0.4291449090652547	0.6147348062880215
0.4744257265457125	0.5283947054236467	0.5671762213405607
0.4278496626255763	0.5905299468021210	0.4340322237291288

0.5718371424838302	0.4091340581371203	0.5661817697130787
0.3559222508286656	0.4030985841846047	0.6078473894217354
0.3459754152800647	0.5103929311378903	0.5168756173101582
0.3777738179674853	0.5554961295566602	0.3102779589991495
0.2696550736770524	0.5153830872015154	0.5254185536440518
0.5588663451420539	0.5216070133367133	0.3825812759795110
0.4998850167833604	0.5000244890525827	0.4998706280722811
0.5396194520439952	0.3548637773254821	0.6182965394427284
0.4231870098447962	0.5051510880062943	0.5084303245270921
0.5325390205792516	0.5499315095273143	0.4513537711359663
0.4916475634238577	0.6158431206969056	0.6686239498839617
0.5023039173909859	0.6227567875788245	0.4486243781231218
0.5508527997985763	0.4423571590474182	0.3653910881684831
0.4975920069175201	0.3770650071853065	0.5516483557855696
0.5179912242837819	0.5413233893179957	0.3142725912963920
0.6401216855434756	0.5169488886152774	0.3707447682212435
0.3182883648972715	0.5398729514997371	0.5857344747489620
0.5139350350018197	0.3379662565424258	0.3993695455404155
0.6254557485207860	0.5200938821820297	0.6603473501830619
0.5608419666329855	0.3573955992126006	0.5039822590544681
0.5763103591936339	0.4140510670064642	0.2983558927539429
0.3594738599892492	0.4833205021917094	0.6290267160899099
0.6814262536269518	0.4602058629104535	0.4140232052188166
0.3864210356674938	0.6099817384095089	0.3698350607545816
0.4816541381123458	0.7017718508538405	0.5284355200810490
0.3025413876118296	0.5292823000614357	0.4525146787539944
0.6083431714830837	0.4226440373472956	0.4934754667022919
0.6399898021528497	0.3506103256726661	0.4953005810530707
0.3132129482053665	0.5831548601444583	0.5150902229754329
0.3339473564617036	0.4658266446688790	0.4101738566680510
0.5849236014711172	0.4931553392968967	0.3138678665643059
0.5563578878921205	0.3989099430992862	0.4340440804372291
0.5595256321993195	0.5690677243193756	0.6681500038225938
0.6220372521830855	0.4444647220167472	0.6896502192579785
0.5489310200226147	0.4109047373198243	0.6784611223968732
0.4601290165960125	0.6448097565905282	0.3818307485400835
0.4410401647828744	0.4781247677937431	0.6176259262502328
0.5545117826863650	0.6871062653584096	0.5622846082216654
0.4916532607821503	0.5692909489322353	0.3867085555126242
0.3793174965414756	0.4481372477824939	0.4761922750311153
0.4859368482898096	0.6619616389881849	0.6004715526879062
0.5400053837727461	0.4809071951664838	0.5635608657758158
0.6653877226826693	0.5340483135345998	0.5894522426782750
0.4842916169832847	0.4895187939275917	0.3680492853147048
0.5169208682749562	0.5861364124788518	0.6002460229742079
0.4037313520194014	0.3496063203252374	0.6479314420152285
0.4898711471154873	0.5391933411010894	0.7008011367524368
0.6863484686320790	0.4168599427668756	0.4847140123309077
0.4816356491211213	0.4583631476389223	0.6858808471149513
0.5463621488580628	0.6844527107046666	0.4802612539155103
0.5982948229922544	0.6501351047556650	0.3539603519988243
0.4672447095653396	0.4499939947784860	0.5485586441514040
0.4124410769694054	0.6732828263840210	0.5645628236225275
0.4718754539437685	0.6954542910102322	0.4459988323586253
0.5153143377451954	0.5101472765213851	0.6321819940762938
0.5252038160965654	0.4712326993526614	0.4329936591582143
0.4457483889816841	0.3372392722057366	0.7020501708267558
0.4366758507733825	0.3136184045350132	0.7299151055311014

CO/Cu_{147} $E_{ads} = -0.90$ eV
1.00000000000000
31.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 31.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 31.0000000000000000
Cu C O
147 1 1
Direct
0.4153370887170150 0.3866525787559681 0.4365703287498279
0.6034853586360497 0.4657520425025973 0.4231179425121375
0.4181820945248986 0.5368689110297472 0.3735699145556561
0.4236274228859280 0.5864568162259080 0.7015441220411621
0.3967382922506227 0.6629874526682826 0.4313984473056103
0.5876411655988439 0.3265666709638714 0.4352593719385054
0.6299315290878480 0.4364941162626156 0.3549411035242522
0.5302993308241546 0.4290811252648974 0.5019175542375904
0.7302072990227887 0.4846106111152327 0.4739268419493559
0.6271546042159336 0.5957067188039000 0.6284429479131066
0.6610734388484786 0.4575299464374565 0.6188917450592035
0.5910991176277108 0.2867205461647895 0.5058717410792172
0.6188304273839910 0.4761813250767058 0.5551643862216598
0.4241266594641400 0.3919801941310033 0.5176272941663645
0.4879542287869893 0.3707014481941739 0.4700884605052091
0.4068079233751037 0.4273372036371462 0.6672994372902216
0.4696840733163491 0.5710412527157807 0.4979504896658518
0.6969434335299450 0.4708221006635684 0.5468855959251862
0.3427330473331229 0.3945727241580067 0.5269076428519215
0.4158575932387413 0.4613044090666700 0.4040789597847122
0.5097875961703374 0.4605165572225117 0.2993463833194067
0.3905092936599692 0.3404162924002759 0.5666730613285026
0.3699983144278672 0.5636121168707208 0.6448319235440210
0.3726741598421345 0.4041694420372051 0.3712942929784467
0.3809684249510445 0.5238671904813684 0.4447660849075211
0.6985642061798506 0.5474212682421261 0.5147750770416563
0.6448085110537803 0.5965819706047359 0.3920985541106397
0.4578204446402139 0.4435095723806525 0.4683892842981364
0.4403394818556687 0.3560140991031708 0.3671426239109019
0.6109251426286454 0.5456716822806816 0.4416695079892826
0.4829138399007996 0.4135821624808405 0.3998767770761540
0.5353084590185287 0.6745166083466828 0.3988852848322734
0.4537852488499126 0.3156367626788691 0.5199518570015779
0.4753985543229820 0.3785860405073406 0.6630657386891352
0.6533123591091324 0.4019264314149155 0.5585413216293406
0.4143549776667763 0.5074052087601333 0.6858776657166330
0.6373902749554050 0.3912194150179728 0.4233551964725663
0.3112519834486324 0.4591019303020992 0.5673393685652165
0.6095517576555223 0.6596787724950144 0.4331652754588159
0.5595930179725102 0.6437654785757306 0.6326042808145067
0.6138617751096568 0.3900132756032460 0.6297163968526726
0.5082847857476397 0.3838922068097715 0.3314493930484715
0.6890188903672709 0.5409975819308652 0.4324442511402187
0.5923189450052212 0.5724122185453094 0.3323297781858137
0.5246086217122296 0.6205624091306886 0.3365039287481841
0.5766121293608325 0.4949013690351178 0.4913008923313841
0.3968569586158251 0.5339133431544391 0.5769628905547147
0.3894626000206464 0.4545397251870123 0.5585375496963509
0.4391483834780463 0.6425555305919295 0.4959538162737542
0.5281134563847698 0.3047408840319495 0.5539042773758602

0.4491747806587367	0.5574089544216445	0.6348377190770009
0.6640431568140855	0.6093934325326177	0.5551993553570315
0.4401798666392612	0.4305704056272757	0.3321181102235755
0.3466090826038871	0.5981862399274515	0.4414221007496557
0.5825812734762797	0.3690896570489014	0.3657385979313769
0.6031501573118804	0.3372907413901877	0.5684046706129384
0.4089196964775537	0.7134555299128778	0.4938950497547916
0.3915902835458055	0.5772115441638601	0.5068013230012846
0.5759961807430087	0.6081987501564575	0.4823765019051883
0.5846485237879329	0.6133382395985100	0.5632543314049867
0.4344652441795712	0.3994202917568726	0.5981987794937720
0.4435867479163927	0.6009336523244964	0.5660776811435489
0.4455176675059185	0.3127810665303274	0.4379141702263274
0.3810947356359191	0.3341889027854265	0.4859029168883661
0.3388601735306785	0.5425289646451288	0.3809334210762989
0.5183898275131408	0.2980912354730886	0.4716223680787174
0.5656203485385006	0.6006920011116309	0.4020138457555195
0.3740795492744209	0.4794654337696972	0.3398272476426833
0.3360138205846455	0.3906280173845199	0.4448063180945112
0.3600578839749040	0.6493073459559521	0.5048060156874666
0.3732854776274617	0.3302633181613353	0.4049847519485898
0.6573832969007515	0.6055000724965959	0.4730660078429770
0.5837063697463174	0.5385126998731496	0.5959820335745228
0.6266842379410399	0.6697060510982460	0.5947396564784038
0.4431814773405670	0.5078821984288706	0.3035303432213409
0.4174806254558008	0.6308837826362249	0.6340738302091257
0.5816080023006631	0.4631093258180906	0.6265880136856847
0.5119933942685460	0.6292746295101627	0.5300470454361028
0.4507216176897404	0.5885798758439472	0.3221903949079384
0.6190565537794785	0.6660252793483938	0.5140257015055643
0.6537407276689158	0.4897238173168844	0.4825813665311749
0.4647114694085474	0.3254389349793737	0.6008832040000434
0.3013841572022855	0.4525716144306883	0.4851912881874069
0.5576436515730311	0.4925707593192419	0.6964391208402928
0.6204689100570160	0.5520644840636606	0.5233047665890613
0.4593093014456391	0.5183584522072012	0.4370556716327935
0.3627314481755191	0.6087288699277987	0.5765940912945371
0.5421481868097590	0.5564449445866336	0.5314558161686258
0.5076690707074930	0.4310335172769577	0.6147858879898088
0.4747121939885144	0.5284602123978035	0.5672257263695941
0.4278947264037001	0.5907175781756587	0.4340775532756784
0.5717073987698666	0.4094932190200528	0.5660543015673749
0.3550932141442516	0.4034409006475408	0.6076495691030335
0.3463332014966527	0.5103263071364206	0.5172388850803765
0.3775853294063062	0.5551451631823872	0.3106407933518934
0.2699247350292177	0.5154859962664733	0.5257702835027466
0.5588811163355112	0.5217664490789368	0.3824689236643266
0.5000006340538258	0.4999990974818415	0.4999938795614460
0.5399200898547676	0.3551378122987955	0.6181864628737596
0.4234994889774363	0.5051273313107968	0.5085472508474240
0.5326521682265809	0.5501073341344755	0.4512165348018997
0.4917580078408388	0.6162384284266558	0.6683694109917985
0.5023486020290348	0.6229857694819442	0.4484210187494675
0.5508924357228637	0.4423727024681151	0.3653007930955247
0.4977434995203006	0.3774397717203914	0.5518097496875312
0.5178941672195163	0.5412965283158891	0.3145267586683802
0.6399880272978493	0.5169893088536395	0.3706066921790533
0.3187908159234096	0.5397530177330103	0.5860704078075246

0.5140651109174161 0.3378564921062701 0.3995241953013273
0.6260282752436134 0.5206198427275474 0.6600013209093274
0.5608645563522007 0.3575462166448944 0.5038761795428007
0.5762172958461722 0.4139178840158329 0.2983026103876183
0.3600995028415518 0.4830130873149971 0.6293554699585265
0.6814769107880145 0.4602355950196117 0.4136947495752408
0.3862476627877247 0.6099697467274513 0.3700606058647383
0.4816179630954160 0.7018688608952917 0.5283744413672068
0.3028401587435613 0.5292661107616655 0.4529596985082661
0.6084422957934869 0.4228122817432952 0.4933454855325131
0.6400245238958684 0.3506996251956538 0.4951879479251275
0.3135428338262282 0.5831311646930276 0.5155274467853402
0.3342895287650268 0.4656962532888076 0.4107348456825680
0.5848611761957483 0.4930937172970344 0.3139188215140197
0.5565238873487616 0.3988951935159280 0.4338409048275635
0.5597543197591053 0.5693170817626881 0.6678389126610704
0.6228022239526154 0.4448325925564966 0.6892048225709292
0.5499782869643832 0.4109026494405809 0.6775397575291884
0.4600492245010798 0.6449773952289062 0.3817978854902276
0.4419109111453600 0.4778298661566234 0.6188693691400198
0.5544828867288932 0.6872700748918074 0.5621166661768739
0.4918077416832037 0.5695234379253039 0.3866528572149756
0.3795361421044097 0.4478709898827268 0.4768316788660063
0.4859520903830079 0.6620166825541717 0.6004222725367944
0.5405066815872882 0.4816115331919972 0.5631456474445768
0.6655980629181762 0.5342768143686256 0.5892078726375140
0.4843722523124092 0.4895091216532740 0.3680922680508339
0.5171070170133153 0.5859028799908338 0.6001570780296046
0.4016222138223720 0.3491630507919065 0.6465683913159058
0.4903724394725467 0.5403751951836728 0.7006669348677196
0.6864405085011943 0.4169479114292874 0.4844650698828312
0.4815672284314322 0.4574825642044867 0.6910911668555372
0.5462505715749884 0.6845026231864287 0.4800474035422150
0.5981374518808904 0.6505846537815908 0.3531383758736183
0.4674248716666329 0.4499780567608834 0.5490349101906715
0.4124977887685347 0.6732569247271882 0.5645805057516892
0.4718770191550128 0.6955694507342292 0.4459355790824507
0.5149296843826958 0.5094253930291255 0.6329970356172769
0.5253363663301910 0.4713502703507526 0.4329607110245275
0.4758712222778228 0.4443618669500874 0.7492364048954270
0.4722862677474870 0.4361670280016886 0.7853097458922593

CO/Cu_{147} $E_{ads} = -0.87$ eV
1.00000000000000
31.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 31.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 31.0000000000000000
Cu C O
147 1 1
Direct
0.4154075909114055 0.3867093936587166 0.4366100948470307
0.6034376904016865 0.4658440062222365 0.4228911833729632
0.4183818937008660 0.5368566635678635 0.3731885599210703
0.4235431205162708 0.5862735292091371 0.7015696396145898
0.3968215235030987 0.6629313816803908 0.4311849746437378
0.5876251680339365 0.3265069123194931 0.4348982433434290
0.6299020573275877 0.4367360108096249 0.3546768694581572

0.5303425515001756	0.4290961114391208	0.5017411221732084
0.7301293545948396	0.4847725282363223	0.4738728836714086
0.6269042354095704	0.5954271748466986	0.6287326395806888
0.6608970553975854	0.4574621496457603	0.6188275541697422
0.5911244886497591	0.2868921122499472	0.5056224970083836
0.6187417804235301	0.4761887905338034	0.5549828510741882
0.4240902133539630	0.3919191716953378	0.5176609235566828
0.4880077325440368	0.3707184360044351	0.4697222056832961
0.4073070156922285	0.4266990842061282	0.6706392088184110
0.4697952620355436	0.5708796940696376	0.4978947682818590
0.6967506894516450	0.4707911283174815	0.5467481980476042
0.3427499928072620	0.3946516117532850	0.5270669281541427
0.4158640213684814	0.4613949491180012	0.4037888856132417
0.5098095135592123	0.4605970283998007	0.2989635782653580
0.3905757820996013	0.3405369252766431	0.5666255370623501
0.3699381770129067	0.5634400738821799	0.6447786214777321
0.3727872366039685	0.4043284505499740	0.3711633947904335
0.3810029674514783	0.5237659481707400	0.4444447213460289
0.6985823650365467	0.5474367914433846	0.5148917393557539
0.6449291517406266	0.5967289547267296	0.3922886612019339
0.4578662660873726	0.4435716832883954	0.4682192129336519
0.4405217080674885	0.3561564839616753	0.3670259930997593
0.6108912345774890	0.5457742061407082	0.4416003310923591
0.4830292823173646	0.4136302245128422	0.3996044409672694
0.5355253897077379	0.6745406142087808	0.3990507587076595
0.4538689205613193	0.3156659155789394	0.5200936271714187
0.4749338433524680	0.3785988553927668	0.6663290916172527
0.6532696457021628	0.4019107346885509	0.5583320037434238
0.4145783974156165	0.5073348246254406	0.6859766920138486
0.6373598541698312	0.3912649935339652	0.4230353871087531
0.3113425018501171	0.4591173347484395	0.5672646000797580
0.6098218777212252	0.6599183695500943	0.4334101778913579
0.5593976094303427	0.6434331137281819	0.6328605129756242
0.6136866009910230	0.3899759521525556	0.6296986540984694
0.5082294404312399	0.3840101814503316	0.3310506515973536
0.6891490479502125	0.5411497580912265	0.4325166881642543
0.5922201600564367	0.5725474736183215	0.3325188356414489
0.5249147405365107	0.6204006038548870	0.3367052560184912
0.5764615913998032	0.4949656709251061	0.4912539310767929
0.3965660131731876	0.5339923521015338	0.5767045520790843
0.3892346522842739	0.4545475688778253	0.5580506061268800
0.4391733890827325	0.6424595351054363	0.4957469790989780
0.5280843077648095	0.3048721609945004	0.5538588732480008
0.4488417428042509	0.5572341132594020	0.6346429780748245
0.6639762114662630	0.6092216347913881	0.5553098066792191
0.4402385448598875	0.4305807825249940	0.3318183146303534
0.3466696481384806	0.5981234711827765	0.4410403294743637
0.5825520072408972	0.3692605392641476	0.3654334361354412
0.6027840795832285	0.3372647705376730	0.5684250576052287
0.4091202365513520	0.7133665941699474	0.4937463358848681
0.3916256889785135	0.5772155740116386	0.5065226267685800
0.5759433258030614	0.6080644490127703	0.4824366435740964
0.5844106232545130	0.6129625566941492	0.5635311681562757
0.4345809127169940	0.3996146442324443	0.5984476904157330
0.4435699139412147	0.6008280078441907	0.5658715460944240
0.4455457540074062	0.3128231117498589	0.4379463605027922
0.3810732341561534	0.3341383207489613	0.4860263896609200
0.3390793216974499	0.5424764963165942	0.3805767551562988

0.5184541669422595	0.2981953242108170	0.4713644874430155
0.5657473801493549	0.6007389302623921	0.4020237352344753
0.3742348362860767	0.4793771300377558	0.3393880401831417
0.3360647484347178	0.3906301063678897	0.4448379872634043
0.3600813514312128	0.6493106075873694	0.5045277895766652
0.3734939225791709	0.3305213718119582	0.4051860560747133
0.6574882041596873	0.6056563615345716	0.4731942444825939
0.5834586250388735	0.5381675917988649	0.5961998486952634
0.6263736668583659	0.6691960831832211	0.5950221276088209
0.4433229460001563	0.5078479620866078	0.3031390056854206
0.4173872967661609	0.6307008044791971	0.6339644859891116
0.5815001664116954	0.4628408700900333	0.6264045317015843
0.5120454710754085	0.6291746103712118	0.5299755611464402
0.4509169454198005	0.5885654820766418	0.3218449341172185
0.6188932334744098	0.6657559993148694	0.5141528615465217
0.6536889258894125	0.4897317209410200	0.4824131600468305
0.4650214941318550	0.3264031487184713	0.6013967679025846
0.3014563062346889	0.4526560177455759	0.4848695453219355
0.5565109405314872	0.4916323132436277	0.6965512448258601
0.6203874350127638	0.5520848408504536	0.5232462542837527
0.4592997418053323	0.5182807980515470	0.4367771462840412
0.3626583761077114	0.6086694401730101	0.5763384621717947
0.5420147557373660	0.5562318547488529	0.5314685718666846
0.5076113606935009	0.4300307587799971	0.6138813948693561
0.4744748300521537	0.5282128601179276	0.5672097804031909
0.4280267701896565	0.5906318314091663	0.4338212801525416
0.5718481737449049	0.4093289471061552	0.5657794194858664
0.3559360177342759	0.4040485771494832	0.6081905951265458
0.3463198391008950	0.5103991065482741	0.5170053089015876
0.3778675061729477	0.5551772924218950	0.3102665552398683
0.2700238112572877	0.5155646792345162	0.5254009562847883
0.5588662095370868	0.5218879512373631	0.3823208509963824
0.5000106845575212	0.5000115683697357	0.4998345300505966
0.5394278137929045	0.3553908768527057	0.6185834071844575
0.4234757928376225	0.5051529604422068	0.5083792165074646
0.5327067808577032	0.5501306018882772	0.4510533188390121
0.4915343689113540	0.6155658244785212	0.6685504782439361
0.5025074475175191	0.6229108750540286	0.4483385056170844
0.5508982180907959	0.4425397846230830	0.3649447205667659
0.4977701988108147	0.3772956777792937	0.5512897100614349
0.5180288823717785	0.5413964582496016	0.3141779059951446
0.6399394830281725	0.5171748818022219	0.3706043752435231
0.3188168048224442	0.5393688567428504	0.5860210845259711
0.5141733967104934	0.3377282136402064	0.3990873928248276
0.6255127819497849	0.5202430459178592	0.6602465407254109
0.5609444924228896	0.3576038535854406	0.5036606034206889
0.5762676143828129	0.4141529952642197	0.2979694557615029
0.3604998197552158	0.4826075133799989	0.6297402298346150
0.6814930180739321	0.4602726220834156	0.4135482521912934
0.3865118813264634	0.6099257548125259	0.3697532256436147
0.4816440843422695	0.7018278335508973	0.5284450712551241
0.3027766591018144	0.5291868001076960	0.4525256249169995
0.6084473016424600	0.4228819622061825	0.4930893835748116
0.6400398261590593	0.3507731022323219	0.4949684237531407
0.3135767882165484	0.5831389110200477	0.5152062627697449
0.3341443550087107	0.4657025042439216	0.4102782887993628
0.5848959182698993	0.4932356848777826	0.3135765009712101
0.5564599628983870	0.3989040280394099	0.4335386934777117

0.5594115118923674 0.5688150521640649 0.6680471806027156
0.6225988794257393 0.4447410904416120 0.6892518291330351
0.5498043917057676 0.4111291393126914 0.6776179833018252
0.4603254761547546 0.6448775675877024 0.3817533224618296
0.4408615094071129 0.4775086758255638 0.6180780439703975
0.5543624097425253 0.6871142963050660 0.5622299986380281
0.4920049679827347 0.5694643328825556 0.3864932888683455
0.3795262978209156 0.4479060956510745 0.4764660988505362
0.4858800371683800 0.6617498011528058 0.6004553781368327
0.5403593218043392 0.4813617167941174 0.5631245356100717
0.6654140864158810 0.5341822454713446 0.5892836061621228
0.4844556565955976 0.4895493125828710 0.3678134640873930
0.5168549753270937 0.5855224146385073 0.6003535824385906
0.4014719032103125 0.3490162053142310 0.6462463365649248
0.4897906663111545 0.5390695556834676 0.7007233337170304
0.6864618533489555 0.4169935595475158 0.4842309180562254
0.4814892131519621 0.4575805655147684 0.6890018055955287
0.5464181618010109 0.6845895902862588 0.4801508468774890
0.5985664208326188 0.6509398929876502 0.3535798322242848
0.4673061092454582 0.4498684619066948 0.5486900127065711
0.4124988925759025 0.6730423991363111 0.5643817731322739
0.4720512399778253 0.6956447692028780 0.4459643530790728
0.5144501433071870 0.5088306574875783 0.6327587659389272
0.5253252043489284 0.4713140595062738 0.4326900701124965
0.4490696018250713 0.4090393549704024 0.7200172974548233
0.4442169165725177 0.3987777100932572 0.7563531361278503

CO/Cu_{147} $E_{ads} = -0.85$ eV
1.00000000000000
31.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 31.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 31.0000000000000000
Cu C O
147 1 1
Direct
0.4153982708917637 0.3866690071027808 0.4356468210410483
0.6033810373645342 0.4656091861238068 0.4232608223496427
0.4182271780074570 0.5369398293922009 0.3732996325398343
0.4237663307224389 0.5861753521996418 0.7018559631689191
0.3965133963346150 0.6626657141549744 0.4317314283191575
0.5875816798772387 0.3264160543538132 0.4350783067600665
0.6299629079604765 0.4365758091966292 0.3550091928375781
0.5303213865092232 0.4289610944815844 0.5017383667106607
0.7299720724447094 0.4842560168469655 0.4745789178381233
0.6272136716279956 0.5957915743015690 0.6285002396960037
0.6607303334848050 0.4574034203936590 0.6192538148020988
0.5908471488133470 0.2865803293885457 0.5058958752504402
0.6186298686300101 0.4760229332505115 0.5554172056234212
0.4239415078715434 0.3917485907999874 0.5165086435507842
0.4879794642108780 0.3707276932768266 0.4693490634106212
0.4078705314036521 0.4275843558255819 0.6714628896155659
0.4696315956996617 0.5707261372899605 0.4981726315001596
0.6967542815091948 0.4705074053341541 0.5473687602291890
0.3427685653468281 0.3945229441072817 0.5261311341948490
0.4159190619196724 0.4613925721259962 0.4034997626818922
0.5101927159995185 0.4608746320216640 0.2989910224129783
0.3905279648585099 0.3405541527963759 0.5670357476563437

0.3701284647423295	0.5629537062413837	0.6452077361575971
0.3727275410025273	0.4042225207506712	0.3705390407610886
0.3809174680837473	0.5237256902973875	0.4446611199551231
0.6984760571309779	0.5471995171220435	0.5150930309250991
0.6447550645857562	0.5961824890804461	0.3924182800456637
0.4578125535153102	0.4434757790594172	0.4678985274642966
0.4405066038632519	0.3560219621421176	0.3663616513827873
0.6107649758673350	0.5454423937756534	0.4418911460120946
0.4830484332602093	0.4136312469512406	0.3992912126481906
0.5349608201298611	0.6742361761278494	0.3991619705339460
0.4537114637799148	0.3157204136513042	0.5192823894379558
0.4753000058643557	0.3795863369910204	0.6668160357493101
0.6528580323495149	0.4016501288242453	0.5589777549708816
0.4152880006944600	0.5069362248568523	0.6864769655350103
0.6373723955982941	0.3911029263128509	0.4234886860453916
0.3111881853213725	0.4589317125142131	0.5671964537651386
0.6091871775170989	0.6592217338191589	0.4335329226812533
0.5595039392695772	0.6439824542360201	0.6326187130670015
0.6130988609962912	0.3899645711153312	0.6301774719672080
0.5085210923449853	0.3842289002122686	0.3309434531565185
0.6888859307491068	0.5407933759107183	0.4329313393187484
0.5922748607474503	0.5721499244071739	0.3325006606935312
0.5244221593788070	0.6203291998188669	0.3366581477209989
0.5763560865386230	0.4947671998307646	0.4915431980384335
0.3965606564973950	0.5335510027473843	0.5771259287635304
0.3890453433768881	0.4545299273508168	0.5578137477111531
0.4388996421077968	0.6422694882003351	0.4962649371883649
0.5278569523321065	0.3047195323112243	0.5538978865772650
0.4490837197989200	0.5572982945792559	0.6349558826188834
0.6639631514856266	0.6093867787731957	0.5552273937814733
0.4405035961966705	0.4309342138563293	0.3315112370244996
0.3465444262529722	0.5980079940122786	0.4415193865498215
0.5827689278645427	0.3693033367342289	0.3655203384917031
0.6022849783633288	0.3370710020753152	0.5688441401895142
0.4086650336411388	0.7130832142058104	0.4942509774867986
0.3914775518005167	0.5769942791262584	0.5070406417397330
0.5757271309645760	0.6078024642953470	0.4826711279474903
0.5845165141231506	0.6132384115314947	0.5635079297781079
0.4344992345010698	0.3997772513566659	0.5965125957817139
0.4434167308239211	0.6007328199711964	0.5662714033615402
0.4455177823170344	0.3128365233226645	0.4372362611166212
0.3811192567392671	0.3341638243065920	0.4855772744937609
0.3390736049164466	0.5426447409568959	0.3807339494239244
0.5183528284379041	0.2981590441784961	0.4711685549755925
0.5653242178060334	0.6002009399237173	0.4021038102378027
0.3743712991754211	0.4796858535195259	0.3393670848951663
0.3360983003933055	0.3905482035894814	0.4440547154871974
0.3597538347880280	0.6491168397621654	0.5050874284136649
0.3734513111738160	0.3303489455003961	0.4043057009771824
0.6573712163210279	0.6054220987467668	0.4732465428571701
0.5839046758574898	0.5385360766085256	0.5960875177263312
0.6266601207129949	0.6698202145803709	0.5945850128365684
0.4434580635924223	0.5083225505780518	0.3032085531300223
0.4173842864930281	0.6306512563783255	0.6343403877419125
0.5813787360898873	0.4630682589433822	0.6267386137888081
0.5119484378163142	0.6291695417879782	0.5300518578422534
0.4507426087482497	0.5888098867053453	0.3216820445361959
0.6189804198218372	0.6660104320032061	0.5140534271906896

0.6535726118876070	0.4894019153511459	0.4829981263679343
0.4643822333031086	0.3260945190852668	0.6004967867154867
0.3014688955049510	0.4525283693408000	0.4846092070520857
0.5571462533900142	0.4926768481065202	0.6967698333310861
0.6203372817422639	0.5520372118101708	0.5233655124007879
0.4591381797408836	0.5181767501183303	0.4368329840849123
0.3625868296483384	0.6082497253377821	0.5769314929855963
0.5419357110982452	0.5561567123655686	0.5318983353134972
0.5071728053731438	0.4299980851710195	0.6142199255267013
0.4744267194261967	0.5280796521931167	0.5674922883521741
0.4278376653096404	0.5905002505432613	0.4341765433564616
0.5713623078971958	0.4091346421711615	0.5662539192157824
0.3555234226669531	0.4035267493664413	0.6070744858861027
0.3462013160656732	0.5103152506377028	0.5169747836582023
0.3777906564657140	0.5556164113090442	0.3102730560799659
0.2698565825167228	0.5151991950871879	0.5256753502496880
0.5587813299200080	0.5215466265239538	0.3823278573461871
0.4999836873345794	0.5000061006427144	0.4997331569010323
0.5386969002779135	0.3551365699749401	0.6191709787074355
0.4233704471017407	0.5050749469603125	0.5084135974125845
0.5325515916993506	0.5499242500033388	0.4511977829792108
0.4916428264184010	0.6162354415054130	0.6685818084842814
0.5022022937053171	0.6226885382931376	0.4486061622872405
0.5510421336133683	0.4424327492754670	0.3650080727840859
0.4978068934092294	0.3771306618057225	0.5510019718394013
0.5180315865096293	0.5414126143957029	0.3141444562877809
0.6399527264797327	0.5168094736322217	0.3707354414016684
0.3188335606816330	0.5388694165624749	0.5864090989113400
0.5142909901549473	0.3378691771824866	0.3989117051724990
0.6258680594753402	0.5205987344215176	0.6602854675963220
0.5609063666450956	0.3574395452383496	0.5036001777940502
0.5767105382121850	0.4143148455328630	0.2979069667782157
0.3605204762214099	0.4819157109647697	0.6302917460345743
0.6813362476551901	0.4599903676664716	0.4141646760134998
0.3863250283138877	0.6098770601410433	0.3700862101382828
0.4813794220970680	0.7017448808420375	0.5284974904851567
0.3027779804864261	0.5290885548692205	0.4527348074572651
0.6082988221059503	0.4226277374250660	0.4936331833807291
0.6398158868931825	0.3505443863305450	0.4954318661034898
0.3134903571628657	0.5828577574559434	0.5157082268657879
0.3342901034315784	0.4657872390216523	0.4101364896962636
0.5851875622882035	0.4931914978232883	0.3134038099256663
0.5565321063300225	0.3987957721374544	0.4336981905345555
0.5599814102784315	0.5698393037716064	0.6680048371536990
0.6222953131865676	0.4449327099775248	0.6895761677157491
0.5490684822158138	0.4116178129621656	0.6781729526112200
0.4599073854338414	0.6447783319998306	0.3818499434026574
0.4408283220002992	0.4771441130521923	0.6184219435160375
0.5544049641408388	0.6872593343960048	0.5620602473428601
0.4916842208454301	0.5692872791076292	0.3865081678933218
0.3795663060531047	0.4478226283849800	0.4761253193619166
0.4858165161364024	0.6620359367917092	0.6004855080871717
0.5401915134535791	0.4812913659541613	0.5634132938050475
0.6655158764976056	0.5342342049486422	0.5893975839178767
0.4844257915512713	0.4894924703867239	0.3678512327282291
0.5169219881870550	0.5861976562800958	0.6002473222789941
0.4023472828416989	0.3503613702061402	0.6470760804753379
0.4904993098865561	0.5400964128747724	0.7009336408636976

0.6863856253208834 0.4166159395261768 0.4849149659187694
0.4828701247443544 0.4598889378357185 0.6864243033994909
0.5461031646964829 0.6844570836065362 0.4801676311600561
0.5979197474607838 0.6502206536494685 0.3537909868464408
0.4673696520100120 0.4500124961908710 0.5482635482627468
0.4122019654177003 0.6730195237926527 0.5648889545755528
0.4717127759892265 0.6953035063749116 0.4462131751845907
0.5155677227273018 0.5105555953088401 0.6323076703266288
0.5252848271929264 0.4711033024790360 0.4327386004373628
0.4211851391204106 0.3739632283664727 0.7062945356491801
0.4161293075231964 0.3606598430026672 0.7416434172940899

CO/Cu_{147} E_{ads} = −0.85 eV
1.00000000000000
31.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 31.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 31.0000000000000000
Cu C O
147 1 1
Direct
0.4152810876512957 0.3867049758332191 0.4367809165275124
0.6035062877817375 0.4657866687153863 0.4229307214763614
0.4182925223631054 0.5367510230626322 0.3733915564944533
0.4235382703277528 0.5858740718197920 0.7017142487769700
0.3968409016399798 0.6627579102751284 0.4314220778773248
0.5875999369890622 0.3265725422026034 0.4349891835296185
0.6299758118060694 0.4367155156973382 0.3546595495950935
0.5303387582871264 0.4290848106212229 0.5017957009554462
0.7302871366731865 0.4847903734715540 0.4738117143422109
0.6270595855526345 0.5953355620583284 0.6289196666528817
0.6609537672936061 0.4573380535779984 0.6188305681351506
0.5910363805145338 0.2869296285238160 0.5056624968379536
0.6188852344171184 0.4761550095888951 0.5550465152714456
0.4239674869525615 0.3918693030907892 0.5178983558302223
0.4879116743276763 0.3707085790726000 0.4699506319259500
0.4052688258332581 0.4276930136517552 0.6677655315907937
0.4697481019843199 0.5707493304961043 0.4981116240814307
0.6969109430056827 0.4708729107917834 0.5467588366361711
0.3425270250463118 0.3944854812354356 0.5269380880102863
0.4158465809636659 0.4612553959803655 0.4039308297333419
0.5098573866385619 0.4605782298466167 0.2990485431876233
0.3905512627539868 0.3404413774836226 0.5669259529711493
0.3699441874927908 0.5633135734857044 0.6448720130277097
0.3727740517114188 0.4042470695964341 0.3712628196223099
0.3809342298700867 0.5237392785099133 0.4445766213350382
0.6985806263013974 0.5474184606013724 0.5149133302389437
0.6449668638510421 0.5968361908793519 0.3923166559492935
0.4578359920257273 0.4435132709113003 0.4682619493302510
0.4404622104938883 0.3561541019661035 0.3672468099840923
0.6110002887821546 0.5457288050105772 0.4416056461941208
0.4830238373520391 0.4135826603773854 0.3997951198722842
0.5355593269562993 0.6744034794193405 0.3991430362646190
0.4537359513034016 0.3155532025336340 0.5204536412512647
0.4746966665693834 0.3793166724121635 0.6662227730251854
0.6533799201195372 0.4018931018864765 0.5583715195035990
0.4146129396398885 0.5067652605347766 0.6860841315948104
0.6374188614490257 0.3912936136364678 0.4230543133542407

0.3110169685020487	0.4590876837572800	0.5671004506434684
0.6098358456969488	0.6598989160041379	0.4334789361707688
0.5594470273995511	0.6433114264962619	0.6330889626030286
0.6136337931561349	0.3898112451676891	0.6297627776550920
0.5081965318643898	0.3839865684361002	0.3312112039097230
0.6891560941392645	0.5411534368143559	0.4324484071016332
0.5924672821570450	0.5725213507547262	0.3324801186413563
0.5248805304402395	0.6203057839211467	0.3367100523024248
0.5766311291539831	0.4949385728617277	0.4911553656621698
0.3966118863472041	0.5337507248021112	0.5769348902752803
0.3891618552169793	0.4544379019882444	0.5582720219855765
0.4391923671830183	0.6422933390369295	0.4959337254180266
0.5280461705506220	0.3048417130453267	0.5540123922392471
0.4489140938354069	0.5570384011608059	0.6347616342393123
0.6639751117669065	0.6091620652149954	0.5554417573691504
0.4402016804659171	0.4304693063754420	0.3318963900134936
0.3466589794982986	0.5980479100327427	0.4412276286589271
0.5824831186452604	0.3692689187757518	0.3655461941958481
0.6029380437259944	0.3372431643849885	0.5683848929860402
0.4091296778353676	0.7131781658008277	0.4940492737662045
0.3915210112082390	0.5771108803527784	0.5067246234696499
0.5760149310154711	0.6080583684084194	0.4825388331558813
0.5845416920089580	0.6128546905592802	0.5636696770999349
0.4347196720367976	0.3995861511127611	0.5988610829487807
0.4435625636456326	0.6006472343238983	0.5660686630075186
0.4455012643819035	0.3128231942259314	0.4381972325565500
0.3809693882614441	0.3340795608541058	0.4861601476832706
0.3389162032822015	0.5424251402238528	0.3806970420940869
0.5183441880790274	0.2982139903656149	0.4715606293095622
0.5658110726163053	0.6007310801843265	0.4021244167894973
0.3740938994006069	0.4793485072021420	0.3395935882031728
0.3360067863979677	0.3906290456895087	0.4448607043941071
0.3600591055439220	0.6492053826311730	0.5047683402972587
0.3734764279899268	0.3303824110823379	0.4052840239267703
0.6574319717175411	0.6055342273073290	0.4732898970306694
0.5836157768137418	0.5381127250566566	0.5963055776062087
0.6263916109645639	0.6691209932496243	0.5952546656518105
0.4431710929071739	0.5076413774463023	0.3033659998131320
0.4173955337514990	0.6304828395815223	0.6342200935654716
0.5814545525971002	0.4626927868854014	0.6265758961813581
0.5120263185826094	0.6290409375922790	0.5301874742861937
0.4510387805883070	0.5883795233023873	0.3220657971934032
0.6188845461106199	0.6656824815346616	0.5143380808973791
0.6538092098237842	0.4898308086395485	0.4824689122250475
0.4651182141631822	0.3265049341969338	0.6019171791900192
0.3012957737693401	0.4526351897020652	0.4849558679395007
0.5569442548612024	0.4918343704255443	0.6966258149010747
0.6204132651419372	0.5519970992105866	0.5233529157624895
0.4592718724007852	0.5182507681758233	0.4369466709146694
0.3626684635074102	0.6085879620255330	0.5765194801518554
0.5420461738612586	0.5562262751365412	0.5315303829239109
0.5080518905541594	0.4301122515043618	0.6131238007403357
0.4745613617661616	0.5280620589198204	0.5673455263150688
0.4280076297048427	0.5904951400824592	0.4340103637030307
0.5721624256638757	0.4093683246808648	0.5655421623911402
0.3549876498978051	0.4034293694145616	0.6075045120682558
0.3461586077778739	0.5103243081001658	0.5171234405390585
0.3778207831307495	0.5551516462711915	0.3104493435685770

0.2697469331849633	0.5156238147732711	0.5255055884740878
0.5589660520890892	0.5218845634970232	0.3823749068629695
0.5000046908559853	0.4998793618301010	0.4999411810188567
0.5396300539099542	0.3554041954936883	0.6184435182457085
0.4234144623568210	0.5051232890454163	0.5085089219233727
0.5327233139370823	0.5500846330332837	0.4511961257221411
0.4915622974593065	0.6153022472200883	0.6687202989891008
0.5024967913156242	0.6227770618214974	0.4484772011921456
0.5509400630810154	0.4425604750624694	0.3650127452721913
0.4976521046357488	0.3772325026910897	0.5512945245997496
0.5180159241078112	0.5413166493126949	0.3143115867644539
0.6400266464921454	0.5171115231426331	0.3705084084532103
0.3185162595983653	0.5396569558776132	0.5859479105680380
0.5141009072155852	0.3377955649118461	0.3993436910472031
0.6258197525278990	0.5201907050691765	0.6603156704315291
0.5609080435388879	0.3576186125658051	0.5037507768199722
0.5762212745168305	0.4140659371401607	0.2980251961589765
0.3597237662118955	0.4830402552824843	0.6292445601819898
0.6815159817456284	0.4604284662619426	0.4135550556693458
0.3864712612678338	0.6097450184559474	0.3699511914132918
0.4816597378313738	0.7016699832451502	0.5286989541533689
0.3027733339317946	0.5291979650906099	0.4526945575557099
0.6085240484098395	0.4229215974893553	0.4929797227670828
0.6400050442566310	0.3508291135007215	0.4949066883100399
0.3134010570140894	0.5831494412395557	0.5153387569780020
0.3342053594628509	0.4656547938754249	0.4104837577321976
0.5849186455639688	0.4932301964081605	0.3135774008382450
0.5564868320043965	0.3989464629066842	0.4336563970572346
0.5594976704739385	0.5687023440477494	0.6681637502055625
0.6227704704976768	0.4446622537780779	0.6892752948656173
0.5501041529101807	0.4110196519356846	0.6778087871625439
0.4603111217311533	0.6446723574832744	0.3819828595954326
0.4413748274235553	0.4773680043516962	0.6184258182506240
0.5543948148063164	0.6869745356447600	0.5624894991943568
0.4920003437260110	0.5693934412585946	0.3865895816980662
0.3794455431688645	0.4478891014418023	0.4767049562679547
0.4859126347559126	0.6615127508796612	0.6006759110057012
0.5406402457507961	0.4814997041840317	0.5629045199627865
0.6654974606993022	0.5340941816955356	0.5893818704707527
0.4844163738948413	0.4894467392664175	0.3679497801128119
0.5169388348038895	0.5853205766000430	0.6005334097147766
0.4015367276909891	0.3494253130024459	0.6468304063697230
0.4898326149011994	0.5387447660854676	0.7008504752325488
0.6864711345234501	0.4170633137789334	0.4842130371185133
0.4812205166918443	0.4578735288374087	0.6894414538602106
0.5463873188756589	0.6844255682847815	0.4803455458742468
0.5984253574208233	0.6509164905485991	0.3535253631938154
0.4671618795712287	0.4498099450160308	0.5486385130378185
0.4125282517205211	0.6729195712151469	0.5646398030402384
0.4720880517933402	0.6954444464688539	0.4461868730624717
0.5147179634108238	0.5085768968231448	0.6328440812377781
0.5253570781418365	0.4713878054688649	0.4327725193451606
0.4738856346945204	0.4059279737314867	0.7253113971132282
0.4708235715888703	0.3937944568251196	0.7609688390963902

CO/Cu_{309} $E_{ads} = -1.15$ eV
1.00000000000000

38.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 38.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 38.0000000000000000
Cu C O
309 1 1
Direct
0.4932121988543686 0.4599027756762545 0.4525813588007072
0.4999908117838379 0.4999148321740263 0.5000196154450313
0.4440440161572174 0.4728747689003323 0.4939854083991592
0.5495830683471310 0.4648333505933314 0.4858235747244925
0.4646929858400241 0.5189512836674950 0.4521704054053785
0.4699864872076906 0.4858482961710072 0.5528540555105704
0.5323620994120887 0.4187883713877555 0.5638413302949633
0.5299363832768177 0.5140366671211176 0.4471118938132340
0.4134219658380145 0.5551928447652795 0.4656561359834921
0.5559655848521431 0.5269116510721383 0.5060855261029499
0.5068028733334190 0.5398863577294043 0.5474924966354464
0.5034855716414238 0.5604330721961933 0.4852200046522420
0.4894771783311410 0.3973173294070768 0.4667579436624797
0.4360474587363868 0.4316202237096913 0.4455061567277518
0.4393751270339242 0.4105415831927407 0.5089498573011640
0.5469878084173693 0.4024284905195332 0.5006791760774290
0.5436326611614675 0.4232852767660532 0.4372493784392429
0.4570779365872856 0.4786120415576961 0.4029104586837713
0.4658919016590321 0.4238544537524847 0.5689873447968733
0.4070283314711560 0.4918220237848192 0.4450586105096047
0.4124164055272457 0.4579247423280044 0.5477611510026861
0.5236134891401341 0.4734881199050744 0.3977298175211394
0.5352513948100909 0.4808188350324186 0.5478516370039497
0.3923539365160447 0.5081498618713239 0.5082687627192962
0.5865204275311706 0.4447496416044143 0.5343503190263418
0.5811317590737189 0.4785504928512095 0.4316505682267243
0.5053929877163423 0.4661769316870118 0.6026705417355084
0.4945846736452789 0.5337582709556814 0.3973051884601219
0.4503576033195300 0.5350425170435339 0.5141356859538022
0.4188231560942741 0.5213879215634450 0.5683213310208279
0.6075605724711686 0.4916575247601351 0.4917498600258872
0.4675828827520255 0.5810621555531257 0.4361541443038012
0.4763536314782110 0.5263118133373178 0.6022363490726602
0.5930697091995822 0.5080713076055775 0.5550197458891657
0.5875459872031128 0.5418836430710638 0.4523438273555316
0.5429422673746224 0.5213008390139591 0.5972435966821406
0.5340691689164800 0.5760106261750564 0.4309644349199750
0.4564264286123137 0.5764956121187358 0.5627755222262905
0.4529330390883140 0.5974379671678721 0.4993125964590895
0.5640503387769863 0.5682434125559482 0.5546372329133235
0.5606332544844436 0.5891494004792596 0.4911256911933081
0.5105286940734596 0.6023738337666570 0.5333266329063289
0.4929114565073171 0.3778767475554284 0.5298165585941608
0.4863909859262902 0.4192821871160871 0.4044586647767270
0.3872608850724615 0.4454573792085774 0.4879362963275183
0.5999083254278031 0.4291801067018087 0.4714478871863927
0.4289148669605797 0.5384884769976527 0.4035948084483890
0.4395471426605554 0.4715329813408408 0.6064946803754147
0.5710700475594774 0.4615406811151653 0.5964036827178956
0.5604082124101043 0.5283500758724180 0.3934611137524281
0.4000157980268718 0.5707070425380855 0.5285422332818163
0.6127509148117374 0.5543873632070744 0.5123498939886727

0.5138486567260511	0.5805006758943856	0.5956435789168417
0.5070486658525699	0.6218490515837060	0.4702136915951061
0.4313754793230594	0.3676439808591574	0.4599940865676130
0.5407311220604345	0.3592970229732879	0.4515915855753780
0.3984864938065675	0.4501479251633032	0.3951021747927565
0.4073777842484682	0.3945187510230492	0.5638993812578211
0.5842700257313458	0.3811105878832912	0.5501856493995050
0.5754227464896355	0.4367161398239003	0.3814345122327070
0.4874477776959418	0.4928090599303807	0.3465467219973388
0.5017705996230325	0.4028920458083445	0.6196411304342293
0.3540718226060658	0.5280407330389004	0.4588472904493093
0.3595808901872078	0.4936761903749793	0.5631823365905759
0.6458792757866730	0.4720920514224214	0.5413720659301192
0.6403956264960828	0.5062413189093095	0.4369254525197248
0.5127818483142859	0.5072538542885485	0.6534347758674732
0.4980934350644362	0.5969992497986186	0.3802398904342091
0.4155883462705909	0.6187793541042593	0.4497115550167426
0.4246664552950778	0.5631783125843808	0.6185836588723543
0.6017483221268399	0.5497200304986422	0.6052021652533798
0.5925551021507794	0.6052555713913786	0.4362109988496853
0.4593365734517924	0.6404331691083767	0.5484265213548422
0.5686515642499033	0.6319471431744759	0.5401376050260812
0.4858704898420338	0.3347616015613863	0.4815897653012942
0.4825989700244171	0.3557674754988602	0.4181579564882288
0.4353156736264563	0.3481255149215551	0.5241779194881964
0.4287492612786215	0.3902313849588247	0.3968217812291325
0.5437533893532966	0.3398599835014947	0.5157523416655377
0.5371868312511467	0.3819077454557581	0.3883735509511732
0.3785687025834465	0.4034952281757748	0.4390612951573450
0.3818488884972194	0.3823696608069628	0.5029883421102533
0.3492646248533508	0.4642625670773607	0.4386090820578372
0.4499973174548658	0.4376897550927441	0.3537860492600984
0.3546662342325037	0.4300968905902663	0.5420979090100086
0.4619873437395329	0.3614785685555169	0.5846187365197696
0.5979396434644650	0.3659456427283562	0.4863061359798759
0.5945401363643040	0.3869119290524009	0.4223071726094912
0.5169776341556821	0.4324899554567699	0.3486241844702959
0.5290150215039074	0.3564907379542840	0.5794304542075517
0.3345158745585328	0.4806510282701799	0.5022912857870796
0.4208289061104506	0.4978890292982331	0.3533795236237097
0.4351060196642679	0.4089626281966958	0.6234351792058339
0.3703569208464157	0.5112123728446289	0.3958943060005852
0.3811500388652671	0.4432684594488185	0.6020117326040055
0.6377827310748548	0.4086438320443713	0.5202108395937370
0.6323485120673943	0.4426208457029799	0.4167253081018724
0.5543710349555636	0.4877076390678188	0.3430690409675445
0.5685442325249048	0.3988106807106440	0.6131134578363946
0.6231281703808622	0.4247568947741631	0.5833946398444186
0.6122931190901961	0.4927634957952113	0.3772217092195307
0.4749358567367864	0.4516580409371577	0.6573501601683870
0.4585762514915450	0.5534277284884601	0.3477539190651177
0.6589479056096931	0.4559327497150878	0.4772870005756951
0.3409771378917988	0.5440465638768428	0.5227897185626855
0.3767729748969110	0.5750393893229139	0.4166128827499154
0.5413539551709712	0.4463749875139109	0.6522326478120047
0.3876774716906370	0.5072001127470840	0.6227449946136130
0.5251012353465456	0.5483737656266668	0.3425744563691560
0.3621319101067004	0.5914146478764026	0.4798301865810293

0.3676085624271154	0.5573384615753860	0.5832608410010066
0.4313724689927644	0.6011842746767068	0.3868247704482655
0.4456961114539844	0.5122486012288648	0.6568827779629273
0.6296420811692941	0.4886175273364254	0.6042110025444007
0.6187172184635136	0.5565692241911315	0.3980057487942739
0.6653734761018546	0.5192744374756650	0.4981132729517245
0.5792030911042783	0.5019309769355971	0.6467055418623117
0.5648902103952704	0.5909934922041047	0.3765325882909166
0.6507236236516676	0.5363590632186733	0.5623734257757035
0.4054528073711537	0.6128836200681669	0.5776174367313899
0.6452187997229342	0.5697475801663485	0.4581470877442472
0.4020191798307597	0.6340145541846764	0.5137121485649828
0.4709072824543373	0.6433763310217718	0.4205291633371854
0.4834434269855493	0.5673081121767968	0.6513662841029108
0.5511688180369296	0.5626268782355655	0.6462560120145182
0.5378927199928767	0.6382813900152418	0.4153515747615349
0.4630423681476396	0.6178368940581674	0.6116002296526635
0.4561669480766194	0.6598798446981065	0.4842059165196044
0.6215673273603730	0.5964020367829058	0.5616210812884901
0.6181164442597991	0.6173471514557861	0.4973119841297429
0.5718872989427479	0.6095136233393207	0.6034592581240977
0.5645951187264470	0.6515375647082261	0.4759835368864456
0.5176318879737275	0.6438576829469209	0.5819355815215079
0.4625855649946713	0.7043819938632360	0.5337009258950931
0.4795155958569194	0.3781574152475167	0.3557466808303566
0.4893283123733529	0.3156795868671068	0.5450452554764292
0.3297639042486595	0.4176986258345235	0.4818291602880790
0.6508820667845484	0.3931692307241115	0.4569041556958124
0.3926672156970115	0.5580204680663203	0.3544427829346705
0.4087885308929147	0.4571101907186942	0.6608232611513889
0.6072981553259815	0.4418418931397077	0.6455942461206833
0.5911421138913103	0.5428663122712998	0.3390929905329160
0.3490389274119067	0.6067932919261771	0.5430465327372667
0.6702313410655415	0.5821359036076067	0.5184391948326081
0.5207214224958020	0.6216005424379458	0.6443384243526969
0.5105948496657995	0.6840325171177398	0.4549505774187514
0.4269859990340944	0.3036009926029086	0.4748709480859023
0.4237487841453401	0.3248677584594840	0.4107043870836052
0.5376222000037492	0.2951625763122241	0.4662681104972471
0.5342814665860989	0.3163171603890359	0.4020899594387687
0.3397269950054723	0.4218025413006561	0.3877539418885256
0.3485644958436581	0.3653585499093149	0.5585060147743985
0.5923849800885639	0.3215671188998570	0.4364404327000333
0.3904585793650258	0.4084049112098345	0.3450788178566406
0.4026052628193477	0.3308014844792384	0.5799675212044162
0.3729559369192229	0.3383086622771413	0.4534435091658559
0.5815611996015613	0.3173087309663275	0.5660051743453424
0.5694093218402886	0.3947346890888633	0.3311153707443037
0.3609983360789616	0.4693136663215084	0.3445018477371813
0.3754800659438757	0.3788810715571593	0.6191943085164032
0.6363815191697141	0.3435545496705865	0.5361745668612525
0.4805207554861478	0.4515599645919299	0.2957866979318620
0.4981898379261950	0.3393140397224494	0.6362784664248832
0.6274695353642150	0.3998033868332588	0.3655174485322470
0.2946879388604033	0.5005895388424986	0.4523080529035073
0.3002508006721702	0.4657425083350902	0.5577974018998754
0.6215553615847856	0.3600278155634708	0.6001026223863496
0.6072503574611579	0.4505201339044503	0.3254758827802035

0.4709249906353262	0.3872559289285299	0.6755356699139985
0.4510965070059524	0.5124254658524583	0.2953335733899551
0.5381544356299983	0.3820052751682674	0.6703184759050694
0.5182595142725954	0.5073030300433260	0.2901490510134251
0.3159127442417774	0.5480581374901623	0.4091001410317146
0.3270863638215216	0.4790661643081865	0.6184694473460012
0.3011451208808218	0.5646397677788553	0.4729373420246414
0.3067257203258241	0.5298030823578423	0.5785842006939830
0.6986185747079006	0.4353660071245257	0.5270096817867732
0.6931633401973685	0.4701666797428530	0.4215024487043726
0.6839882036029511	0.4517010256199903	0.5909794268691889
0.6727865184301933	0.5208826736001473	0.3816135074718826
0.4816989043772273	0.4926635067729989	0.7096302959705293
0.4617264781737441	0.6178300172262089	0.3295064261436927
0.5489057588879415	0.4873164489065907	0.7046666923970073
0.3782078767059828	0.6398278159293511	0.3998285668039032
0.5289461205825676	0.6127142412290307	0.3242280258818430
0.3928401102789859	0.5494107888871653	0.6744342166991897
0.7052066914764177	0.4994224021044894	0.5478491591381932
0.6996566910196426	0.5342406305047067	0.4423549537222349
0.3726256598441102	0.6000938733933313	0.6344000590083452
0.3633932727269208	0.6564377895030320	0.4636948449928891
0.5196515227200190	0.5483913565362081	0.7041471614579340
0.5016079560563047	0.6605758780507519	0.3635712409091392
0.6391174880600016	0.5298206819849314	0.6558924427094044
0.6244009141327392	0.6209530183917498	0.3808849040543366
0.4182850090681050	0.6825627208013787	0.4338432966320841
0.4307793891284993	0.6051827525678074	0.6688169986651732
0.6623864036017376	0.5783564113417979	0.6143543647814833
0.4076771565936232	0.6782009214369790	0.5635183648558222
0.6512631631048417	0.6344219638885571	0.4417545388676872
0.6113591707463996	0.5918279772015997	0.6573088388852789
0.5971808487467301	0.6688355875508273	0.4203142349048103
0.4659638812578737	0.6833438991606041	0.5978417257863892
0.5142008025786851	0.6648515064475981	0.5184364346483025
0.6272041661366807	0.6609247876733604	0.5475102559138068
0.5769403294950030	0.6741859709173486	0.5898105823247126
0.5731730703314598	0.6957941707068014	0.5254645846785609
0.4790677950787743	0.2929323932903441	0.4329666996964435
0.3711498014081885	0.3621649783070177	0.3902256921378064
0.3776786042421175	0.3197061412917542	0.5183246446753507
0.5948321695809996	0.3031789120346158	0.5014089787724463
0.5881693268539218	0.3452881310050221	0.3732962320521556
0.3124190120383738	0.4835698215770781	0.3893048847626577
0.3232617629024167	0.4151757111872635	0.5964635214292182
0.4136635960504834	0.4568792563958564	0.3040396781291164
0.4312229094336381	0.3464226497444776	0.6392454031078764
0.5477733684504071	0.4466191381883139	0.2936787154872080
0.5653267127338710	0.3362167051112955	0.6288057167092298
0.2828282245989022	0.5165287960341827	0.5168302552763808
0.6745926125517036	0.3884840212802254	0.5692411896998267
0.6637282919735845	0.4568010325767570	0.3620946775431975
0.5107425270427770	0.4317559467679214	0.7071505914977132
0.4891613388586727	0.5681333823287205	0.2927494530706089
0.3252647021288145	0.6114139205604118	0.4307134555063530
0.3362609015403421	0.5432281850432016	0.6378913068618850
0.7170813190974605	0.4834237401642349	0.4832474582241295
0.4345196839363190	0.6636967073404401	0.3710859064852625

0.4523044083629997	0.5533121027344755	0.7062525641942941
0.6876984386091418	0.5159837531328190	0.6108719490346601
0.6765252125226130	0.5847049364576971	0.4037993575924337
0.5863795980008911	0.5427195401136700	0.6962268903191983
0.5687039111016871	0.6534061193238827	0.3607486429112658
0.4121213974503433	0.6544648397329634	0.6265787787589902
0.4051302853196742	0.6966383201064715	0.4986014846636340
0.6306853214282675	0.6380656775576622	0.6118553209971430
0.6222429670240145	0.6799018385919600	0.4823273219892185
0.5215246135951678	0.7064727923434275	0.5671778364946568
0.5406401088791291	0.2774625258542124	0.5308615501131958
0.5305426176680821	0.3404930195523129	0.3396657907830248
0.3210616819349486	0.3754939302925956	0.4325682732447465
0.3243858020535785	0.3541862138597935	0.4969494877985579
0.4213869690988896	0.3489379379359756	0.3480971667261989
0.5102685673119390	0.3915270279181685	0.2995546695249993
0.5256232991812768	0.2941972991614702	0.5950007965051970
0.4428260328748998	0.3967287485982208	0.3048146629556335
0.4313240256503618	0.2857217557912434	0.5392479084069560
0.4580940327876112	0.2992965473167602	0.6002950311356751
0.2915969251396963	0.4366729527985977	0.4321570570946629
0.2970816947060017	0.4020979851681189	0.5363524287970429
0.4757078867523246	0.3142533737739753	0.3695762084051680
0.2767163371664866	0.4531819460513586	0.4962603820213180
0.6488230657454576	0.3294186213773968	0.4718674591831244
0.4821326587688754	0.2722686455203672	0.4964571342090064
0.6454847555338052	0.3506844389782642	0.4073815609552767
0.3846979310758152	0.5171293266850924	0.3038846381009205
0.4043501020264390	0.3940461836197675	0.6778607456175564
0.3337225864677393	0.5305161578762924	0.3467764047660034
0.6889387802777555	0.3723788949887211	0.5059565941235805
0.6834889671907811	0.4066907026490704	0.4017431882661065
0.3499757401437371	0.4287048913051286	0.6563044710277709
0.5852355893622544	0.5019143041440506	0.2884784858730691
0.6046622684164319	0.3786049294471668	0.6622865981036901
0.7102899061673472	0.4200834421938719	0.4626611482801805
0.4443092488194667	0.4370531244495036	0.7120005973553045
0.4226502301490330	0.5731194945658247	0.2982652420177176
0.6597170083147010	0.4047733297952865	0.6323992830387116
0.6434800050732423	0.5069634697404143	0.3228703599232897
0.3402029811807543	0.5948526381758686	0.3675788610532225
0.3565469387253268	0.4930332622255273	0.6770865308738906
0.5771930519409765	0.4265239416292195	0.7017733015466137
0.5556577599882196	0.5630206071274055	0.2878815601790538
0.2897139821210273	0.5799616950409296	0.5373974377669553
0.3951644757932464	0.6212227494859321	0.3375988685598338
0.4148173396371303	0.4981411631032396	0.7115226706190287
0.3109627832021269	0.6276970653382596	0.4940096280533270
0.3164651252384538	0.5933131098542465	0.5982906807929660
0.6662387634266310	0.4688966220864149	0.6532970065893452
0.6498693495616437	0.5712920964130136	0.3437990460749385
0.6152042072643368	0.4823293592807177	0.6962351987608559
0.5955704119520999	0.6060336401845268	0.3220462080514580
0.7232605397147758	0.5467099527561143	0.5038627198304418
0.3546468648024322	0.6492212985375336	0.5925180928880222
0.3511252812185798	0.6706321011896125	0.5280560635066923
0.7085605284676851	0.5631659808504770	0.5680516307964288
0.7028917653874817	0.5977419499179679	0.4637809271748044

0.4742598062356369 0.7056978542241855 0.4049233736274598
0.4898396949849911 0.6083393996990120 0.7004598412774728
0.5573269025684606 0.6031172065495011 0.6954198752654309
0.5417347324865900 0.7004523975630125 0.3997839503996078
0.4695724510187654 0.6593095795503774 0.6603569261943283
0.4594082252967808 0.7222313156574576 0.4690924932276976
0.6793485591154842 0.6240939429128808 0.5673532104066672
0.6755492778993660 0.6455975211320493 0.5033611290760589
0.5783559952629127 0.6508035258384358 0.6523490559701242
0.5686410293813172 0.7138451455527872 0.4609419634449254
0.5245551311351865 0.6854365651569311 0.6304641751482177
0.5179560808640280 0.7272694871163639 0.5036539475232041
0.4858376659507565 0.2549433361084045 0.5600411635955226
0.4725920227729736 0.3379901310899238 0.3081251721800777
0.2735827303676003 0.3905356299718171 0.4757673997983389
0.7007057635657886 0.3579281138797017 0.4427055101081507
0.3573247032422966 0.5771115027357619 0.3063819747469619
0.3786494914287050 0.4429959757747371 0.7139380904308097
0.6425949776485217 0.4224676915915606 0.6936854635954299
0.6213669403514033 0.5570590362277917 0.2860669065850400
0.2993092146601779 0.6421066263080760 0.5573252236063356
0.7265897971350058 0.6092598069347264 0.5242046246151808
0.5273078826186623 0.6618810109893943 0.6920644099390548
0.5141577664392545 0.7447463140936877 0.4400517262335862
0.4964596264118520 0.4393386908841505 0.5147854300684641
0.6590897097863686 0.6155565798346412 0.6526871717442634
0.6793906530971220 0.6273534501904049 0.6731323396370663

CO/Cu_{309} $E_{ads} = -1.14$ eV
1.00000000000000
38.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 38.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 38.0000000000000000
Cu C O
309 1 1
Direct
0.4932482346560265 0.4599461238181489 0.4525470377906903
0.4999582553215667 0.4999764910128703 0.4999606171753612
0.4440303734590755 0.4729153313394533 0.4940106117934751
0.5496165592397383 0.4648899977429003 0.4857865472783134
0.4646790531061599 0.5190318621960859 0.4521352673407886
0.4699889480335306 0.4858820464352893 0.5528841343307175
0.5324646685579835 0.4189106557163945 0.5638946280615479
0.5299546061607610 0.5140874122171306 0.4470357856810009
0.4133459056481174 0.5551813220533517 0.4656589818854150
0.5558863781821490 0.5270416605683848 0.5058900932503255
0.5066624272496290 0.5400130561194422 0.5473766609720332
0.5034039835304777 0.5605120550865836 0.4851235284635043
0.4895902293309434 0.3974249287489778 0.4667727102548775
0.4361017886330814 0.4316347206476128 0.4455504367376261
0.4394279664501258 0.4106436063552126 0.5090243801225581
0.5470485077060893 0.4024694925622297 0.5006411323348966
0.5437274787723891 0.4233772491508648 0.4371691596693134
0.4571096396956386 0.4785735683812583 0.4029152400169557
0.4658993723341951 0.4238741008055461 0.5690274344044988
0.4070211396123936 0.4917760211246797 0.4451170591285771
0.4123870801234039 0.4580091672041141 0.5478310598106592

0.5236770498229005	0.4735435573856874	0.3976560761383387
0.5352322484916212	0.4809061247001926	0.5477856617240956
0.3923027678704226	0.5081893146346010	0.5083420397499430
0.5865267735410706	0.4447478222976187	0.5342578177643248
0.5811417247669373	0.4785903754718905	0.4315441939638032
0.5053499069555253	0.4661596725762671	0.6026637644044424
0.4945714956710749	0.5337638764000353	0.3972290779580773
0.4502946203367271	0.5350875175463338	0.5141579720282721
0.4187521446656242	0.5213946185091110	0.5683419469331148
0.6075915181606307	0.4917869093677011	0.4915481268408512
0.4674934597945364	0.5811054937171427	0.4360564181287337
0.4762240783762017	0.5264368380652077	0.6022363507632362
0.5929778222343635	0.5079876853234370	0.5546253504149934
0.5875498004438461	0.5419653802847070	0.4521694577035727
0.5425815411666314	0.5212653351217320	0.5971103690523633
0.5340155506973916	0.5760481332812984	0.4308516631330549
0.4562710360711981	0.5765743887885310	0.5627817232119203
0.4528113537153650	0.5974589498959821	0.4992674973975114
0.5637216280271077	0.5685045653582551	0.5541973685433269
0.5604828523666460	0.5892848534985891	0.4908603591917328
0.5102871751935134	0.6025055789164259	0.5331433585972858
0.4930628182551675	0.3779963636793365	0.5299280779483402
0.4864815345981598	0.4192902217317256	0.4044397465972712
0.3872593711715890	0.4454506366446266	0.4880306193202544
0.5999917880782906	0.4292743374681503	0.4714031719235724
0.4288921154439776	0.5384258686485310	0.4036016506021221
0.4395687262456528	0.4715905516970224	0.6065682657554525
0.5711405382441691	0.4617517661567351	0.5963709044849098
0.5604249740970154	0.5284094511713756	0.3933478447804926
0.3999192739852986	0.5707393276860739	0.5285731213753715
0.6126633383006881	0.5545176739453499	0.5121349331675623
0.5136853742402581	0.5806091482496242	0.5955440315664010
0.5068852922921776	0.6219216451350713	0.4700465826646706
0.4314656927296223	0.3677470341676564	0.4600386255378140
0.5408380287527225	0.3594095259816711	0.4515604860931228
0.3984336953135151	0.4501663680255459	0.3950307716093978
0.4074187357545297	0.3945936478963018	0.5639636176567998
0.5844309868792549	0.3812667569806153	0.5502417450814978
0.5755035038243346	0.4367912299023189	0.3813163994906708
0.4874714849419564	0.4928223049686050	0.3464792787002586
0.5019027360238114	0.4030270949369868	0.6197644445773598
0.3540116276997026	0.5280263096067885	0.4588947271873241
0.3594987779105400	0.4937243955639046	0.5632688884773041
0.6458702182043811	0.4721175872838188	0.5412172299688743
0.6404097703814060	0.5062665159138001	0.4367407961077678
0.5126880778134248	0.5072503635831156	0.6534166088863065
0.4980620194153882	0.5970018319900551	0.3801631113147155
0.4154964479092642	0.6187642115583027	0.4496983223993745
0.4245143664837595	0.5631699334485680	0.6186167449391714
0.6009704046735930	0.5495340495631608	0.6043524846990443
0.5925019316984853	0.6053540600815507	0.4360393710100695
0.4591539834355435	0.6405095616389895	0.5483791684158343
0.5685753056083629	0.6320641937772613	0.5400720166160570
0.4859971267771422	0.3349364387732860	0.4816818943033589
0.4826841501865256	0.3558790896472617	0.4181650628101426
0.4354820237077600	0.3482579685603780	0.5242459889087537
0.4287732158742247	0.3902708547550136	0.3968372628428458
0.5439126589706903	0.3399970581609691	0.5158323890080557

0.5372940168875380	0.3819216316163632	0.3883105475204344
0.3786212546412643	0.4035068711363518	0.4390748328260762
0.3819140604171620	0.3824381179283688	0.5030401714966883
0.3492906882593778	0.4641609255472502	0.4386537295178106
0.4499932839696689	0.4376393578049048	0.3538159352583485
0.3546442514075483	0.4300842263054110	0.5422051168559744
0.4621386739586698	0.3615775273569878	0.5847427917235771
0.5980485300060894	0.3660131735119405	0.4862713812530228
0.5946263307681589	0.3869903153378101	0.4221877178824298
0.5170025877702837	0.4324897989958774	0.3485843936103771
0.5291831356093605	0.3565881812953158	0.5795632781903800
0.3344940206689142	0.4805972640583897	0.5023522345129540
0.4208767874175433	0.4978519845782189	0.3533856458008756
0.4351425506152516	0.4089906490327816	0.6235263858684036
0.3703437261844826	0.5111699277877900	0.3959767516280711
0.3811080981569598	0.4432996821033746	0.6020719258700179
0.6378655433677388	0.4087212677695720	0.5201516611119334
0.6324239589498044	0.4426928123055582	0.4166491758437886
0.5544159090491371	0.4877266012218051	0.3429460666993522
0.5686558299903023	0.3989445104701681	0.6131486443234756
0.6232166151431532	0.4252017243518260	0.5834288239338528
0.6123562665700644	0.4928187509387016	0.3770766689167603
0.4749545288906813	0.4516941428058852	0.6574161345407689
0.4585130491304267	0.5534507408264108	0.3477311523824073
0.6590355102257007	0.4560068512113384	0.4772065871282072
0.3408645091007104	0.5440285048774228	0.5228683441773158
0.3767547353970808	0.5750251994121083	0.4165741187515440
0.5415727100316141	0.4467472583163587	0.6521914028890701
0.3876535634009829	0.5072118903416158	0.6228328555011420
0.5250878211886527	0.5483833609744411	0.3425061612796690
0.3620655615727472	0.5913782302555604	0.4798498417311980
0.3674873956333627	0.5573630562298942	0.5833421688143415
0.4313035137852450	0.6012133005149076	0.3867578720430437
0.4456736037466266	0.5122696402753317	0.6569783344097012
0.6297162433817850	0.4894596449659313	0.6044365355401778
0.6188036894125928	0.5566704606614299	0.3978704444109135
0.6653838974109059	0.5194153256155042	0.4978505247741873
0.5797062621391781	0.5026375542153244	0.6466027836798567
0.5648780200421489	0.5910106197079090	0.3763770357078388
0.6506378047531356	0.5361875675002039	0.5619946696072069
0.4053109288934025	0.6129636671379990	0.5777233804967336
0.6452144699827237	0.5698611944547217	0.4579143173441396
0.4018437921777340	0.6340110406922539	0.5137222525657430
0.4707234173768895	0.6433806099124033	0.4203459612691445
0.4832406444830002	0.5674414006752109	0.6513575678362731
0.5507701012789411	0.5624979244925530	0.6461814419526795
0.5378300368212199	0.6383212398932385	0.4152423280906629
0.4628226304507206	0.6179391026762326	0.6115984172624543
0.4560358316452321	0.6599029483293752	0.4841603941583958
0.6216104617743202	0.5962347432657700	0.5615710871300464
0.6180174227664077	0.6174663252360082	0.4971612673848818
0.5717491502422369	0.6093869770271982	0.6035886174734930
0.5644733583607723	0.6516413042201946	0.4758174135808839
0.5174865822141403	0.6439452112706059	0.5818431395806515
0.4621910813036959	0.7044940035557897	0.5335609869358503
0.4796114620410339	0.3781489674308605	0.3557560548127184
0.4895534709604444	0.3158165163218423	0.5452137748999945
0.3297911016119790	0.4176524151407436	0.4819389193929207

0.6509528515925390	0.3932161784940698	0.4568173954137671
0.3926428559695954	0.5579971878147472	0.3544490137699059
0.4087676019982570	0.4570990475669109	0.6608939316637188
0.6073698450985812	0.4421441795030375	0.6455106859759240
0.5912137397284726	0.5429059413356447	0.3389931964362624
0.3489287699152472	0.6068024036455025	0.5431426245315639
0.6701332743804697	0.5823136029631029	0.5181874969748527
0.5205237056470768	0.6217630932162237	0.6442159964931985
0.5103778281832044	0.6840798602407603	0.4547416000468263
0.4270843213293032	0.3037116860973009	0.4749014929381205
0.4238498772289830	0.3249112065131488	0.4108043338928555
0.5377840071627059	0.2953280827593799	0.4663187136969318
0.5344330288839361	0.3164800818293830	0.4020873143058422
0.3396705181115726	0.4217428454024468	0.3876884020489991
0.3486385662196322	0.3654562745020506	0.5586107599059514
0.5925403294119369	0.3216818577717483	0.4363608723232675
0.3903882581771305	0.4083766743276735	0.3450014031569231
0.4027603642401295	0.3309212604958950	0.5800693004999572
0.3730829216122568	0.3383231231226385	0.4535260796876590
0.5817123568631861	0.3174816357233733	0.5661204942522284
0.5694849704772017	0.3947637941429096	0.3310184856290333
0.3609921214452568	0.4692224237154102	0.3445504081481534
0.3754972042195842	0.3789445052270786	0.6192912047327650
0.6365322651415528	0.3437127301721001	0.5361765402784662
0.4805548269013155	0.4515398941188232	0.2958306859598016
0.4984093153405125	0.3394373113495970	0.6363930659002495
0.6275714688776076	0.3998736147845325	0.3654353469718889
0.2947277211345476	0.5005116503592085	0.4524012352854596
0.3001948026865331	0.4657165576180847	0.5578942430733899
0.6217427735893818	0.3603021388331458	0.6001525026280492
0.6072971220518171	0.4505788288469410	0.3253256989325731
0.4710287707178207	0.3873744580628010	0.6756582273552474
0.4511491504916745	0.5124412007293233	0.2953984139306168
0.5383407894555120	0.3822456419632529	0.6704200512356728
0.5183026431740010	0.5072783160137019	0.2900186964566190
0.3159663792364455	0.5480383997320113	0.4092078149053068
0.3270640335574171	0.4790659111812072	0.6185850194967534
0.3010099481769229	0.5645857067933392	0.4730217227314632
0.3066003209840891	0.5298131474278969	0.5786632919212124
0.6987283800172307	0.4354652961816702	0.5269021287221646
0.6931817558834562	0.4701671917698327	0.4213532445659094
0.6839268824897096	0.4518681814097759	0.5907940582943603
0.6728409433537083	0.5209125475646867	0.3813940848355643
0.4816897543142153	0.4927159528242987	0.7097222016501566
0.4616588949527468	0.6178271446163925	0.3294326331595506
0.5488669892584201	0.4874470232523676	0.7045315001578105
0.3781191459642479	0.6398088384561509	0.3997849586269224
0.5289032504485198	0.6126951322262022	0.3241616224193217
0.3927298577280460	0.5493406249104711	0.6744915437196054
0.7052287792741473	0.4995343356449656	0.5474925012920112
0.6996382845674060	0.5343124938064586	0.4421637371715139
0.3724080220398879	0.6000857184798353	0.6344810828467111
0.3633042509323827	0.6563773321368390	0.4636921444259212
0.5193899667972421	0.5485176674195186	0.7041133838652470
0.5015158174909398	0.6605698565019509	0.3635221328307190
0.6404966609909064	0.5313162404732049	0.6569730232934464
0.6244070126445833	0.6210217000022289	0.3806810217997648
0.4182027294598878	0.6825219812228338	0.4337886331058163

0.4306021662739647	0.6051983458702757	0.6688260202479258
0.6618650831706568	0.5790363930053307	0.6135943024837718
0.4074344067177177	0.6782543458796253	0.5635519100886868
0.6512559770975792	0.6344119876070639	0.4414494131755623
0.6109184692160218	0.5924512673323397	0.6565480040596754
0.5970676115267554	0.6689415705309256	0.4199327684199947
0.4655959758451056	0.6833447053826868	0.5978655358924416
0.5140301158463118	0.6649407664072191	0.5183206547825623
0.6269293744456984	0.6616129807199932	0.5463732869697412
0.5760429886853508	0.6750455770967966	0.5892154003419959
0.5727800397533307	0.6960305510101297	0.5250269427297829
0.4791584980169528	0.2930621085940445	0.4330412347690419
0.3711802118300232	0.3621378560946913	0.3902417053808806
0.3778236675238272	0.3197658605136570	0.5183701062334086
0.5949550520502441	0.3032775378956720	0.5013849902963774
0.5883431944396279	0.3453361056462731	0.3731266212850446
0.3125630545197844	0.4834295197317993	0.3893690570415804
0.3231477659475113	0.4152116964147847	0.5965975649855960
0.4136257047313702	0.4568256395449948	0.3042108204422829
0.4313110197780287	0.3464742605282733	0.6393408170746725
0.5478752685804464	0.4466401820652534	0.2935874374928512
0.5655658035515475	0.3364065110701951	0.6289551715271277
0.2827509250611176	0.5165148127164750	0.5169724872216652
0.6746403014651744	0.3885982845616940	0.5692340364791652
0.6637424386530228	0.4568590514485249	0.3619600826408368
0.5108602254954582	0.4318085050956902	0.7071637782101283
0.4891428713268643	0.5682056000592663	0.2927059284447260
0.3252343621625874	0.6114373125119992	0.4307234154828517
0.3361704301511085	0.5432037234656782	0.6379326025366624
0.7171231662840285	0.4835153436018348	0.4830207509469057
0.4343722610596569	0.6637644206758107	0.3709168958341112
0.4521508425457141	0.5533602580992047	0.7062926275086365
0.6880678831400537	0.5159058444623519	0.6102072698903575
0.6766827513829187	0.5847331233244241	0.4035222256889968
0.5857578170168863	0.5428575618596532	0.6964597385120523
0.5686584487621992	0.6534336719737235	0.3605387723411261
0.4117811973404703	0.6545125714570937	0.6267567916258067
0.4048967962921418	0.6966485798625419	0.4985876513338758
0.6287042327570452	0.6387132115965100	0.6093515323967257
0.6221028576316859	0.6801236947156746	0.4816244298434199
0.5208127882074305	0.7067960275498343	0.5669273501595745
0.5407904334078544	0.2775600300774516	0.5309086167176413
0.5307327611542042	0.3405516288859979	0.3395265811465452
0.3211617356884791	0.3754768464687097	0.4326232543753838
0.3244984125314759	0.3542050815377802	0.4970040852465689
0.4214464912904309	0.3489719393288664	0.3481651862482317
0.5102735363506946	0.3914927670761992	0.2995586653180696
0.5258918803640140	0.2943366841797950	0.5951917639667973
0.4428147017271958	0.3966780124446632	0.3048411653727331
0.4315455520106330	0.2859442355691633	0.5394685040983190
0.4582419345369078	0.2993655841749519	0.6003913289878580
0.2916296968626221	0.4365502781264838	0.4321911732707721
0.2969974940213355	0.4021543518411611	0.5364977379747872
0.4757818552605889	0.3143439270631361	0.3696333888041098
0.2767344944507565	0.4530774089829523	0.4963128815161421
0.6489201205361187	0.3295546401689436	0.4718172425459569
0.4824341275124467	0.2725000187621243	0.4965941682292756
0.6455695536690403	0.3506916798292581	0.4072646382343632

0.3846839681121348	0.5170820654219713	0.3039412056279107
0.4043982270075892	0.3941106020575549	0.6779214740083896
0.3337349619048557	0.5304440930850037	0.3468362766832918
0.6890311266922267	0.3724476829544110	0.5059527646926461
0.6835842186130288	0.4067638518082204	0.4017114777793826
0.3499275832773686	0.4286309795304024	0.6563763499512151
0.5851988859384537	0.5018834490726128	0.2882924697786330
0.6048612433222873	0.3789011496229003	0.6623567024592639
0.7103825682650208	0.4201674154961859	0.4626152352836703
0.4443897929903003	0.4370427307579144	0.7120957883095403
0.4225781263281445	0.5730789161434183	0.2982568567915633
0.6597907354385442	0.4052214612273837	0.6324036214773734
0.6434797673516393	0.5069221084470747	0.3226556959455891
0.3401625009879893	0.5947880493468611	0.3675669101035373
0.3565749765960873	0.4930172275831279	0.6772087807301334
0.5774227689956720	0.4269315658398482	0.7016899092777613
0.5556501595282742	0.5629887408899751	0.2878291086565219
0.2895392724547816	0.5798827526757505	0.5374043496373299
0.3951004893764021	0.6211830663270683	0.3375642441018701
0.4148502275892331	0.4981455054200853	0.7116360295754336
0.3108903322589242	0.6276026976292908	0.4940535629310756
0.3162448285886046	0.5932304261981419	0.5983303347081090
0.6662107144862587	0.4695643084948414	0.6531889501877384
0.6499805397894954	0.5713493187354792	0.3436136110781439
0.6153838857332208	0.4829081888148989	0.6959914137354462
0.5955580166236039	0.6059944299950256	0.3219196738309305
0.7232077964595828	0.5469265171410804	0.5036993391662294
0.3544180331654157	0.6492642581101600	0.5926548081246982
0.3509628833788906	0.6705560034693295	0.5280943865036309
0.7083223203255364	0.5635011530078219	0.5678079520465512
0.7029010170169695	0.5978094730927607	0.4635746620079190
0.4740329584161296	0.7056748388293652	0.4047372265847763
0.4897510138270126	0.6084969301307813	0.7003998178196689
0.5572254462609834	0.6033541650234430	0.6951159553093353
0.5416158099544149	0.7005176925942979	0.3996367224831459
0.4693476049268929	0.6593604203410545	0.6603958777912492
0.4592058102911508	0.7222794221031951	0.4689982365211054
0.6788569921205573	0.6244676546391780	0.5673748801016223
0.6754623664497375	0.6457591989868935	0.5030063732140397
0.5785464386495428	0.6509591389899857	0.6518788944247172
0.5684251438501177	0.7139644892301772	0.4605502139276511
0.5242326595732728	0.6856003593490010	0.6303439688633062
0.5175498972843042	0.7274004795344778	0.5034164868245008
0.4860820340853956	0.2550800387270070	0.5602006052952198
0.4727196503635709	0.3379854677906206	0.3081680983588394
0.2736428327856731	0.3904887934461100	0.4758955128873654
0.7007841673836539	0.3579906181248422	0.4426563775628722
0.3572486386186250	0.5770000960458678	0.3063827550743284
0.3786731397293753	0.4429690512243606	0.7140110760378291
0.6427584740100936	0.4229396317805431	0.6936312957525433
0.6213843009067421	0.5570711083864159	0.2859154889586232
0.2991415955075422	0.6420753538214928	0.5573646172839999
0.7263860886193861	0.6095323883667607	0.5240825309125163
0.5272670416679883	0.6620479657007559	0.6918551234829694
0.5139024463994289	0.7448221375751549	0.4398284858213645
0.4965235032277830	0.4394250963243995	0.5148172619499488
0.6619989947024408	0.5795146492281946	0.6673346134658622
0.6824712512673432	0.5895817911800179	0.6884375151553354

CO/Cu_{309} $E_{ads} = -1.01$ eV
1.00000000000000
38.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 38.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 38.0000000000000000
Cu C O
309 1 1
Direct
0.4932535376455147 0.4599722395140143 0.4525715927903307
0.5000035278492855 0.4999974167160271 0.5000051346969021
0.4440743665387409 0.4729386460006613 0.4940221497849261
0.5496418481304882 0.4649575906736557 0.4857931749732027
0.4647019682645769 0.5190137726974247 0.4521603862332045
0.4700083235374191 0.4858944931523456 0.5528679328344115
0.5325269767027621 0.4190007152281051 0.5638924389881257
0.5299648006375347 0.5140855321326534 0.4470733919542403
0.4133987961018932 0.5551723232345463 0.4656807082427569
0.5559657966322799 0.5270795226825831 0.5060169950633814
0.5067706940426594 0.5400144805000558 0.5474308631619195
0.5034712569913102 0.5604829997764592 0.4851296224192594
0.4896207025528063 0.3974760810068500 0.4667932120518193
0.4361531080434962 0.4316360889584781 0.4455682057580705
0.4394743204350065 0.4106436870858203 0.5090131414938275
0.5470753172289753 0.4025089761692440 0.5006654026618332
0.5437287482294514 0.4234262062500747 0.4372085731506535
0.4571477293669362 0.4785911939875880 0.4029139509015220
0.4659779222409923 0.4239584624525649 0.5690492722461040
0.4070469903974982 0.4918220610572399 0.4451368107752735
0.4123989462716702 0.4580173098457034 0.5477944918075549
0.5237374048271018 0.4735632277254335 0.3977010095535176
0.5353007940728102 0.4809990649380105 0.5478404195474422
0.3923279211830359 0.5082289972544880 0.5083326190453460
0.5865540839976725 0.4448741857252540 0.5342743903948034
0.5811987442471848 0.4786448772496942 0.4316214713591652
0.5055227624611872 0.4663743956982216 0.6026365303881646
0.4946262584942389 0.5337880358696635 0.3972743112415130
0.4503237701216616 0.5350854623856740 0.5141646903637865
0.4188570840072739 0.5214083856356561 0.5683648343404538
0.6076205432096428 0.4918722364658609 0.4916983702957523
0.4675296829456370 0.5810669838595666 0.4361004427670842
0.4764877808749642 0.5264443562905085 0.6022093960367004
0.5931428498113941 0.5083114659512905 0.5549613915084654
0.5875440969385860 0.5419595775443758 0.4521655891758540
0.5433516489048184 0.5216510820771740 0.5970936866439781
0.5340949171754387 0.5760494382145360 0.4309306729904944
0.4563711663658832 0.5765646910304710 0.5627884390370328
0.4528581055033690 0.5974520718715197 0.4992969562192104
0.5640794339239202 0.5684371689128839 0.5545353571125907
0.5605631310666614 0.5892531437242260 0.4910175490939508
0.5103880902050260 0.6024444203297907 0.5331649020245237
0.4930918899241507 0.3780631968107421 0.5299158626295489
0.4864728535660783 0.4193472961319872 0.4044505044080263
0.3872952958364876 0.4454724142685678 0.4880543362631495
0.5999786561060394 0.4293020829218509 0.4714448018394233
0.4289283535397593 0.5383767566419992 0.4036134549066513
0.4396191199918640 0.4716151212525793 0.6065228520762044
0.5712496029165650 0.4618455810007381 0.5963878841838849
0.5603853343796378 0.5283834088562247 0.3933165969322207

0.3999865425091295	0.5707223241945588	0.5285644643097047
0.6127288147576273	0.5545475711762163	0.5120782716504914
0.5138290407155202	0.5806473442212782	0.5955606626718862
0.5069018022483239	0.6218873328779033	0.4700929431560207
0.4314652513429464	0.3677858724305729	0.4600759549234261
0.5408573500623284	0.3594538463395634	0.4515923265740372
0.3985262255129193	0.4502247617611093	0.3951572556385660
0.4074889148524324	0.3946313732282887	0.5639808511656946
0.5844446541797377	0.3813311540943722	0.5502347167943045
0.5755286532602536	0.4368050887761474	0.3813650964763965
0.4875200256190047	0.4928405406928220	0.3465216798546003
0.5019093002863609	0.4030346810944593	0.6196776421206198
0.3540322227008615	0.5280094997292460	0.4589418007057048
0.3595691052775168	0.4937516375845230	0.5632866385294663
0.6459280189967240	0.4721582442707403	0.5411440879558086
0.6404137725973036	0.5063394188351324	0.4367248640757320
0.5126772466420719	0.5072527577792882	0.6533184648005043
0.4980841485707358	0.5970013633048442	0.3802178832314184
0.4155453064289091	0.6187474090959472	0.4497393857128070
0.4245052316570201	0.5631725302114855	0.6185389433343075
0.6026836380935183	0.5503723807289070	0.6051639115287211
0.5925627375034186	0.6053091268678426	0.4360330447872577
0.4592124632550313	0.6404745351751674	0.5483868841223095
0.5686408463516001	0.6320764065942701	0.5400107853874038
0.4860241605712913	0.3349953658740271	0.4817145006598038
0.4826754715658323	0.3559135963589485	0.4182178879239598
0.4354848345317084	0.3482759325328190	0.5242810840268084
0.4287925414061293	0.3902520311038132	0.3968377544547805
0.5439551777828074	0.3400453693319279	0.5158652060809830
0.5372695734094352	0.3820134830528727	0.3883823727336821
0.3786475037707411	0.4034886816308635	0.4391131336271226
0.3819679288700435	0.3824117248229541	0.5030741763358000
0.3492812730394919	0.4642114476032274	0.4386930606917777
0.4500208379906668	0.4376581444869866	0.3538388304793320
0.3546912321083290	0.4301019537878369	0.5421798273636511
0.4621456742919390	0.3616387352869326	0.5847128584653938
0.5980524471892311	0.3659960296004149	0.4862544679596259
0.5946776409026431	0.3870402573196937	0.4222942478009640
0.5170349107111338	0.4325557004774757	0.3485784006056243
0.5291893833860792	0.3566575401902254	0.5795145061585971
0.3345038284345720	0.4806591707256460	0.5023928089458104
0.4209053419363231	0.4978550431056065	0.3534037773040698
0.4351465522695671	0.4090224680156536	0.6235055624339604
0.3703325077747237	0.5112048875622992	0.3959734064319624
0.3811783911874613	0.4433301943128918	0.6020958379677427
0.6378194603658239	0.4087067612718618	0.5201335143253448
0.6324049577219585	0.4426899817959764	0.4166405334020700
0.5544121182068075	0.4877341132301509	0.3429124622118123
0.5686681226564101	0.3989933427855443	0.6131254862823698
0.6232479831289384	0.4251058782977676	0.5833882237589175
0.6123289279074891	0.4928266949035680	0.3771287272776248
0.4749670631090143	0.4516820068126444	0.6573140024139251
0.4585838477437670	0.5534239531716169	0.3477253969696641
0.6589531616116938	0.4559885716571722	0.4771118869489790
0.3408789339732936	0.5440243923075536	0.5229073398691538
0.3767684672351326	0.5749937526937801	0.4166307602206730
0.5414447298784787	0.4465499074793801	0.6522102526310962
0.3876746052036392	0.5071907308605375	0.6228093613265908

0.5250933839391285	0.5483644999441742	0.3424745044811749
0.3621212488776002	0.5913634794138283	0.4798875961026999
0.3675288906533150	0.5573330243245432	0.5833143106531213
0.4313542466344499	0.6011291709031710	0.3868311299113444
0.4456646071967506	0.5122905515173974	0.6568720483883780
0.6298214240319371	0.4890974090440670	0.6041880675360901
0.6187503881266438	0.5566404306059372	0.3979442318996370
0.6654058821495310	0.5194041879629047	0.4978177316263105
0.5792892787045895	0.5022405825746480	0.6466426177367843
0.5648607131486197	0.5909742972513028	0.3764308685233829
0.6509423744138169	0.5364499786188904	0.5620121901685265
0.4053598711153671	0.6129230748843835	0.5776793407137139
0.6453233786564400	0.5699074888583751	0.4581151035496025
0.4019141918270560	0.6340142129763185	0.5137627174824386
0.4707956008488945	0.6433829905416205	0.4204615842066717
0.4829849458019035	0.5674766026623719	0.6513583678751719
0.5501977193334193	0.5624298683298065	0.6462197390631633
0.5378202323312026	0.6383011057802838	0.4152376291833825
0.4628586973007130	0.6179217744669485	0.6115775879496720
0.4560291429541029	0.6599118030930502	0.4841531148603663
0.6220208632030289	0.5963021556999588	0.5615948409482943
0.6180243451862435	0.6174844564591452	0.4971328411444670
0.5715500080555074	0.6096830443730635	0.6033422180213072
0.5644168438537718	0.6515803153283434	0.4757377297912726
0.5174320485462485	0.6440292448121220	0.5818102784307149
0.4621591365662374	0.7045161510673786	0.5335552942984140
0.4795442796784813	0.3781857820609044	0.3557726232383682
0.4895299982191986	0.3158679814245333	0.5451847042023623
0.3298270566988490	0.4176749281800095	0.4819122228517391
0.6509690167075581	0.3932393651151971	0.4568665804947608
0.3926307174195924	0.5579202446236660	0.3544646643803249
0.4088394226242598	0.4571369459548932	0.6608781779731304
0.6073753054045489	0.4421237011638688	0.6455669178173281
0.5911284446008122	0.5428544345030769	0.3389876949648140
0.3489519662399611	0.6067569501977169	0.5431153446195877
0.6703103313661783	0.5823991614971590	0.5184186625432370
0.5205193322837359	0.6217882858791847	0.6442674070236768
0.5104122840079821	0.6840680308616253	0.4547957525570122
0.4271154383112285	0.3038044468560223	0.4749868223335348
0.4238169128391709	0.3249014566163033	0.4107140483997304
0.5378032198745043	0.2954027599981667	0.4664101503905920
0.5343945995222037	0.3165943237355640	0.4021437277468027
0.3398228862022202	0.4218338478521045	0.3879299058392172
0.3487031656957726	0.3654629906119186	0.5586022409520568
0.5925210652533950	0.3216735240923811	0.4364182908528422
0.3904461670727435	0.4083442820497646	0.3450634971224872
0.4027850164861949	0.3309592055255651	0.5800522245883204
0.3730538603789018	0.3383281554128032	0.4535118750882638
0.5817691877527548	0.3174938824710714	0.5661245920319277
0.5694410162129959	0.3947863417443244	0.3310827701162835
0.3609936194945574	0.4692986779661835	0.3445955440054920
0.3755109356821144	0.3789167561363776	0.6192523703130893
0.6365317444744870	0.3436700875568910	0.5361615097971457
0.4804180427245435	0.4515078393757609	0.2958331081392629
0.4984333793287734	0.3394681901528132	0.6364099712103537
0.6275605713600741	0.3998549309174124	0.3653930089867408
0.2947030975391122	0.5004964827269760	0.4523994502482978
0.3002400869477805	0.4657486174555553	0.5578958672343216

0.6217074924958479	0.3603469658874736	0.6001162259445820
0.6072702369106077	0.4506613365706598	0.3253734598276959
0.4710534756700532	0.3873604427941307	0.6756187806516806
0.4510441667161874	0.5123412951850072	0.2954017141621875
0.5383378501335103	0.3821988881687973	0.6704234803269784
0.5183283698386653	0.5072816738877339	0.2900442495703387
0.3159328911986521	0.5480280159430571	0.4091279977584271
0.3270529522462676	0.4790748911262686	0.6185430329269093
0.3010880664006856	0.5645591923062052	0.4731167080413413
0.3066436235416550	0.5298011807279243	0.5786445184654364
0.6986990298905991	0.4354961513229759	0.5269066093816906
0.6931876937416024	0.4702618883262363	0.4213735994708674
0.6840606941493410	0.4518139396860884	0.5908209326594852
0.6728524591054619	0.5209586000112589	0.3814572063345426
0.4817074731531731	0.4927411904968220	0.7095421196456305
0.4616453081307952	0.6177643860056899	0.3294956652016875
0.5489492247870520	0.4875821890936221	0.7045402202558860
0.3781880590220617	0.6396892406846166	0.3998614853667182
0.5289396943884241	0.6126201206068544	0.3242039968052177
0.3927195355357401	0.5493672700917595	0.6744486663834146
0.7053331253403637	0.4995801533447652	0.5475699531511152
0.6996844328973058	0.5343353345060368	0.4421093466520813
0.3724334042091338	0.6000897282517414	0.6345008241369492
0.3633835136499929	0.6563423110561848	0.4638025759394510
0.5195368967185975	0.5485218799095136	0.7041101512785116
0.5014864349926902	0.6605578930456127	0.3634859033943744
0.6390601759417969	0.5305088112748292	0.6559053868653431
0.6244338431824288	0.6209959376951283	0.3807513084853554
0.4181923725574554	0.6825099787669280	0.4338558681687258
0.4305594268706235	0.6052289900772609	0.6688346205565399
0.6627731908772619	0.5794869939614430	0.6145696401612598
0.4074746561884922	0.6782898525325517	0.5635597511164800
0.6512982605344657	0.6344348402685946	0.4414047893373448
0.6094623013155144	0.5918090062602509	0.6554712979740570
0.5971433241050410	0.6688876981265489	0.4199535914141658
0.4655969025682785	0.6832902096692882	0.5978349998635322
0.5139880682254847	0.6649068793632308	0.5183119773099263
0.6270330490007231	0.6616582778193363	0.5464572279819905
0.5760806296780276	0.6751776992753801	0.5892423750222384
0.5727884296641170	0.6959845103884639	0.5250415820564182
0.4791036977192745	0.2931811423886057	0.4330725217058244
0.3711519804295675	0.3620262279932620	0.3902591163268450
0.3777985239378635	0.3197297416897291	0.5182871471276400
0.5949959553628588	0.3032554022305113	0.5013922006236332
0.5883244957897626	0.3454994172259344	0.3732373546182658
0.3124408708408515	0.4835022282973469	0.3893917678610230
0.3232523639181492	0.4152444120525147	0.5965391427782080
0.4136331685920198	0.4568253056665754	0.3040814363782078
0.4313535099434198	0.3465188333835011	0.6393590485423372
0.5477936954378965	0.4466200158647715	0.2935584140765148
0.5654847617803095	0.3364005669932110	0.6289151092659808
0.2827095615868880	0.5165189871518021	0.5169013283995522
0.6746750029003831	0.3886328066249659	0.5692170648874483
0.6636871920595611	0.4568401420370632	0.3620149013929406
0.5109048209688141	0.4318682876304428	0.7071794552397600
0.4890735833939038	0.5681315098047748	0.2926727027624376
0.3252840823431006	0.6113326167267547	0.4307703226987807
0.3362259762686267	0.5432008196261656	0.6379452579062795

0.7170686343733826	0.4835403495578521	0.4830882198344875
0.4344805347699897	0.6636400085571910	0.3710437016573707
0.4522104277715041	0.5533695072200905	0.7063001827982986
0.6879348081261684	0.5157433178489346	0.6104984762526281
0.6765586790332833	0.5846777466378944	0.4035807598138167
0.5863010830187171	0.5431262994120697	0.6960762706019723
0.5686036939146428	0.6533981787711758	0.3605902818712240
0.4117141362028559	0.6544564660106393	0.6267204793082564
0.4049147125117828	0.6966973065464234	0.4985999961843679
0.6285147178848853	0.6387204160160014	0.6096377695311096
0.6220954511066230	0.6800668858676902	0.4817020508124887
0.5208547532173319	0.7067999339950866	0.5669185912259661
0.5408142063360877	0.2776256597043791	0.5309713778652486
0.5306310913699047	0.3406132836750542	0.3396371088171824
0.3211596274727047	0.3754578208172925	0.4326958259865114
0.3245135535425475	0.3541469311090200	0.4970638642801405
0.4213683023890282	0.3488977327402544	0.3481107686508118
0.5102658196781217	0.3915475168238213	0.2995365303526388
0.5258612906534780	0.2943760086632354	0.5951306215613112
0.4427935370564319	0.3966744173749951	0.3048315676231294
0.4315149160980479	0.2859190084052776	0.5394156212945609
0.4583230519528213	0.2994255597986819	0.6003664933511459
0.2916037286785397	0.4365802880295050	0.4322786916253216
0.2970843369625498	0.4021947844790798	0.5364795785214006
0.4757121543937226	0.3143562226534890	0.3696946848834056
0.2766926885980650	0.4531309315477352	0.4963894921542751
0.6489727169224001	0.3295349546848616	0.4718514007360337
0.4823820375268369	0.2725475416233654	0.4965540891072228
0.6456203007340015	0.3507737995324020	0.4073471097745398
0.3846750155811950	0.5170645091597684	0.3039202147039775
0.4043679053248576	0.3940848803208243	0.6778981068228332
0.3336315919663709	0.5304309532058209	0.3467765010000877
0.6890221582909705	0.3725040909566775	0.5059562465889148
0.6835780549769049	0.4067940899789090	0.4017214890641996
0.3500406680050908	0.4286720568660867	0.6564201732840201
0.5851251945160656	0.5019134636455730	0.2881661460736632
0.6047925829421839	0.3788805228567375	0.6623280596281309
0.7103134188674098	0.4201881779010492	0.4626483800468769
0.4444034392735817	0.4370653221782336	0.7119943052086257
0.4226154644681767	0.5730290740442049	0.2982298580096849
0.6597795820849182	0.4051047960942301	0.6323791126183015
0.6434259815157981	0.5069774259234370	0.3227260119866426
0.3401230073282026	0.5947217946453364	0.3676307125048137
0.3565182909241695	0.4929938338374389	0.6771764063585503
0.5772871058295479	0.4268342187223057	0.7018115957999097
0.5556289721823638	0.5629061983902757	0.2877143064539736
0.2895009821879760	0.5798810316761989	0.5373560172085234
0.3950812194148174	0.6210710207700936	0.3376714437619494
0.4148584081666919	0.4981451603831459	0.7115279341769655
0.3108890647025820	0.6275396052117466	0.4940230684586085
0.3163329432827350	0.5932475975132122	0.5983028218527853
0.6663747846768483	0.4692677229933006	0.6532446548619796
0.6498131058549785	0.5712731575425749	0.3436424112065901
0.6152391607558371	0.4827246797814728	0.6962173662164535
0.5955627768119657	0.6059100114669849	0.3220019529243148
0.7233530305705926	0.5468873370152585	0.5034695281008925
0.3544215009712905	0.6492099728305331	0.5925884913423639
0.3510279571178726	0.6705324917871118	0.5281516754749603

0.7089563554381855 0.5631658497029127 0.5671409173265228
0.7029483660860076 0.5978329477352573 0.4634886410602657
0.4741306231746337 0.7056589674167529 0.4048174456413000
0.4896053224642248 0.6084559531785216 0.7005075731181502
0.5570225499742725 0.6033723570547542 0.6953170168442644
0.5416312702321342 0.7004898225220998 0.3996422779752309
0.4692825957550280 0.6593109349293023 0.6603645671964337
0.4592376168791644 0.7223274186322680 0.4690396929712565
0.6790178829651230 0.6251712478535335 0.5667140600487494
0.6755337294765539 0.6458862623803100 0.5027927342166789
0.5784335443213012 0.6512740697969446 0.6519233144025813
0.5683991821258702 0.7138826916900007 0.4605916804661574
0.5241287386514178 0.6856760425317363 0.6303209161918730
0.5175939299466640 0.7273487805740588 0.5034270913170732
0.4860525857868325 0.2551101546069164 0.5601245008956197
0.4726844915082647 0.3379926505236541 0.3081838382726683
0.2736414949492763 0.3904923279107465 0.4758782158683968
0.7008070125249761 0.3580329183469042 0.4426765697082321
0.3572362612549422 0.5769677146364363 0.3063975800814065
0.3787281935356863 0.4429931438760670 0.7140192881940493
0.6426792150626233 0.4228799543450947 0.6936417145165900
0.6212970012618040 0.5570310250822166 0.2859127147354510
0.2991445786655860 0.6420401459839991 0.5573097395019814
0.7266058745012935 0.6096162356295695 0.5238381175876990
0.5271742090538279 0.6620305460383120 0.6918607922837703
0.5139575941091707 0.7448021926593729 0.4398611425957192
0.4965424303558050 0.4394530239111509 0.5148217617436589
0.6995672283453459 0.5975291162483638 0.6406710289872634
0.7227578859118904 0.6089150194344550 0.6566375772273049

CO/Cu_{309} E_{ads} = −0.97 eV
1.00000000000000
38.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 38.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 38.0000000000000000
Cu C O
309 1 1
Direct
0.4932801908852603 0.4599735864786285 0.4525939171843831
0.5000580323695544 0.5000082055972188 0.4999882286170018
0.4440602750873219 0.4729286091028634 0.4940448212132146
0.5496105128159507 0.4649142442132551 0.4858222363003533
0.4647183948076465 0.5190428149761299 0.4521732865427104
0.4700196692366821 0.4858965638604683 0.5529162262971831
0.5324772836828371 0.4188992092277397 0.5639019705642395
0.5299399593437802 0.5140803921640502 0.4471018007907909
0.4134449321662823 0.5552112655542670 0.4656879220317940
0.5560723745489013 0.5271324703691503 0.5059691904754348
0.5066996348696465 0.5400227945150684 0.5474210664685307
0.5034216177386479 0.5605085203212384 0.4851562662833495
0.4896714954688842 0.3974820920140125 0.4668013303948892
0.4361303255841087 0.4316028059711531 0.4455996598806790
0.4394596616851393 0.4106998080867959 0.5090623635190005
0.5471248413794710 0.4025401271947307 0.5006806517097955
0.5437806375802877 0.4234155686445345 0.4372147823230467
0.4572061287312837 0.4786203686593979 0.4028927743938297
0.4659750491214381 0.4239402270767526 0.5690832301769947

0.4070146373068704	0.4918257289893522	0.4451691816443493
0.4124345634916002	0.4580301665826937	0.5478606768049022
0.5237257994926902	0.4735619079365180	0.3977252444993182
0.5352568252146009	0.4809373059257942	0.5478244368150217
0.3923693260515199	0.5081793025262088	0.5083813573482683
0.5866002217490239	0.4448224250794762	0.5343141071448699
0.5812003079346149	0.4786210843172048	0.4316222710183792
0.5054287142994588	0.4662180071721365	0.6027058973923903
0.4946129166919539	0.5337942712238620	0.3972958013082660
0.4503397617784967	0.5350825013264109	0.5141790733153566
0.4188486129268013	0.5214150772219162	0.5683959834287557
0.6076034815765101	0.4918558112998550	0.4916333215099207
0.4675563439539696	0.5811214759969716	0.4361072354788235
0.4763167038149630	0.5264642925529912	0.6022761877996655
0.5929699821356184	0.5081891276834825	0.5547965426118199
0.5875511565698520	0.5419694604321018	0.4521880007009326
0.5428523149206754	0.5214017509683296	0.5970998164280276
0.5340724248727819	0.5760785180984886	0.4309346361286078
0.4562678841560167	0.5765932071338264	0.5627909535731526
0.4529146092007229	0.5974711815127652	0.4993106110541187
0.5638739327018126	0.5683673235759523	0.5543696143251342
0.5605409746839064	0.5892563808289163	0.4909517250795282
0.5103845766862151	0.6025198525862442	0.5331967351663371
0.4930586037117947	0.3780488703852676	0.5299064132140302
0.4864596307360866	0.4193222859492296	0.4044646361856353
0.3872729708019061	0.4454558234256103	0.4880050858544451
0.6000725828018252	0.4293363937949028	0.4714513588342624
0.4289040662874615	0.5383843928681927	0.4036285815857778
0.4396059883205054	0.4716091652484098	0.6066093795870083
0.5711324561340029	0.4616426592929080	0.5963566493708718
0.5604323664698200	0.5284161871495767	0.3934147963672167
0.3999644582288802	0.5706970487341615	0.5285534567535041
0.6131457960839688	0.5547499348425646	0.5120516688895941
0.5135948836509763	0.5806747222380628	0.5955187262210951
0.5069816008927595	0.6219432497317696	0.4700983410795799
0.4315265404936978	0.3677913627380952	0.4600954244440978
0.5409073270989601	0.3594676172909325	0.4515836941285601
0.3985577461335725	0.4502326295272853	0.3951543380885674
0.4074608169903253	0.3946624131556103	0.5640039842291634
0.5844309494818112	0.3812189751423390	0.5502742804019566
0.5755539045087820	0.4367941604231990	0.3813768611718369
0.4875333059029904	0.4928568000439672	0.3465323145904158
0.5019231998542961	0.4029714810036403	0.6197681724012235
0.3540856815515103	0.5280507423148058	0.4589588542219524
0.3595819675796826	0.4937128036520539	0.5633072301209220
0.6459626086905365	0.4720122065451948	0.5410345890652356
0.6404658470594248	0.5063494967269103	0.4367363759696540
0.5124949632995882	0.5071536866308556	0.6534810332554823
0.4980928378225755	0.5970434326633334	0.3802275365763827
0.4155880303343032	0.6187791025989028	0.4497218615131893
0.4244801205771317	0.5632204311977473	0.6186191712063273
0.6015168083201233	0.5497931712513313	0.6048177839468946
0.5926022800849065	0.6053517120985623	0.4360388353145783
0.4591177127467382	0.6405412450448484	0.5484112824360347
0.5685487198975256	0.6321994926373141	0.5399008362500048
0.4860225855835539	0.3349712378230898	0.4816914989570880
0.4826874614633556	0.3558695915515366	0.4182201754760893
0.4354654923152864	0.3483006834696755	0.5242673310952646

0.4287702578385585	0.3902490713855675	0.3968419517027085
0.5439385447309110	0.3400770840224818	0.5158461756993330
0.5372608698068668	0.3819995988032500	0.3883665861472144
0.3785852903032365	0.4034994092662736	0.4391105294584547
0.3819350430486296	0.3824228286132373	0.5030638354496649
0.3492654469444694	0.4641412537318453	0.4386878349991212
0.4500100305319246	0.4376175422371363	0.3538120065472743
0.3547018935404979	0.4301115193937389	0.5421479393439093
0.4621546331074931	0.3616430542372677	0.5847365828692622
0.5981005494930580	0.3660396644917127	0.4862593214953621
0.5947389264419946	0.3870617805444000	0.4222972335762255
0.5170463103198858	0.4325363389001872	0.3485981841443576
0.5291646350260605	0.3565788603879049	0.5795417163613233
0.3344999773491552	0.4806202448618991	0.5023760617676443
0.4208657677474297	0.4978756135876399	0.3533828899861151
0.4351034242333292	0.4090039730764757	0.6235437618266428
0.3703198251891490	0.5111808397783627	0.3959834358318967
0.3811796854060089	0.4433344115142090	0.6021473872419790
0.6378984020910482	0.4086404681579474	0.5201388299368148
0.6324670515689482	0.4426902057641172	0.4166629809865944
0.5544551845031955	0.4877382230944542	0.3430074115763313
0.5686787405483702	0.3988783182663089	0.6131752864696052
0.6232596780943932	0.4249701016177688	0.5833569473188773
0.6123745661204379	0.4928397246170504	0.3771628754592588
0.4749115970815173	0.4516031163061608	0.6574450083636686
0.4585736952792750	0.5534609049765673	0.3477433214375724
0.6590917874703648	0.4560705443476149	0.4771295123065740
0.3408896817714060	0.5439858934338359	0.5228880441413353
0.3767514787070895	0.5750303460835990	0.4166295029869564
0.5414559280980250	0.4465544677366018	0.6522541747770033
0.3876426734431107	0.5071774736621919	0.6228513387989895
0.5251173452152480	0.5484172085436801	0.3425679965524849
0.3621091774089208	0.5913682275548089	0.4798623168041755
0.3675464788662898	0.5573344098249212	0.5833368453580292
0.4313453567159467	0.6011353111484082	0.3868172287127901
0.4455793521159266	0.5122866875643547	0.6570051525338264
0.6296786995065555	0.4888484300776230	0.6039712557900473
0.6188177034801278	0.5566801520528609	0.3979161765675718
0.6654682067104974	0.5195048574622223	0.4976736129554208
0.5791528178515395	0.5021317300578979	0.6466177975799771
0.5649030957431493	0.5910146100538525	0.3764685769810691
0.6507379136105574	0.5359483821263133	0.5612174815097395
0.4052973124229913	0.6129588685145458	0.5776995871768469
0.6453042520849581	0.5699056744503288	0.4579928870630165
0.4019272004183420	0.6339756844929920	0.5137338466371122
0.4708583276991127	0.6434256008535576	0.4204560928132210
0.4829976612508877	0.5674776225991792	0.6514012635466704
0.5500238864412680	0.5623753281992395	0.6461906672346395
0.5378542153331536	0.6383561814906775	0.4152607926566941
0.4627846394199426	0.6180086644528088	0.6116238953240979
0.4560868643444835	0.6599235748969841	0.4841483408487584
0.6214830668897600	0.5964483274766755	0.5607933069923067
0.6181334414408345	0.6174783399154004	0.4969841481439245
0.5712655741108065	0.6097194109656497	0.6031193477178174
0.5645554929201209	0.6516503830114302	0.4757502290526663
0.5173391365991973	0.6441244744764936	0.5817681352589402
0.4621800712490482	0.7045702598510261	0.5336172006048721
0.4795583110638086	0.3781822029147460	0.3557752131518509

0.4895250891277595	0.3158633225683311	0.5451622367261238
0.3297897819250406	0.4176482914256275	0.4818866968751184
0.6510525842500455	0.3932691355524497	0.4568984363745839
0.3926361528039162	0.5579319720458275	0.3544667757933052
0.4088375527859527	0.4571334698037974	0.6609834627123863
0.6073712226225997	0.4420630097761045	0.6455259421464429
0.5911676337547860	0.5428854193094375	0.3390285573433201
0.3489546763230195	0.6067428226530753	0.5430973874390618
0.6716610443218090	0.5830749384570459	0.5182671364105196
0.5204654781006832	0.6218133757075514	0.6442213694663949
0.5104715720394670	0.6841301927169039	0.4548327823021661
0.4271678612710986	0.3038498773344080	0.4749765120707365
0.4238099620822698	0.3249394798829863	0.4107289643471682
0.5378124406744147	0.2954344368892248	0.4663665660582261
0.5344344304722777	0.3165653119207026	0.4021154297439421
0.3396755838716761	0.4217528821580641	0.3877970725519627
0.3486704156265854	0.3655362221237421	0.5585889678225952
0.5925630964129550	0.3216486121589585	0.4363807989773688
0.3904635554021652	0.4083527530572879	0.3450400233714273
0.4028197018381758	0.3310003957195162	0.5800779938854302
0.3730290575329064	0.3383722133642195	0.4534850973006427
0.5818079412080716	0.3174449273278009	0.5661765123806517
0.5694951777923354	0.3947878107868564	0.3310844896679616
0.3610165152069298	0.4693019957241960	0.3445804342899129
0.3754947714244082	0.3789217249333405	0.6193170610796226
0.6365870380548696	0.3436503100036962	0.5362419713544893
0.4804804606965536	0.4515020874450376	0.2958496304650537
0.4984231740186045	0.3394183810322687	0.6364702241667959
0.6276130217679297	0.3998967523351679	0.3654269806248851
0.2947374196519624	0.5004266107643487	0.4523703536378904
0.3002756496218517	0.4656947416669843	0.5578750712624440
0.6218031746355380	0.3602242775965528	0.6001801653112391
0.6073100199730875	0.4506186430914751	0.3254331240868623
0.4710549314221273	0.3873166709923097	0.6757127910982504
0.4510682523355031	0.5124125911696202	0.2954180919420404
0.5383279458946806	0.3821791543658258	0.6704989410485179
0.5183343934442377	0.5073001431035504	0.2901712131503473
0.3159669718251795	0.5479820674624090	0.4091474698679282
0.3270550433854683	0.4790796933356357	0.6186090916456030
0.3011564830397124	0.5645611457027975	0.4730962827029757
0.3067073514374015	0.5298123879115394	0.5786743987714721
0.6988332666504008	0.4354645569562059	0.5269089715614174
0.6932849514619898	0.4702368940505308	0.4213442354356447
0.6840319256546437	0.4520273216197367	0.5908251696985701
0.6729466515048718	0.5209450012242947	0.3814309509958364
0.4816884161648003	0.4927172005740897	0.7098354906238465
0.4616868208938290	0.6178273149426233	0.3294999024489615
0.5489373374902670	0.4875728610072335	0.7046029485052501
0.3781921826194991	0.6397478171766935	0.3998206596965370
0.5289384271723006	0.6126917747595861	0.3242717088585579
0.3927005415988740	0.5493957590219984	0.6745501728080010
0.7053284608448158	0.4996020691911847	0.5476394387982315
0.6997836268622099	0.5343542799631550	0.4421400512808006
0.3724054274724568	0.6001023672612250	0.6345569371816115
0.3634130621507433	0.6563222274762145	0.4637402306565072
0.5195208184413569	0.5485039849720966	0.7041711258018252
0.5015579183959066	0.6605954199310130	0.3635169623614564
0.6389934908408954	0.5307039276171945	0.6553983226509585

0.6244997515682542	0.6210935125885657	0.3807207924840010
0.4181991813068567	0.6825538113885484	0.4338134134749286
0.4305395232484651	0.6052339721009037	0.6689103181700422
0.6604027918304956	0.5782742771145654	0.6122176521751170
0.4074657655389197	0.6783577185194186	0.5636036304214104
0.6513844684681090	0.6345110750092312	0.4414259758897847
0.6095647954102935	0.5916248414559022	0.6549440791901199
0.5971851161571238	0.6689810042597221	0.4199358429754704
0.4655738740735845	0.6834385563485085	0.5978823428157182
0.5139909982833949	0.6650191244738625	0.5183082159316207
0.6270275401550873	0.6616591810625079	0.5465300869618511
0.5762196122556129	0.6750365042987848	0.5892484038461405
0.5728487045031813	0.6961182216460435	0.5250300339443794
0.4790828482901523	0.2931044573417617	0.4330284885167466
0.3710955714650804	0.3619699212621430	0.3902450825052832
0.3777858318322325	0.3197945080100285	0.5183131445764525
0.5950131101732500	0.3033295848753869	0.5013893532077534
0.5883204347354415	0.3454797005885772	0.3732592613825115
0.3123624726190156	0.4834745554894716	0.3893777400694615
0.3232737279873939	0.4152681885610166	0.5965582090486051
0.4136285494742657	0.4568303080713049	0.3040445432848313
0.4312837810141173	0.3465222761158499	0.6393754833990003
0.5478130126787709	0.4466538988577353	0.2936235804476588
0.5655189302595345	0.3363325879331221	0.6289228486360260
0.2827540017245647	0.5164651250282417	0.5169155735764452
0.6747702153936508	0.3886628280220428	0.5692688183506710
0.6638135142676185	0.4568788496621811	0.3620502549017842
0.5108789921023960	0.4318482576936349	0.7072614738293823
0.4891133402087963	0.5681497421173580	0.2927397661736379
0.3252247690301948	0.6113470093199248	0.4307163498141708
0.3361955237949888	0.5431563413552025	0.6379701123105014
0.7171553705563504	0.4835894025173064	0.4831109573043412
0.4344620313604290	0.6636561760041779	0.3710662305985324
0.4521867890159340	0.5533543955379591	0.7063771955253070
0.6875668606611637	0.5165407350833140	0.6105442245469580
0.6766553446944771	0.5847223113678847	0.4035296484319573
0.5863923108836129	0.5431635246663642	0.6959430543675753
0.5687187867960188	0.6534800817450764	0.3606425787326453
0.4116910011060966	0.6545216906189417	0.6267239810082224
0.4049743161258200	0.6966575467108330	0.4985942099591064
0.6288873927554930	0.6379503065620945	0.6096935767614406
0.6221799095383210	0.6801137427333032	0.4817133730036822
0.5209457979381373	0.7068652605677972	0.5669571012666478
0.5407862121764696	0.2776571367619708	0.5310090835126655
0.5307065975802502	0.3406185108090937	0.3395810912500932
0.3210936784353877	0.3754072376543536	0.4326334624480792
0.3244871088222993	0.3541272962968831	0.4970408189944309
0.4214174340298764	0.3489030745189839	0.3481631111235735
0.5103171352037975	0.3915269073243043	0.2995496137390821
0.5258564024587405	0.2943119749105064	0.5951610671558409
0.4428203546654449	0.3966633920840598	0.3048012491206358
0.4314901110384534	0.2859697755318316	0.5394477599444228
0.4583392782003453	0.2994330062472403	0.6003757553316278
0.2915353631550726	0.4365378569606104	0.4322032235324093
0.2970245259827738	0.4021647470236612	0.5364823718048872
0.4757905969606906	0.3142993758209136	0.3696832961465764
0.2766749239337555	0.4531088891501476	0.4963563792060706
0.6489603768738345	0.3295156875728890	0.4717916750468216

0.4824236156618378	0.2725200866737331	0.4965619446048478
0.6456316988971577	0.3507479021332578	0.4073776575451298
0.3846765268260076	0.5170997631501578	0.3038988904493102
0.4043568419830274	0.3940744793568662	0.6779574028140763
0.3336639770562871	0.5304615823332947	0.3468403032360936
0.6890812496559856	0.3724009489054514	0.5059663637279612
0.6836365502583290	0.4067286241329003	0.4016620275402092
0.3499936979069030	0.4286605792195892	0.6564115046289628
0.5851721284852263	0.5018828766619381	0.2883083571223758
0.6048485768296792	0.3788706260317845	0.6623797175681512
0.7104004127972718	0.4201716892970746	0.4626075720092830
0.4443698943933254	0.4370250256674852	0.7121463584054845
0.4226357553100094	0.5730960411431570	0.2982444788517810
0.6598497141718811	0.4051484894933576	0.6323773013001803
0.6434681097470462	0.5070045618845074	0.3227448586669235
0.3401366282024857	0.5948113034790600	0.3676210807959607
0.3565215011287726	0.4930022906283141	0.6772427049407712
0.5773680112161443	0.4268794657160874	0.7017523458493766
0.5556316798840490	0.5629750457771048	0.2878499290632930
0.2895354215428195	0.5798193690250107	0.5373878155804925
0.3951401813139347	0.6211160263804774	0.3376229803172198
0.4148236824762402	0.4981422368909803	0.7116880996029347
0.3109079074151683	0.6275703952671537	0.4940259491058974
0.3163625279582620	0.5932665651389257	0.5983200134159899
0.6662770610502476	0.4694977571793619	0.6531364821717286
0.6499372298702262	0.5713297420745868	0.3436053772772301
0.6153137388001452	0.4828723572363848	0.6961194668608996
0.5956183043715367	0.6059410550999632	0.3220271861347189
0.7233241488767133	0.5469656485070329	0.5036699200594208
0.3543834970069930	0.6492483678910801	0.5926149916240926
0.3510401511770873	0.6704782349009729	0.5281809521784490
0.7084833974677189	0.5635086759663499	0.5677491620912113
0.7029890391210876	0.5978631525807446	0.4635778640180894
0.4741193313251802	0.7056910489963433	0.4048399608608036
0.4896868621519861	0.6084894974447848	0.7004490306783158
0.5571730162010987	0.6033256982759270	0.6952209023166500
0.5416252604725879	0.7005731800569041	0.3996067756125531
0.4693120910821871	0.6593774157970583	0.6604180663260586
0.4591946189111417	0.7223358921527158	0.4689654205450854
0.6789498195120179	0.6245823454449126	0.5673338604469983
0.6755476038321901	0.6458530990933379	0.5029862261644364
0.5785420023117235	0.6510486615951185	0.6518242778537250
0.5684356230182966	0.7139829005864217	0.4605485291906135
0.5242044639554578	0.6856991965256881	0.6303158049533052
0.5175422434418839	0.7274775329990394	0.5034316528551295
0.4860175587657480	0.2551163153453523	0.5601276440294012
0.4727183099477093	0.3379870701043576	0.3081890088338861
0.2736482888127624	0.3904870954828542	0.4759224710014183
0.7008743663816228	0.3580144582546125	0.4426923901654724
0.3572548740483547	0.5770004216958333	0.3064018904166644
0.3786700554086042	0.4429671222291325	0.7140694053435795
0.6427546767111485	0.4229840654004106	0.6935915771980331
0.6213388295378630	0.5570549269404232	0.2859381783550195
0.2991409541670523	0.6419986626564262	0.5573024137747972
0.7290251951238145	0.6108319059270138	0.5243463457860776
0.5273077142542523	0.6620154463925866	0.6918065753770360
0.5139739688715975	0.7448819025270381	0.4398696006525912
0.4965495005121067	0.4394778863241233	0.5148346318120864

0.7725801879623685 0.6319573495276719 0.5290540114689019
0.7996534171991426 0.6450712260123604 0.5320599953402216

CO/Cu_{309} E_{ads} = −0.95 eV
1.00000000000000
38.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 38.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 38.0000000000000000
Cu C O
309 1 1
Direct
0.4931972055109170 0.4598784501702136 0.4525258091843180
0.4999848143042091 0.4999510151013554 0.4999496487163866
0.4440716825766201 0.4729053449486198 0.4939871420359237
0.5495395082862508 0.4647533125341533 0.4857042427627795
0.4647470014363891 0.5190431412335389 0.4521534137242413
0.4701348355423283 0.4860153706885645 0.5528827872646699
0.5325386582518622 0.4189622922578614 0.5638286139395808
0.5298597207807791 0.5139334299600593 0.4469613605671919
0.4135117542483364 0.5551885742144985 0.4656915141994567
0.5559423859283938 0.5269242156864220 0.5057869716370269
0.5071403355549832 0.5401380520929814 0.5473321995386884
0.5036098466708375 0.5605173513603098 0.4851455223129267
0.4896011164255461 0.3974126159082439 0.4668211374765979
0.4361085317037747 0.4315332153890135 0.4455081670206156
0.4394902202163282 0.4106745455886758 0.5089989931550754
0.5471141007646980 0.4024928160840507 0.5006817568151977
0.5436335862423601 0.4232502110922892 0.4371331367102630
0.4571167851364031 0.4786086086104997 0.4028654948216486
0.4660190798053550 0.4240009836477718 0.5690215105487199
0.4070345523972734 0.4918064462157382 0.4451014706066787
0.4125616813520250 0.4581033347857176 0.5478351417247284
0.5235790306720317 0.4734028545581786 0.3976238861968914
0.5354198281447591 0.4810091976499887 0.5477645695052997
0.3924942041185427 0.5082345232788972 0.5083715147331985
0.5866762324484962 0.4448746652973670 0.5342275399863156
0.5810979042899223 0.4784688098244198 0.4315327174329510
0.5055419767072143 0.4662936051687698 0.6026395945954562
0.4945909889275691 0.5337700064340615 0.3972717079151958
0.4504882404765025 0.5351119889289363 0.5142103954771776
0.4189612720917559 0.5214827334074338 0.5683796948790339
0.6075298290800005 0.4915976850625332 0.4914344654022150
0.4676516799942916 0.5810725141986579 0.4361231009632247
0.4765256985444220 0.5265667401075129 0.6021576776776530
0.5931658582914722 0.5083212461487053 0.5547757173783441
0.5874548891564180 0.5417552176818162 0.4519467222749242
0.5430964763060402 0.5214434368719039 0.5970157251809903
0.5341844683854411 0.5759963575624956 0.4309343155875128
0.4565159984722851 0.5766069624637439 0.5627384200934735
0.4530568831287154 0.5974773649968872 0.4992968248087237
0.5645455080812942 0.5685894683127258 0.5543018282047529
0.5607752579879751 0.5892948682908710 0.4909890645015732
0.5106416726616176 0.6025693129462250 0.5331067363857391
0.4930517472299905 0.3780510714812725 0.5299049617663016
0.4863858512064630 0.4192374505708884 0.4044169318790313
0.3873623532755849 0.4454422649512267 0.4879038031888010
0.5998870262426331 0.4290763797958860 0.4712819243611411

0.4288934930553279	0.5383736675848421	0.4036282086120553
0.4397197384237027	0.4716777891100867	0.6065743630091526
0.5712485044221076	0.4616999487147825	0.5963008487771396
0.5602423186110730	0.5281660761664264	0.3932197959653603
0.4000821762200422	0.5707467158626909	0.5285413522106417
0.6126661490099697	0.5543305387275609	0.5117835937007581
0.5139242881477826	0.5807429474667143	0.5954049105416401
0.5071241855472591	0.6219379092067168	0.4700791523289596
0.4314740556649150	0.3677491931584854	0.4600157904209274
0.5408554536059476	0.3594149545165806	0.4516460071604370
0.3985223926104229	0.4501646107503776	0.3951025598638322
0.4075016751992677	0.3946871890079835	0.5639630331565126
0.5844492093278779	0.3812586100378555	0.5502677242144768
0.5754110493427590	0.4366209082448528	0.3813039284376658
0.4874791739796985	0.4928625003520203	0.3465348851298088
0.5019560636076221	0.4030166136841423	0.6196752420559967
0.3541145596095376	0.5280600542119153	0.4589422515066490
0.3596962395353985	0.4937651925733781	0.5632888214659643
0.6460146016796474	0.4720414545659488	0.5409807183637169
0.6403418480607291	0.5060698406250578	0.4364914356169013
0.5126486989785496	0.5072601003146635	0.6533728598992053
0.4981195623478090	0.5970118345700681	0.3802643615981600
0.4156417366110794	0.6187243491617173	0.4497177189772206
0.4246918497542421	0.5633049759200609	0.6185668943779004
0.6016884499607240	0.5499185674434810	0.6048345824534930
0.5926696048036492	0.6052886177012157	0.4360331708030870
0.4593442800609726	0.6405324288962794	0.5483814361829342
0.5687460180664760	0.6322905906767727	0.5399321746283905
0.4859615154966233	0.3349208870484561	0.4816909891333579
0.4826351861906406	0.3557797886637856	0.4182528683839887
0.4354620278121956	0.3482824930318834	0.5242348637892101
0.4287077671061934	0.3901647518245202	0.3967501787598869
0.5439048007274483	0.3400538118407717	0.5159024972794323
0.5371390027707657	0.3818433152171659	0.3882974822193793
0.3785528600011903	0.4034298549455114	0.4389890754324914
0.3819923801528289	0.3823646490904556	0.5029750043380250
0.3492846800282005	0.4641386919537803	0.4385743036694869
0.4499386274728754	0.4376272476450837	0.3537661305276272
0.3548844115293120	0.4301501509184179	0.5421098611532064
0.4621444909030608	0.3616730397655177	0.5846816566545096
0.5980168288261229	0.3659127798340774	0.4862439921779489
0.5945289943191938	0.3867685211077392	0.4222029044154728
0.5169316061617629	0.4323931106986638	0.3485092495632342
0.5291692220045404	0.3566380888662765	0.5795307687214152
0.3346531717300136	0.4807008687158402	0.5023273401245887
0.4208095360740870	0.4978458535174005	0.3533543786029051
0.4351985029171541	0.4091059291980532	0.6234957861022936
0.3703021673200204	0.5111678505227890	0.3959429384622764
0.3812848535914626	0.4434239568666591	0.6021403380001875
0.6378920150976959	0.4086331821988495	0.5200624613226891
0.6322999022375746	0.4424370158343466	0.4165063007787568
0.5542307589506977	0.4875329821134252	0.3428259273977280
0.5687174252214061	0.3989560908360256	0.6131284833707114
0.6233079507990829	0.4249871453053156	0.5832844649443799
0.6122067058780012	0.4925978503277549	0.3769912279342684
0.4750205729260089	0.4517233472168349	0.6573860456760939
0.4585289862013416	0.5534714538128950	0.3477584483195842
0.6589132831341967	0.4557248085292721	0.4769068701315530

0.3409963881803820	0.5440537424477507	0.5229219287601062
0.3767572496510848	0.5749804150728141	0.4166310435549144
0.5414947310512330	0.4465667139951793	0.6521942218509968
0.3877423683837289	0.5072805133154739	0.6228279227283429
0.5250205010036360	0.5483318376377349	0.3425039649901231
0.3622202045549455	0.5913797139924186	0.4798916861929708
0.3676684613006482	0.5573887669270383	0.5833630879369577
0.4313621805913930	0.6011048773178022	0.3868678119934068
0.4457350918995515	0.5123836154076433	0.6568986303205078
0.6297883634733763	0.4888835424135870	0.6039789757252203
0.6186157755420278	0.5563986891117744	0.3976320850924090
0.6654100850328485	0.5191768128428920	0.4973699136716240
0.5792491451548986	0.5021354604453794	0.6465900236006628
0.5649251414839476	0.5909000380001795	0.3764545636914826
0.6508317669163209	0.5360042918305064	0.5612983200903294
0.4055013699163904	0.6129759583444477	0.5776659703464754
0.6452098581920487	0.5696284804111484	0.4576465866739071
0.4020763930676579	0.6339950350488426	0.5137614693560909
0.4709157413059733	0.6433821593695142	0.4204901683914756
0.4832485543220288	0.5675701688783137	0.6512533199447066
0.5502955386949541	0.5624829043338324	0.6461026911678128
0.5379143768882679	0.6382822219313585	0.4152200822454485
0.4630760889239724	0.6180175488562786	0.6115407490238052
0.4561411758162323	0.6599063793533189	0.4841098177884256
0.6227462968208036	0.5970244112996712	0.5608745121096566
0.6182202230115924	0.6175718203981325	0.4970235886819463
0.5716171224673545	0.6098464124898588	0.6030836139583453
0.5646550391161353	0.6516839070323126	0.4757225262862909
0.5176359579182862	0.6441875406618039	0.5817151083339636
0.4623197491521872	0.7045816667301995	0.5336348945377222
0.4794215799462174	0.3780765948690516	0.3557369597718866
0.4894974844039214	0.3158621502928399	0.5451584131960098
0.3299122025182946	0.4176455129761789	0.4817738619271943
0.6508982734903441	0.3930216641106003	0.4567557875077516
0.3926189884226333	0.5579042914701839	0.3544613616621512
0.4089216937965343	0.4572470674662855	0.6609309134782617
0.6074582680181561	0.4421020816959128	0.6454820796827203
0.5910034457806530	0.5426566680057759	0.3388539030892484
0.3490777647327113	0.6067665262156151	0.5431313797973504
0.6699205157093655	0.5822563609399323	0.5181456549175176
0.5207656916123591	0.6218986618015181	0.6441286995253124
0.5105698256388913	0.6841134206401548	0.4547904092398169
0.4270645848841180	0.3037930112324206	0.4749815918542172
0.4236588744180345	0.3249287790640826	0.4106835786331712
0.5377622762420413	0.2953992831962052	0.4663977686494493
0.5342810081188062	0.3164785542992599	0.4021767966174561
0.3396420596193065	0.4217058440763297	0.3877199627276398
0.3487223091966110	0.3655089631947226	0.5585329996488915
0.5924168167169149	0.3214982592697573	0.4364438961744987
0.3903700631955258	0.4082863217861459	0.3450385667999402
0.4028121929463583	0.3310075516096064	0.5800450715806675
0.3729864004479682	0.3383401155660224	0.4533853891235622
0.5817873071806074	0.3174567027473106	0.5661965931974525
0.5692197987926741	0.3945694745455363	0.3310323036837178
0.3609259204702228	0.4692933854750241	0.3445378246759334
0.3755750671190107	0.3790171655145467	0.6192810235078834
0.6365367123576264	0.3435976117839448	0.5362282331347294
0.4803668668151629	0.4514577298532200	0.2958652566280188

0.4984163800057850	0.3394984737998451	0.6364231757115899
0.6274710935531529	0.3996703063817422	0.3653648095171942
0.2947491119731646	0.5004412837104866	0.4523120577070761
0.3004197763925139	0.4657498909174677	0.5578605770694143
0.6217734122811452	0.3602577224462896	0.6001409026442627
0.6071517660397477	0.4504508056604285	0.3253188869882430
0.4711223696621714	0.3874431188797227	0.6756546537965671
0.4510543991444108	0.5123930138953295	0.2954153478472306
0.5383473316095827	0.3822309342548181	0.6704416332075716
0.5182074041734759	0.5072374285841886	0.2901353282246567
0.3159523691665718	0.5479622175102474	0.4091305805952564
0.3271200919553979	0.4791673935473783	0.6185979873710958
0.3012442986170361	0.5645863954732944	0.4731458656393348
0.3067923171519801	0.5298511701486932	0.5787115161886383
0.6988198464885883	0.4352351392756202	0.5267407546454227
0.6931547583957707	0.4700960236828836	0.4212249612340992
0.6840821363010063	0.4518939706394248	0.5907922090988543
0.6728354994428734	0.5207463021540977	0.3813515677513488
0.4818028342366275	0.4928642196728921	0.7097353739198160
0.4616554466369180	0.6177982743110080	0.3295247358465581
0.5490021142280235	0.4876747672665734	0.7045501761929466
0.3782143113350298	0.6396914912368685	0.3998754450725527
0.5288684865753699	0.6126133059313527	0.3242422131935243
0.3928235952422038	0.5494933395516812	0.6744312420628783
0.7053265080158612	0.4991405439435943	0.5473862923383137
0.6996628548495151	0.5342259217870462	0.4420710440692974
0.3725764029948598	0.6001031968862327	0.6345276724217567
0.3635234716421388	0.6563145697937376	0.4638085449774465
0.5197437295734313	0.5486329478932916	0.7040185830277226
0.5015291843889406	0.6605124016863209	0.3635273815357727
0.6391271765534262	0.5307285820963829	0.6554011100018108
0.6244299573438093	0.6209305123526876	0.3804677070094700
0.4182383524428301	0.6825114885742262	0.4338255246701972
0.4307426752877629	0.6053336238179310	0.6688658103041558
0.6606209237208788	0.5781693626093043	0.6121449371870747
0.4076971266985808	0.6783586367824275	0.5636104936432327
0.6512488414563374	0.6343032203924364	0.4408842038566424
0.6098532539403456	0.5917552586216125	0.6550059620865789
0.5971616204365988	0.6689468762663047	0.4197438506181811
0.4658977736810851	0.6834462023243739	0.5978162200117463
0.5140882114538828	0.6650604762137926	0.5182430373758131
0.6271712660891977	0.6617443364324072	0.5462799010203749
0.5765082169993822	0.6752101716443868	0.5892413819758676
0.5729799670387229	0.6961925222547382	0.5249536795435892
0.4790000477937940	0.2930737262931806	0.4330572852323705
0.3709286333624329	0.3618680932728972	0.3901284836220983
0.3777679589383136	0.3197070690045438	0.5182862284783433
0.5949392248876630	0.3032620076777751	0.5014676408022385
0.5882084120734348	0.3452867908752679	0.3731541758501286
0.3122937504583169	0.4834857277276993	0.3892628377045724
0.3234207529015932	0.4153691252377513	0.5965092051305469
0.4135888766885817	0.4568205396382738	0.3040384042140115
0.4313362875832062	0.3466416837711108	0.6393068681188401
0.5477464853381475	0.4464538473446916	0.2934993290385668
0.5655096118213107	0.3363938452337170	0.6289159927725545
0.2829065039995678	0.5165069731900455	0.5169458687406271
0.6747743025530757	0.3886455989421823	0.5691809207999210
0.6635712357654669	0.4565959159438277	0.3618885419972061

0.5109706567878320	0.4319469220353084	0.7072127537599698
0.4890290611154662	0.5681386990075209	0.2927419316481701
0.3253189796000738	0.6113083543732791	0.4307725837456761
0.3362268840589993	0.5432215672518045	0.6379926009308267
0.7170567656516793	0.4835626155263588	0.4830050982143478
0.4344589348830706	0.6636175600524545	0.3711074375391518
0.4523231079211008	0.5534799539762895	0.7062111499244627
0.6877517609976139	0.5162118082543269	0.6106583172111024
0.6766061596848608	0.5845467333322437	0.4035161424233563
0.5865394418403596	0.5432075251112491	0.6958966557850330
0.5687011873518639	0.6533614217065737	0.3605430355908603
0.4119355717125963	0.6544870585106882	0.6266864767473943
0.4051110165787161	0.6966875098145723	0.4986110015964507
0.6290505054948519	0.6382501020354892	0.6099641208663485
0.6221422743349967	0.6803089214223955	0.4813456738903286
0.5211360102983548	0.7069319266518556	0.5668803628304332
0.5407158917929593	0.2776318507520853	0.5310185856726530
0.5305014335271487	0.3404330466770214	0.3395420928794455
0.3210885821930213	0.3753376387651067	0.4324908203376679
0.3245833657417157	0.3541272671395468	0.4969242288582071
0.4212863672327960	0.3487723310936306	0.3480339988686831
0.5101425374594234	0.3913591440019816	0.2994794946449322
0.5258294732358489	0.2943713905834769	0.5951629618973514
0.4427119081794971	0.3965866991162171	0.3048226073765708
0.4314541312940323	0.2859456760091398	0.5394441456467866
0.4583197932865961	0.2994690241824897	0.6003643634063033
0.2916236380565828	0.4365279346169736	0.4321139862134237
0.2972803037842626	0.4022013378762040	0.5363782268684723
0.4756208619729861	0.3142553956269094	0.3696863686454359
0.2769066292785821	0.4531561104331875	0.4962715520519274
0.6489445015855962	0.3293910841398683	0.4718079470561517
0.4823612236507854	0.2724972153606073	0.4965602341613121
0.6454752795391269	0.3504943094538685	0.4073061763377396
0.3846622629615808	0.5170720903041697	0.3038657047213223
0.4044455679585362	0.3942056420984068	0.6779099822172749
0.3336307452445497	0.5304445785644231	0.3467931848429374
0.6890349554651406	0.3722631040530867	0.5058862028302445
0.6835231916139594	0.4065962212418524	0.4016066057793228
0.3500921506832192	0.4287647515327857	0.6563859282726814
0.5850312730968031	0.5017035389985476	0.2881491177719543
0.6048646138854791	0.3788972150693715	0.6623178294230705
0.7103073303831640	0.4200646544155145	0.4624645945732750
0.4444529602926746	0.4371631313331095	0.7120786949093204
0.4225909341163772	0.5730569132768232	0.2982407101519386
0.6598634050959362	0.4051200994964423	0.6323303717607643
0.6433797299299298	0.5068594586604102	0.3226969779202364
0.3401289541734250	0.5947739268242775	0.3676402994677778
0.3565845437035117	0.4931236137185656	0.6772202900985909
0.5773944641256666	0.4269331833222458	0.7017022666957003
0.5555872938209896	0.5629367526163356	0.2877755801091072
0.2896426404157726	0.5798695562212398	0.5374418091279346
0.3951257802241865	0.6210835855144829	0.3376819202530913
0.4149293852479478	0.4982977723324531	0.7115766003593752
0.3110388550117047	0.6275929880168185	0.4940929791921213
0.3164723702907919	0.5933157490055655	0.5983787701379869
0.6663776207027704	0.4693979579559698	0.6531569384917979
0.6498634423750766	0.5711251921539474	0.3435256538684937
0.6154069469581961	0.4828805800168305	0.6960473667562799

0.5955414019219289 0.6058130980364342 0.3218999564871253
0.7231518375942839 0.5473534185750173 0.5036472196182079
0.3545969991103642 0.6492562660177886 0.5926440728330132
0.3511922707753573 0.6704921523178634 0.5282472312371141
0.7085836665469417 0.5621376836971252 0.5676011019985922
0.7030182323053683 0.5976736806934684 0.4639840136199358
0.4741397332915636 0.7056217148384146 0.4048151897305517
0.4898608552317826 0.6085797154178534 0.7002864482377308
0.5573584134318327 0.6034254832658781 0.6951233343803217
0.5416176894529567 0.7005034552183854 0.3995124019183752
0.4695516100998002 0.6593677449177870 0.6603278644534317
0.4592739789002798 0.7223082818985510 0.4689581628795966
0.6801248687127203 0.6266068309310612 0.5691490563061888
0.6750777600139415 0.6459347139912142 0.5015459113351401
0.5788882951994659 0.6512373949171394 0.6518662466033536
0.5684712621346359 0.7140285111258746 0.4603635548804360
0.5244604397327767 0.6857310071280950 0.6302573405068015
0.5176734951971188 0.7274697057754799 0.5033246636915528
0.4860051717560171 0.2551368873274292 0.5601670800291926
0.4724432854770433 0.3378269541735955 0.3081623972563550
0.2737418565005323 0.3905263770449865 0.4758854100207202
0.7007265655992423 0.3578577612326302 0.4425899911213428
0.3572575928431436 0.5770137897994331 0.3064115186492080
0.3787730535312800 0.4431038431051248 0.7140287254187486
0.6427779378373297 0.4229387514592046 0.6935682135176701
0.6212052622342341 0.5568507249492611 0.2858510140589135
0.2992897078445587 0.6420424779229478 0.5573670366147776
0.7259636228720152 0.6101497159509861 0.5249997008526244
0.5275802228548795 0.6621200946954318 0.6917320913145638
0.5139861620998346 0.7448618763086260 0.4397408693855050
0.4965832809794737 0.4394745829460408 0.5148154581545664
0.7247030506681521 0.6473593558340974 0.5715643499478126
0.7500897523358681 0.6633227732395659 0.5777933749387442

CO/Cu_{309} E_{ads} = −0.93 eV
1.00000000000000
38.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 38.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 38.0000000000000000
Cu C O
309 1 1
Direct
0.4932698387388055 0.4598954134901110 0.4525525649055268
0.4999926323176817 0.4999494168586688 0.4999892235178777
0.4441092898960514 0.4728642830959293 0.4940177129353228
0.5495623247116240 0.4647059763311123 0.4857656267284265
0.4648263024250125 0.5190855551120653 0.4522222966050402
0.4701374663230383 0.4859832201184621 0.5528803003914073
0.5324363050365505 0.4188466007142061 0.5639168757547580
0.5299372477002969 0.5139823889588457 0.4470418928414560
0.4135834014719234 0.5552324270314348 0.4656748065456364
0.5559713482327073 0.5268686787087290 0.5058763305272918
0.5070811339655166 0.5401437190186194 0.5473260189156565
0.5038061423382469 0.5605702897254253 0.4852584019485606
0.4896212748213555 0.3974094886930385 0.4667832197170124
0.4361766533252651 0.4315066894925655 0.4455044348570187
0.4395005227865219 0.4105713756269623 0.5090657256102823

0.5470205168065747	0.4023691149265982	0.5006618404844203
0.5436752671286991	0.4232461205821212	0.4371525051452627
0.4572728898380176	0.4786557816588806	0.4028591583055238
0.4660355138074962	0.4239655841332604	0.5691244463807451
0.4071694911089211	0.4917890755500529	0.4451118506667016
0.4125912684451990	0.4579810942188103	0.5478538058229724
0.5236785129093996	0.4734932516827976	0.3976753124971975
0.5352589067891639	0.4808531540852747	0.5478051106269419
0.3925611996957085	0.5082194742609950	0.5083745063864527
0.5865977839754358	0.4447083930802960	0.5342383842268460
0.5811837597171331	0.4784575571319135	0.4316154761360951
0.5055430509908146	0.4662930947493628	0.6026929007184942
0.4947273870314618	0.5338197057376548	0.3973277543143429
0.4505200920712601	0.5351339314117809	0.5141805543527193
0.4189904200248090	0.5214390333185249	0.5683946468469047
0.6075675325626738	0.4914502786669265	0.4915024195315791
0.4678148140259762	0.5810732739024044	0.4362069778344576
0.4765676309635582	0.5265201594470462	0.6021375651288466
0.5929716269880713	0.5080374658428405	0.5548013341806970
0.5875353184382597	0.5418174894538228	0.4520555609032070
0.5431313510644558	0.5214575241923293	0.5970062681676938
0.5343561118884418	0.5760490085788673	0.4309956888887086
0.4565655723070483	0.5766323176775731	0.5627255334047102
0.4532088064711418	0.5974781701423953	0.4993377877783763
0.5644323683055117	0.5686023295261863	0.5542686791772439
0.5610987311467800	0.5894084240054894	0.4910761085441092
0.5107759802011749	0.6026392753615416	0.5332032513395298
0.4929908715381496	0.3780043221778722	0.5299434382129425
0.4863936212521230	0.4192879324319834	0.4044168657130862
0.3874374606905271	0.4453693332019061	0.4879496234789689
0.5998235289626999	0.4288865713762698	0.4713229789813325
0.4289867772331726	0.5383746187364918	0.4036579972502616
0.4396804294996861	0.4716414823734904	0.6065715891821247
0.5711657743828175	0.4615607315868338	0.5963021524855292
0.5604543671442392	0.5282653241785489	0.3933863883589634
0.4001279492773915	0.5707346036421141	0.5285544400159891
0.6126538084106707	0.5541444104951442	0.5118442661438609
0.5139452385967684	0.5807751272257543	0.5954187429600284
0.5073311487314576	0.6219683082797689	0.4701807743115960
0.4315162658869813	0.3676792791348424	0.4600491414512693
0.5408295975534733	0.3593824220806714	0.4515754195747186
0.3986278899801976	0.4501596726865476	0.3951205960378663
0.4075134057364320	0.3945951755560633	0.5639683256555733
0.5843438464777811	0.3811264085169669	0.5502715937044715
0.5754540232240857	0.4366598819851747	0.3813375012242617
0.4875449385126870	0.4928974221237371	0.3465246332673589
0.5019217335444086	0.4030401069954495	0.6198004286955346
0.3542331148615719	0.5280452145256878	0.4589642222635865
0.3597404963922706	0.4937084723155702	0.5632658235531011
0.6459449571492929	0.4716772964619690	0.5410119418884797
0.6404244897859966	0.5060118399973220	0.4365360632874064
0.5126828927230880	0.5072767015938149	0.6533413031785014
0.4982967496040239	0.5970237295215427	0.3803786968527124
0.4158025965906774	0.6187297321904908	0.4497680316482646
0.4247004356234436	0.5632233814917028	0.6185308306220554
0.6018856570471232	0.5500087805069940	0.6046400896787021
0.5929767857659699	0.6053945373702794	0.4361947209918783
0.4593553188632531	0.6405294262532143	0.5483888806839043

0.5688783568809506	0.6324892276416668	0.5399471801133594
0.4859621120991811	0.3349337388372208	0.4816883255165640
0.4826258391631810	0.3558259489664086	0.4182121780227073
0.4354148589814371	0.3481567702930070	0.5242299885447897
0.4287144344998622	0.3901136792516664	0.3967706466906736
0.5438070816582786	0.3399486783921367	0.5159336061642729
0.5371203956128706	0.3819053493782250	0.3882524014604206
0.3786466453242192	0.4033961371323744	0.4390166260417715
0.3820002347106049	0.3822892877654138	0.5030277090734071
0.3494099969576988	0.4641135826378440	0.4386450619980635
0.4499207006578433	0.4375859835241605	0.3538025515879842
0.3548631660213010	0.4300562919931813	0.5421185160812410
0.4620519075275628	0.3616307045897501	0.5847321479741927
0.5978373890148262	0.3656516289192844	0.4861864951496288
0.5944670660013267	0.3866623241457691	0.4221738628476279
0.5169598867252542	0.4325261938782612	0.3485379227592712
0.5290796334061942	0.3565793812523864	0.5796142763571966
0.3347093369461565	0.4806790146535209	0.5023735276275225
0.4208964108991169	0.4978966396458805	0.3534036926177678
0.4351162113014307	0.4090589491974753	0.6235313573262462
0.3704067281556316	0.5111623814886831	0.3959963375343694
0.3812588773877686	0.4433371908595238	0.6021079107915260
0.6377539158055578	0.4082937178686086	0.5200348389099863
0.6323034338090492	0.4423124446210988	0.4165517074441739
0.5543789298296614	0.4876788538907693	0.3429497387649912
0.5686094317247341	0.3988621363327761	0.6132138760154895
0.6232268737596939	0.4247770100191982	0.5833170345689291
0.6123210090839339	0.4925766523130273	0.3770614545645718
0.4749576694121021	0.4516800212465805	0.6573843460268386
0.4586332699198364	0.5534517449298433	0.3478091729298579
0.6588928870049705	0.4553876272241497	0.4769285395943595
0.3410379399492496	0.5440513086531098	0.5228992286355334
0.3768195664978001	0.5750215120735235	0.4166709958255283
0.5415384363938045	0.4466877655404655	0.6522120426027920
0.3877027360372300	0.5072109192022395	0.6228047006035757
0.5252060226205432	0.5484521680342008	0.3426543195218190
0.3622427161907065	0.5913684548522385	0.4798573481705115
0.3676869996906794	0.5573266149004172	0.5833283330293598
0.4314954217979388	0.6010937632972437	0.3869555142857707
0.4457126155181149	0.5123711443614222	0.6568514861419884
0.6296570791186421	0.4886317970789438	0.6040255427185738
0.6187703944465288	0.5564602235181573	0.3976960583313101
0.6655452659964807	0.5186201515960962	0.4973497104921785
0.5793652289097480	0.5022631174839619	0.6464253390507353
0.5651320360089634	0.5909577195268311	0.3766400282167108
0.6506837339125886	0.5354789879274542	0.5612830993473802
0.4055011624451613	0.6129494031834339	0.5776417487875054
0.6452061786255076	0.5695593323348059	0.4576032681695761
0.4021232314572233	0.6339455584837537	0.5137580893920092
0.4711202600744673	0.6433685021254800	0.4206072615953826
0.4832837977841062	0.5675508149500178	0.6512203785661915
0.5503593815521549	0.5625252066586390	0.6460081290763870
0.5381739053775089	0.6383462746412808	0.4154192219228146
0.4629914546720086	0.6179646618958359	0.6115858460014122
0.4562795008715672	0.6598764616958788	0.4841264552375162
0.6224167941854220	0.5969607202879273	0.5605288047196709
0.6190912980479699	0.6177783963918542	0.4973172568772270
0.5715941946499592	0.6098940172817416	0.6029976188265690

0.5648861285160613	0.6517215991647399	0.4758639717692221
0.5175196371779842	0.6442643307904324	0.5817728831391773
0.4622839749490243	0.7045550708258063	0.5336283964174959
0.4794081018748906	0.3781353440140826	0.3557171264781632
0.4893758695392164	0.3158089334443100	0.5452153652174216
0.3299548216869011	0.4176231341491579	0.4818476029116366
0.6507818238043312	0.3927440740170465	0.4567469105795322
0.3927095240677940	0.5579588899142156	0.3545350931158229
0.4088899997481297	0.4572312259610408	0.6609323324372062
0.6073995841319343	0.4419597125212167	0.6455109903847587
0.5911861322513718	0.5427089820745747	0.3389431035528735
0.3490814063692091	0.6067163215829121	0.5430911688015314
0.6699007188547962	0.5811513197854505	0.5176943953966792
0.5207187746986548	0.6219157971929345	0.6441282204531130
0.5107086884537353	0.6841507680275627	0.4549024627911616
0.4269800278963108	0.3037662046238824	0.4749870131518771
0.4236154267594009	0.3248933494900993	0.4106556047961917
0.5375907815989986	0.2953594461419579	0.4663731841426078
0.5342106830474747	0.3164748121169840	0.4021047772879949
0.3397263421464410	0.4217242494233449	0.3877500190709282
0.3487231360316689	0.3654618182757745	0.5585507646743487
0.5922921210358993	0.3213330538592545	0.4363329572628425
0.3903908495124548	0.4082762252873844	0.3449292206566283
0.4027497181218537	0.3308817673737796	0.5800852941178779
0.3730480123832486	0.3383711260552659	0.4534451467149316
0.5816161652338564	0.3173676512781386	0.5662333345957233
0.5692855621378808	0.3946785508968707	0.3310196530110466
0.3610570569063139	0.4693020172878020	0.3445676797269037
0.3755176785224255	0.3789174918168301	0.6192989094284294
0.6364042184660921	0.3434145546510829	0.5362052224950589
0.4803167939388033	0.4515514498589626	0.2958454588449064
0.4982280497267377	0.3395012988875942	0.6365277010246913
0.6274051376385120	0.3996033322370699	0.3653425399861718
0.2948782136030860	0.5004469825270590	0.4523693542402891
0.3004371450142000	0.4656916217841762	0.5578459763890339
0.6216850751389547	0.3601494310752723	0.6002077603972061
0.6071775107374336	0.4504831679005806	0.3253562271029670
0.4710965854269291	0.3873516844344703	0.6757135265222231
0.4511341456964907	0.5124032966243987	0.2954021373914594
0.5382319357224522	0.3822639025276159	0.6705249418350990
0.5182615893056247	0.5073149716618494	0.2901787134807818
0.3160295311944650	0.5479892165125929	0.4091591696544922
0.3271189833088811	0.4790857052816280	0.6185743763529699
0.3012923839244068	0.5645861062798756	0.4731285603947038
0.3068473526500398	0.5298308706258884	0.5786371463046237
0.6987207492534375	0.4350705053706752	0.5267636055753955
0.6931610703438826	0.4697831743713392	0.4212267572768478
0.6839970683660461	0.4517566818559932	0.5908009615652181
0.6728872951716210	0.5206233205456935	0.3812608203141543
0.4817967284270678	0.4928610951916307	0.7096747399748925
0.4618296655626583	0.6177926003072503	0.3296623938723655
0.5491199214561512	0.4877339099525914	0.7044490987028964
0.3783033946359058	0.6396729473590959	0.3999176113435132
0.5291333198331991	0.6126765778395479	0.3244382447529792
0.3927874928239241	0.5494178318129327	0.6744049421180486
0.7052807602407580	0.4992325275693569	0.5474355828168620
0.6997260088876095	0.5338980373599588	0.4420292208243671
0.3725691498215118	0.6000539760102923	0.6344653544596859

0.3635888127054105	0.6562410928882770	0.4637733082531715
0.5197419448699498	0.5486301721914060	0.7039036851513095
0.5018064934648351	0.6604880390520760	0.3637556958975648
0.6393377305805346	0.5309934105861345	0.6550818813675388
0.6248661853748396	0.6210687558430199	0.3809976202511575
0.4183719781043343	0.6825153318025678	0.4338392881913445
0.4307219994744674	0.6052441145649539	0.6688407823220838
0.6608183201047531	0.5789022843204293	0.6115190766185892
0.4076650377237453	0.6783515841236644	0.5635915956334819
0.6518628491428907	0.6345715875526857	0.4421615209921196
0.6099202619740541	0.5917930428705994	0.6547743457350207
0.5975521057086974	0.6689755114024004	0.4200463385717595
0.4656803835770749	0.6834383891733617	0.5978592847572356
0.5141715678521191	0.6651414460709986	0.5183435904092677
0.6265604791684740	0.6625203418685549	0.5467730648422929
0.5762105412883560	0.6753885481424884	0.5893538591763229
0.5728250895850691	0.6964930207217016	0.5250964199927224
0.4788875561184516	0.2931503672519557	0.4330543800182984
0.3709878479782467	0.3618857824477434	0.3900994212367528
0.3777120663465638	0.3196371059898083	0.5183263226997428
0.5948049521372064	0.3030680338270653	0.5014415171744326
0.5880790654738121	0.3452212310808943	0.3731209851488771
0.3124618822553021	0.4834975038772774	0.3893668568063940
0.3233775988460474	0.4152618847582404	0.5965304207702957
0.4136068680517992	0.4568719665506954	0.3040760119776227
0.4312275275465010	0.3466039778800083	0.6393674834418435
0.5477150690578537	0.4465904425195963	0.2935959196656432
0.5653962585348006	0.3363413689904977	0.6289538052050344
0.2828785364403250	0.5164717039076010	0.5169071923848215
0.6746550003585047	0.3883883011493765	0.5691940650873082
0.6636668714887536	0.4565085266053784	0.3619271699703486
0.5108953526920775	0.4320022176989432	0.7072088526367375
0.4891465977454397	0.5681834181575165	0.2928375792650577
0.3252409862199003	0.6113407673153732	0.4307096449283014
0.3361902598191186	0.5431421518810277	0.6379645800573013
0.7171383391623993	0.4832393223877627	0.4829909853431715
0.4346443470932442	0.6635703851269261	0.3712320133513534
0.4523368028941797	0.5534452433192238	0.7061640190695946
0.6875996058993952	0.5163188447089100	0.6104557674967600
0.6766698975536131	0.5844348861943760	0.4033957530760145
0.5866328732184777	0.5433265449452913	0.6956980849086009
0.5689886183599350	0.6534193317836906	0.3608515269211214
0.4118442447641629	0.6544504889187773	0.6266811518365508
0.4051160834696499	0.6965858840334640	0.4985738409264690
0.6290248669394644	0.6382891005684810	0.6097794814929575
0.6223179790374238	0.6804097815537605	0.4817170100897269
0.5209385787516524	0.7070261854298303	0.5669913992487792
0.5405297336925836	0.2775707417338074	0.5310556012099943
0.5304494394883417	0.3405077219100274	0.3395342839085116
0.3211366442115123	0.3753497833746732	0.4325389530615553
0.3245393351548110	0.3540309079940177	0.4970033844124912
0.4211986726459955	0.3487230630229959	0.3480111789242747
0.5101193380830159	0.3914973007631207	0.2994937680432376
0.5256592884490080	0.2943015178385844	0.5952370838716758
0.4426800249879613	0.3965971354082141	0.3047949375220294
0.4313110714752360	0.2857394961163754	0.5394651970914397
0.4581765331650575	0.2993941000797994	0.6003641339686080
0.2917332111119790	0.4364763052756225	0.4321642567886870

0.2972393991932870	0.4020770619252533	0.5364041857729296
0.4755455702771765	0.3143040736348698	0.3696803993638499
0.2769541104841398	0.4531401658175253	0.4963344083253676
0.6487508005803490	0.3291050939828932	0.4716972299928081
0.4821844763502355	0.2725257815900472	0.4966011543825286
0.6453962770214117	0.3502886484298008	0.4072652317842733
0.3847254263671294	0.5171296592060339	0.3039052645573755
0.4043835272709843	0.3941369870784742	0.6779545636191782
0.3337855618858271	0.5304816320940038	0.3468437562623100
0.6889191031487327	0.3720458089877768	0.5058432991544811
0.6834479598606986	0.4063118681414481	0.4015620287459883
0.3501090934204997	0.4286922170874966	0.6563895468858200
0.5850650094443556	0.5018635215578117	0.2882370932853330
0.6047367624753188	0.3789009039527247	0.6624623762357784
0.7102272464969043	0.4197488016329559	0.4624789239067442
0.4444252016920754	0.4371567881155580	0.7121014702994717
0.4227099197820050	0.5731401520244770	0.2983125461214228
0.6598010392373921	0.4050285743565065	0.6324116163671845
0.6434110248170870	0.5068279193336964	0.3226282604436614
0.3401420303572449	0.5948499480942189	0.3676866024853549
0.3564938506088409	0.4930934427139118	0.6772008155177286
0.5773806663825665	0.4270084971855477	0.7016869558892259
0.5556520290745972	0.5629677678098073	0.2879546088550257
0.2896343833165516	0.5798254589311729	0.5373916719520232
0.3952578326425215	0.6211141791357691	0.3377717838687308
0.4149035676972043	0.4982838700894401	0.7115366686386566
0.3110438238283218	0.6275812533343721	0.4940371590120368
0.3164921272385353	0.5932649615926052	0.5983138269087153
0.6663476106697311	0.4694714339375250	0.6531772151563925
0.6500018025621598	0.5712412618660432	0.3434988506852265
0.6154715072338123	0.4830333890267557	0.6958563742992655
0.5957865915063560	0.6058460414796143	0.3222554316268966
0.7235300152389591	0.5470177552874443	0.5036302523376253
0.3545673686318427	0.6492079794861340	0.5925965069933711
0.3512108806943743	0.6704402820253176	0.5281835628821456
0.7082146136870630	0.5631217287783765	0.5674014898901160
0.7027310508753661	0.5973077352627876	0.4635686489027918
0.4742794241132955	0.7056305898117141	0.4049265224540921
0.4898432775730590	0.6085514890093392	0.7003055810837457
0.5574152278614459	0.6034608064675916	0.6950474797428915
0.5418864926352028	0.7005451911778716	0.3997464153812095
0.4694848189656156	0.6593648206731546	0.6603607854164394
0.4593619478978183	0.7222938167680779	0.4689706796258449
0.6798995517458448	0.6265868626138946	0.5683644586014782
0.6764748044995900	0.6480352332095618	0.5031608976405108
0.5787707660501746	0.6512627547360920	0.6517929836768561
0.5686358470269393	0.7141101764223954	0.4606128247676484
0.5242318549185688	0.6858117864831389	0.6303676235091364
0.5175437631362845	0.7275949002095290	0.5034102825193333
0.4858077232975576	0.2550473642812348	0.5601977416609748
0.4724925691217718	0.3379303082508119	0.3081311023173691
0.2737827680559878	0.3904965181080728	0.4758883880279212
0.7005435563672037	0.3575889754353186	0.4425766303419597
0.3573540779491993	0.5770609942877136	0.3064653488108520
0.3787562440024054	0.4430949619152659	0.7140345005921154
0.6427683306032990	0.4229691250921279	0.6936065461693405
0.6213432820044656	0.5569610674114295	0.2858832476682679
0.2992892176803618	0.6420052048846159	0.5573148187462598

0.7259300326701629	0.6097862392130271	0.5241336232214056
0.5274934086926012	0.6620793805046190	0.6917900670210559
0.5141343259417210	0.7449100197844076	0.4398372632644288
0.4965358293511776	0.4394088668542312	0.5148278102226423
0.7104786446592387	0.6608501725837234	0.5419030840319945
0.7302373659959056	0.6840123594718110	0.5483473453714079

11.4 *COH Adsorption

COH/Cu_3/Cu(533)	E_{ads} = −3.24 eV				
1.00000000000000					
10.3878408006999994	0.0000000000000000	0.0000000000000000			
4.5828709415000004	6.0103788927000004	0.0000000000000000			
0.0000000000000000	0.0000000000000000	26.5000000000000000			
Cu C O H					
63 1 1 1					
Selective dynamics					
Direct					
0.0032853599999996	0.9972806999999975	0.3042624500000031	F	F	F
0.0028217400000017	0.3308767700000033	0.3042691500000032	F	F	F
0.0026800899999984	0.6645640400000019	0.3042978000000005	F	F	F
0.2572489900000008	0.6186597399999982	0.3218759499999990	F	F	F
0.2571973700000001	0.2857762699999995	0.3217927099999969	F	F	F
0.2571614599999990	0.9524293899999989	0.3219123699999997	F	F	F
0.5099116399999986	0.5747781399999994	0.3415763200000015	F	F	F
0.5095861200000016	0.2417833900000019	0.3416938299999970	F	F	F
0.5096986000000001	0.9088501900000026	0.3416314700000029	F	F	F
0.7627858999999972	0.5310134699999978	0.3609394899999998	F	F	F
0.7629538699999969	0.1970798500000015	0.3608490599999996	F	F	F
0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F
0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0460515907298273	0.2954757436379002	0.4663389280280922	T	T	T
0.0450140792226774	0.6298381944934959	0.4667009358936249	T	T	T
0.0462431325157801	0.9617140782754706	0.4663940258620407	T	T	T
0.3017536826391536	0.2493187357767421	0.4870512233834996	T	T	T
0.3019669549536221	0.5823739515850124	0.4870916901349957	T	T	T
0.3022748384694974	0.9155997430572079	0.4869960881608197	T	T	T
0.5569062494339364	0.2028526069572912	0.5064913648887774	T	T	T
0.5582705968423117	0.5356284368929650	0.5061225813989367	T	T	T
0.5575560001103548	0.8704704902284730	0.5062488819031539	T	T	T
0.8146103109004734	0.1548592486716166	0.5274524287592146	T	T	T
0.8147039192250644	0.4891280491574354	0.5274730568463697	T	T	T
0.8131985125230496	0.8233129004338073	0.5282000592894792	T	T	T
0.0700128842219264	0.1092830887141873	0.5486199933394708	T	T	T
0.0688943126758455	0.4443040362294290	0.5488638405761482	T	T	T

0.0693130279072373 0.7765638242172508 0.5491656461834094 T T T
0.3251920202714873 0.0643685503944034 0.5690343868970024 T T T
0.3227721926026392 0.3987403789673066 0.5696434853962496 T T T
0.3260540464099872 0.7297082726295172 0.5690302961981537 T T T
0.5808928500210453 0.0180851969560681 0.5888724269330369 T T T
0.5819244516432228 0.3477929958078576 0.5872317650483692 T T T
0.5822944191310794 0.6853789358659680 0.5870885289330791 T T T
0.8383970585696584 0.6348163493279827 0.6111450821522232 T T T
0.8390634870072321 0.3022887509038957 0.6098112285091963 T T T
0.8393575877562101 0.9707297444482837 0.6110985123579800 T T T
0.0897797992577200 0.5929187581656096 0.6346121461252584 T T T
0.0942331328796245 0.2578457560355044 0.6318851460092978 T T T
0.0960092823674573 0.9219890978130578 0.6326225399081151 T T T
0.3426509274798978 0.5443237281186279 0.6515756944312867 T T T
0.3460272187834579 0.2140494849299036 0.6526633761714059 T T T
0.3433912354407107 0.8881202780817444 0.6513326882153231 T T T
0.5937076693889892 0.5079870541234198 0.6651888555659239 T T T
0.5995084295819513 0.1678095656148925 0.6716006617154984 T T T
0.5993560938935515 0.8389791466718279 0.6714553608084053 T T T
0.8695830665878079 0.4440545367698565 0.6931732776473379 T T T
0.8728150132326645 0.1081091689668614 0.6934114703771468 T T T
0.8499579431590581 0.7943535586124483 0.6921891740280108 T T T
0.6303509436957703 0.6396157654258434 0.7478188406402249 T T T
0.6338290262903165 0.3168543875969236 0.7473162603894941 T T T
0.3746490121952393 0.6900463495299857 0.7279331782606703 T T T
0.8265342477607551 0.3161725911888887 0.7522647508889534 T T T
0.9347275724765355 0.2316518987675328 0.7915388135223531 T T T
0.8819821463733399 0.2347064816719111 0.8223420690291879 T T T

COH/Cu_3/Cu(533) E_{ads} = −3.23 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
63 1 1 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F
0.2571614599999990 0.9524293899999989 0.3219123699999997 F F F
0.5099116399999986 0.5747781399999994 0.3415763200000015 F F F
0.5095861200000016 0.2417833900000019 0.3416938299999970 F F F
0.5096986000000001 0.9088501900000026 0.3416314700000029 F F F
0.7627858999999972 0.5310134699999978 0.3609394899999998 F F F
0.7629538699999969 0.1970798500000015 0.3608490599999996 F F F
0.7629705100000024 0.8638077299999978 0.3608832600000014 F F F
0.0188077500000006 0.4844866199999984 0.3845455499999986 F F F
0.0188649600000019 0.1508076399999965 0.3844206699999972 F F F
0.0189457299999987 0.8174492599999965 0.3845321800000008 F F F
0.2777182000000025 0.4350678200000004 0.4051130599999979 F F F
0.2779364200000032 0.1018241299999971 0.4049400600000013 F F F
0.2778532499999997 0.7683188099999967 0.4050370400000034 F F F
0.5346647900000008 0.3873898000000011 0.4243529600000002 F F F

0.5347255300000029 0.0542446099999978 0.4245416400000011 F F F
0.5343893300000033 0.7214487199999979 0.4243017399999971 F F F
0.7896143700000025 0.3418778500000030 0.4451831499999983 F F F
0.7893677400000030 0.0085227100000012 0.4452920299999974 F F F
0.7895473399999986 0.6754118300000016 0.4453449800000016 F F F
0.0473018905378026 0.2939453768608757 0.4661538114441868 T T T
0.0459435411978504 0.6289932328614114 0.4663518579663659 T T T
0.0463688086989364 0.9609977813420159 0.4664070094923503 T T T
0.3034465141320268 0.2481044258828362 0.4867066518995955 T T T
0.3029633842554134 0.5802731849520697 0.4874168110966295 T T T
0.3035599919042724 0.9128463653534595 0.4866666280747296 T T T
0.5578953953280390 0.2011609092590874 0.5070056483850109 T T T
0.5595205409661475 0.5332923770911648 0.5064413251611271 T T T
0.5600056989357824 0.8659590039473812 0.5065233275732766 T T T
0.8159865387598302 0.1522228820575720 0.5276927462992518 T T T
0.8169808419037210 0.4849352313153403 0.5271368914782286 T T T
0.8151935819659215 0.8206288923146445 0.5278742066642010 T T T
0.0728138095579922 0.1047316646857013 0.5482524623322007 T T T
0.0716304276662996 0.4426491153859899 0.5481003753043154 T T T
0.0714619291536280 0.7742833779008933 0.5495277056748762 T T T
0.3292771531504286 0.0603860872320467 0.5674802526406708 T T T
0.3261556483507775 0.3958419226305594 0.5706940011206427 T T T
0.3275435420796811 0.7256851529609349 0.5693674130892674 T T T
0.5844384679894858 0.0112739161501310 0.5888702936158552 T T T
0.5842484903585188 0.3454216541571711 0.5881636389289326 T T T
0.5868449406652303 0.6765778297672185 0.5881497130847535 T T T
0.8413225742812500 0.6302598569212492 0.6100144029223529 T T T
0.8450697144626673 0.2947558828866548 0.6096817368232976 T T T
0.8423705707769003 0.9614869898773932 0.6109651897910311 T T T
0.0950638303185727 0.5889079604279743 0.6345131628116576 T T T
0.1025061901639148 0.2506125341524310 0.6290280391597491 T T T
0.0969620080956659 0.9204261115654617 0.6347693378044923 T T T
0.3496719393563694 0.5436002023190909 0.6551884278088451 T T T
0.3485105920234304 0.2125807559407988 0.6520960263969471 T T T
0.3477218735452254 0.8817542509697134 0.6485890357408337 T T T
0.6119268446270496 0.4897752188096192 0.6681452100539644 T T T
0.6048818817016084 0.1545650637582483 0.6702545478976916 T T T
0.5949956357448798 0.8356518527195789 0.6713974544794254 T T T
0.8966241855603627 0.4110984209342163 0.6910711653689177 T T T
0.8607472983506526 0.1096680826193648 0.6919596617718611 T T T
0.8550964507387206 0.7809936239674826 0.6945430010488494 T T T
0.6718870884765451 0.5976849175826970 0.7489775926052715 T T T
0.6143564963273249 0.3217279175127317 0.7459387022185098 T T T
0.3982522257186432 0.7162472788098668 0.7291089853657411 T T T
0.8562624943761605 0.6057277723756229 0.7482201076629877 T T T
0.9426676597705992 0.5557097826060513 0.7907556918571714 T T T
0.0183216789355072 0.5915442752313922 0.7865844054600117 T T T

COH/Cu_3/Cu(533) E_{ads} = −3.22 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
63 1 1 1
Selective dynamics
Direct

0.0032853599999996	0.9972806999999975	0.3042624500000031	F	F	F
0.0028217400000017	0.3308767700000033	0.3042691500000032	F	F	F
0.0026800899999984	0.6645640400000019	0.3042978000000005	F	F	F
0.2572489900000008	0.6186597399999982	0.3218759499999990	F	F	F
0.2571973700000001	0.2857762699999995	0.3217927099999969	F	F	F
0.2571614599999990	0.9524293899999989	0.3219123699999997	F	F	F
0.5099116399999986	0.5747781399999994	0.3415763200000015	F	F	F
0.5095861200000016	0.2417833900000019	0.3416938299999970	F	F	F
0.5096986000000001	0.9088501900000026	0.3416314700000029	F	F	F
0.7627858999999972	0.5310134699999978	0.3609394899999998	F	F	F
0.7629538699999969	0.1970798500000015	0.3608490599999996	F	F	F
0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F
0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0469533666901398	0.2942761326912375	0.4663614565964593	T	T	T
0.0461445988907201	0.6286191553502221	0.4665677479122721	T	T	T
0.0468913969644547	0.9609244981259408	0.4664426689105667	T	T	T
0.3031543866192834	0.2476900890444540	0.4871318521647865	T	T	T
0.3031965957305260	0.5806164482595833	0.4871321656335326	T	T	T
0.3038619522952075	0.9133778721122852	0.4868960576441950	T	T	T
0.5583850044174596	0.2009192252163103	0.5066819025864220	T	T	T
0.5595006486765257	0.5337818034956072	0.5063139467397235	T	T	T
0.5592896710447874	0.8682577941149674	0.5065852945008658	T	T	T
0.8165927008706504	0.1521790053307654	0.5274477576739329	T	T	T
0.8167305221228176	0.4864313304716816	0.5274267148156113	T	T	T
0.8154782377263032	0.8208303595689728	0.5280255211164118	T	T	T
0.0738387452174649	0.1046113508803543	0.5486395416323262	T	T	T
0.0716562580089501	0.4411904199365537	0.5488999651985864	T	T	T
0.0722041360205594	0.7736403225668340	0.5494859529814349	T	T	T
0.3280129929017335	0.0603169290360768	0.5690840683956750	T	T	T
0.3261413266350957	0.3948261013663270	0.5696382885662530	T	T	T
0.3279812325148015	0.7269363303168532	0.5692451958101259	T	T	T
0.5836545930919854	0.0145011962424419	0.5891509565282291	T	T	T
0.5853299385783259	0.3447389038012858	0.5876332302639540	T	T	T
0.5857740407958687	0.6798397519881973	0.5875899158240756	T	T	T
0.8425764154404689	0.6323168877344614	0.6103130312522254	T	T	T
0.8461378167171176	0.2941466947906974	0.6091348164575479	T	T	T
0.8433600365149303	0.9643205311094718	0.6107665613727988	T	T	T
0.0948097254859803	0.5877592104468263	0.6347609689742626	T	T	T
0.0986326995387898	0.2517110675110743	0.6324016082563801	T	T	T
0.1002916571304198	0.9176513054963493	0.6352987846678602	T	T	T
0.3508537541987735	0.5375284582311863	0.6510130547370707	T	T	T
0.3498096048292609	0.2089082997315259	0.6520286769740267	T	T	T
0.3512497100048790	0.8778729076765828	0.6514004756155529	T	T	T
0.6087591247684472	0.4940091252187386	0.6673101876476579	T	T	T
0.6033322522148836	0.1619726544404685	0.6720100073287867	T	T	T
0.6037484298193334	0.8336187957703274	0.6716384214555831	T	T	T
0.8659565256963830	0.4459918672256364	0.6905013048880733	T	T	T

0.8625464517301893	0.1137567301707492	0.6919375885290151	T	T	T
0.8532087453925499	0.7884771296819082	0.6932456426355742	T	T	T
0.6370296337468204	0.6421192157742723	0.7490225677438431	T	T	T
0.6272652359677053	0.3136942539971912	0.7488500752507505	T	T	T
0.3618307752440160	0.6973324900933378	0.7283818050412734	T	T	T
0.5019554426969464	0.5950365435969331	0.7862033545910521	T	T	T
0.4554627915614020	0.6260400213737540	0.8348983069461582	T	T	T
0.5385133976782654	0.6089462148239306	0.8566041450865711	T	T	T

COH/Cu(533) E_{ads} = −3.22 eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H

60 1 1 1

Selective dynamics

Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0476501726852058	0.2934173898988857	0.4661664936455938	T	T	T
0.0474512342141871	0.6272031496776138	0.4660555930559700	T	T	T
0.0470942581131550	0.9607380034800745	0.4662328523746327	T	T	T
0.3037162116351253	0.2467767066381656	0.4866916593490081	T	T	T
0.3034204341662010	0.5805723597316840	0.4866471829001610	T	T	T
0.3032911015125016	0.9134308905551405	0.4866870852288958	T	T	T
0.5587439303286050	0.2009319828482821	0.5066948074083394	T	T	T
0.5586067719901645	0.5343109817030920	0.5068213314906592	T	T	T
0.5590127069880522	0.8671819526661239	0.5067362506782349	T	T	T
0.8158567884284366	0.1533952959491417	0.5276383447312862	T	T	T
0.8157773906244336	0.4854419142805904	0.5269187703464245	T	T	T
0.8158710591899968	0.8210982736187323	0.5269117654746481	T	T	T
0.0721012218904454	0.1075441001678044	0.5491150528666277	T	T	T
0.0720316993231365	0.4402240170496762	0.5486779539192543	T	T	T
0.0723401198983238	0.7720903242425802	0.5489423669578019	T	T	T

0.3264399522500228 0.0606985036892932 0.5688975178185437 T T T
0.3263746959455714 0.3953847781467298 0.5688290417213830 T T T
0.3264102690894760 0.7278306237800704 0.5690080745687716 T T T
0.5845698310210021 0.0135198904314840 0.5883295260952774 T T T
0.5842541724251386 0.3461029783828409 0.5886616291916527 T T T
0.5832212949470299 0.6794771032114910 0.5886855477656461 T T T
0.8367936333877501 0.6354170018441210 0.6064599009887103 T T T
0.8427862241686231 0.2985847273000601 0.6093904830329889 T T T
0.8440554617638347 0.9615137710861554 0.6093073350070732 T T T
0.1021300695943245 0.5806881382501623 0.6353860675123043 T T T
0.1011051836009054 0.2496381366515575 0.6355659425409198 T T T
0.0990113164025534 0.9174100833693902 0.6326447803133959 T T T
0.3547370784217426 0.5393465325298571 0.6516179783079509 T T T
0.3586498642882706 0.2020772185034215 0.6501882702655591 T T T
0.3542162188862286 0.8695362191394567 0.6517979270320590 T T T
0.6062410046472658 0.4944859185339992 0.6720453592353974 T T T
0.6077409117661123 0.1590738106656058 0.6718651011647929 T T T
0.6034543930258524 0.8303372237367631 0.6716804860634750 T T T
0.8563387968083480 0.4533504104414920 0.6902372748980941 T T T
0.8587860184088770 0.1171611310973072 0.6891315387091974 T T T
0.8608649448360294 0.7812577750782148 0.6909908706214548 T T T
0.0467784675969349 0.4586818231388924 0.6951489062215087 T T T
0.1273218000610418 0.3811893506359782 0.7399182242677720 T T T
0.2307130514224584 0.2322560203442960 0.7348774758841833 T T T

COH/Cu_3/Cu(533) E_{ads} = −3.21 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
63 1 1 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F
0.2571614599999990 0.9524293899999989 0.3219123699999997 F F F
0.5099116399999986 0.5747781399999994 0.3415763200000015 F F F
0.5095861200000016 0.2417833900000019 0.3416938299999970 F F F
0.5096986000000001 0.9088501900000026 0.3416314700000029 F F F
0.7627858999999972 0.5310134699999978 0.3609394899999998 F F F
0.7629538699999969 0.1970798500000015 0.3608490599999996 F F F
0.7629705100000024 0.8638077299999978 0.3608832600000014 F F F
0.0188077500000006 0.4844866199999984 0.3845455499999986 F F F
0.0188649600000019 0.1508076399999965 0.3844206699999972 F F F
0.0189457299999987 0.8174492599999965 0.3845321800000008 F F F
0.2777182000000025 0.4350678200000004 0.4051130599999979 F F F
0.2779364200000032 0.1018241299999971 0.4049400600000013 F F F
0.2778532499999997 0.7683188099999967 0.4050370400000034 F F F
0.5346647900000008 0.3873898000000011 0.4243529600000002 F F F
0.5347255300000029 0.0542446099999978 0.4245416400000011 F F F
0.5343893300000033 0.7214487199999979 0.4243017399999971 F F F
0.7896143700000025 0.3418778500000030 0.4451831499999983 F F F
0.7893677400000030 0.0085227100000012 0.4452920299999974 F F F

0.7895473399999986 0.6754118300000016 0.4453449800000016 F F F
0.0468274523145311 0.2941766877398706 0.4663417583805085 T T T
0.0462236273400265 0.6280750575100811 0.4666105964632763 T T T
0.0470730548158258 0.9603924854963211 0.4663653167272841 T T T
0.3033099019177286 0.2469953053006364 0.4873896004500295 T T T
0.3032915040059336 0.5800805963781528 0.4870466546761492 T T T
0.3039306181767003 0.9129587926160312 0.4868653747446317 T T T
0.5585290594685901 0.2002461321056188 0.5066901960459020 T T T
0.5595366019799357 0.5334459086360042 0.5063478441681752 T T T
0.5590668963418537 0.8677637824728137 0.5065763990223715 T T T
0.8165895083672581 0.1518116977911816 0.5272833769592395 T T T
0.8165296037321426 0.4864447230646434 0.5274423131104982 T T T
0.8154012163426501 0.8201977997319716 0.5279474463138456 T T T
0.0736828221327883 0.1043586027816445 0.5484258019068520 T T T
0.0717967862822846 0.4401302238628944 0.5489753060386278 T T T
0.0724097889315516 0.7724953103934169 0.5492570232307159 T T T
0.3279003203365534 0.0586604189675342 0.5695135749008529 T T T
0.3263283002825261 0.3944788322577963 0.5698830105571631 T T T
0.3286079407264708 0.7255482565329103 0.5691684567451603 T T T
0.5832633056221184 0.0130992545580852 0.5888126144422543 T T T
0.5852526283131070 0.3442885297007052 0.5875957215366796 T T T
0.5854930385339117 0.6790249078829191 0.5878272026055669 T T T
0.8427714245924349 0.6315008441207510 0.6104602605269278 T T T
0.8461679469849344 0.2939918706612872 0.6089100879320455 T T T
0.8432307152318756 0.9634462791555762 0.6103542098430808 T T T
0.0945484157594905 0.5869727615756304 0.6348333142916047 T T T
0.0983561676450648 0.2504213226169014 0.6326373835253634 T T T
0.1009493488399897 0.9158249421452354 0.6335328178746522 T T T
0.3503815702354416 0.5378080000485568 0.6519541558047379 T T T
0.3494935897214120 0.2075549192036803 0.6519685829179238 T T T
0.3512964143065744 0.8748278731234009 0.6525008089869075 T T T
0.6115578260247858 0.4887871020410373 0.6676610260465594 T T T
0.6033146436650441 0.1599988620747652 0.6705011224748461 T T T
0.6037934518179142 0.8318077987414654 0.6714068179735975 T T T
0.8650600003085245 0.4474035221562502 0.6910135587642046 T T T
0.8680179272030912 0.1089655145735051 0.6909801650073319 T T T
0.8516273886334744 0.7913524463118407 0.6937207505216705 T T T
0.6347163379774869 0.6411221707549544 0.7491676083610272 T T T
0.6403058496470919 0.2828162025428540 0.7487754576031165 T T T
0.3795332762591954 0.6783413383559562 0.7301264123287083 T T T
0.5290016578382861 0.5482070429236146 0.7881067771402286 T T T
0.4864179671719100 0.5901053550260258 0.8371439940305194 T T T
0.4880907719683520 0.4699399192399909 0.8517772679789886 T T T

COH/Cu_3/Cu(533) E_{ads} = −3.18 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
63 1 1 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F

0.2571973700000001	0.2857762699999995	0.3217927099999969	F	F	F
0.2571614599999990	0.9524293899999989	0.3219123699999997	F	F	F
0.5099116399999986	0.5747781399999994	0.3415763200000015	F	F	F
0.5095861200000016	0.2417833900000019	0.3416938299999970	F	F	F
0.5096986000000001	0.9088501900000026	0.3416314700000029	F	F	F
0.7627858999999972	0.5310134699999978	0.3609394899999998	F	F	F
0.7629538699999969	0.1970798500000015	0.3608490599999996	F	F	F
0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F
0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0469792661906289	0.2941372319035817	0.4661337475065658	T	T	T
0.0457188075968383	0.6289871467859390	0.4663940294625377	T	T	T
0.0462599077363605	0.9609693493589643	0.4663818234245362	T	T	T
0.3030051673862846	0.2480950824196918	0.4867517697762342	T	T	T
0.3025813512017798	0.5805024565720404	0.4873689565956055	T	T	T
0.3032233700707045	0.9131058660950541	0.4866504661774724	T	T	T
0.5574754612106099	0.2014101899190819	0.5068771713456799	T	T	T
0.5591833905300835	0.5335894889591138	0.5063841496710009	T	T	T
0.5594923989478674	0.8663728696644531	0.5065489703773052	T	T	T
0.8155572617808402	0.1523259432496275	0.5276381412123460	T	T	T
0.8163675302008309	0.4855768334415109	0.5272064140863983	T	T	T
0.8146575835509171	0.8209448855082061	0.5279209691463117	T	T	T
0.0720942818104209	0.1052025383418935	0.5481622924966617	T	T	T
0.0708095793032338	0.4427934046339959	0.5481781780592220	T	T	T
0.0707619572904614	0.7745300730207486	0.5495278199224972	T	T	T
0.3285025671204688	0.0602221572912467	0.5676783969999860	T	T	T
0.3250485283436733	0.3960957644447813	0.5704526956279599	T	T	T
0.3269491148772521	0.7262784288288479	0.5692513880381117	T	T	T
0.5835851493239704	0.0121703043707685	0.5887359647220290	T	T	T
0.5835975117192393	0.3455499091289262	0.5878976952836157	T	T	T
0.5859765952304348	0.6770432523927377	0.5881791228094722	T	T	T
0.8406528913176849	0.6309650560715667	0.6103652792849205	T	T	T
0.8441894864606330	0.2954268282190234	0.6095988804572415	T	T	T
0.8414664064348834	0.9616520530847364	0.6111581701969846	T	T	T
0.0932956967165982	0.5894480313258151	0.6346459762868287	T	T	T
0.1014748586991767	0.2505554848705985	0.6291973171940086	T	T	T
0.0966185487691513	0.9202300047089558	0.6343686121588995	T	T	T
0.3483602802248908	0.5431866851957952	0.6541279970472939	T	T	T
0.3476386303474354	0.2125203564844998	0.6519238304489360	T	T	T
0.3471061704537252	0.8812572988760752	0.6492793251969313	T	T	T
0.6105584421491628	0.4890878151651697	0.6679754819638842	T	T	T
0.6040699069615744	0.1553679704676665	0.6702347285244306	T	T	T
0.5950733496961523	0.8359412433659724	0.6708266764830766	T	T	T
0.8951665815377566	0.4123354357601905	0.6912714455890624	T	T	T
0.8618399745432505	0.1091587352309208	0.6915954449511782	T	T	T
0.8540202995393916	0.7828525606716888	0.6960862271772882	T	T	T
0.6666044684251968	0.6011990362776094	0.7478801713636286	T	T	T
0.6198720776525978	0.3153790177732988	0.7463393363424971	T	T	T

0.3955651115152859	0.7067503550888236	0.7290286563998790	T	T	T
0.8532705353203260	0.6062490602308576	0.7486422365707915	T	T	T
0.9425687518824967	0.5580828849286861	0.7905436243337979	T	T	T
0.9329516257300378	0.4647191604314605	0.8133289268911221	T	T	T

COH/Defected-Cu(533) $E_{ads} = -3.17$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
59 1 1 1
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0468989828222703	0.2941678890245853	0.4660631401400437	T	T	T
0.0469655164799434	0.6265620509434058	0.4659618182323015	T	T	T
0.0474269309644200	0.9604631301090691	0.4658964784331374	T	T	T
0.3034352609847772	0.2466072642040587	0.4869069993987338	T	T	T
0.3042702832177326	0.5793761754119515	0.4864639929047243	T	T	T
0.3037133375843695	0.9131670693596661	0.4867578977774087	T	T	T
0.5593835756459313	0.2001133547115259	0.5067383975609303	T	T	T
0.5597255775979733	0.5335038866585080	0.5067667136261704	T	T	T
0.5588610889455268	0.8672533785088774	0.5073970808389348	T	T	T
0.8166610990790559	0.1527705880878969	0.5272427973405200	T	T	T
0.8151456194188356	0.4873876947081968	0.5274958693904210	T	T	T
0.8159021907293607	0.8195993601113827	0.5275440149381012	T	T	T
0.0721888659595251	0.1062898316411136	0.5483111000987293	T	T	T
0.0713387779452717	0.4394836205871968	0.5487244004322491	T	T	T
0.0735082523804209	0.7710723763828966	0.5475439199758085	T	T	T
0.3267952871117856	0.0599469889883153	0.5692650123078451	T	T	T
0.3282452170722649	0.3922661466385051	0.5690087310533940	T	T	T
0.3286715877330693	0.7252440826635151	0.5686383355587949	T	T	T
0.5847736289010683	0.0140288399762909	0.5894807723896633	T	T	T

0.5860050318879715	0.3440353913190179	0.5885040747552281	T	T	T
0.5856121685336149	0.6761179997624325	0.5897454017895782	T	T	T
0.8426875514918279	0.6275549774199831	0.6105431785370854	T	T	T
0.8429513025225575	0.3002063166067401	0.6099246978801816	T	T	T
0.8438898784621500	0.9649517329272612	0.6087148151912487	T	T	T
0.0982585168526171	0.5831179540902554	0.6320279345586499	T	T	T
0.0943785151864276	0.2523865183848528	0.6337909209278294	T	T	T
0.0991995797387375	0.9167175364292177	0.6313971289447053	T	T	T
0.3503010481842210	0.5402885930261689	0.6511652511706174	T	T	T
0.3491516316414973	0.2060567921843415	0.6517747141413750	T	T	T
0.3517606152808881	0.8719442487423450	0.6518264086155199	T	T	T
0.6064048245792861	0.4945494938349739	0.6734730714517596	T	T	T
0.5983434095613944	0.1634675009623763	0.6746020970300250	T	T	T
0.6067625078495738	0.8249919867163555	0.6704519435150260	T	T	T
0.8717912916959136	0.1142762622462996	0.6900503817885379	T	T	T
0.8600782802036164	0.7863968471466762	0.6878345241493307	T	T	T
0.6708737581833972	0.2680346028846827	0.7256661342932560	T	T	T
0.6412023420631883	0.2984215910277683	0.7751962381064388	T	T	T
0.5344260864268549	0.3373197952679519	0.7824049848244030	T	T	T

COH/Cu(533) $E_{ads} = -3.14$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0477952273583061	0.2934243267103852	0.4659161332622623	T	T	T
0.0471550621011298	0.6272206352894614	0.4660601540110149	T	T	T
0.0477843188751264	0.9600172297531990	0.4658718226259667	T	T	T
0.3044955964055832	0.2461071017304899	0.4869041403797068	T	T	T

0.3043140454452033 0.5798322250315616 0.4867607807603049 T T T
0.3048905472367276 0.9122683084657407 0.4865702915015941 T T T
0.5597669022133002 0.2004816363493222 0.5071408420525945 T T T
0.5597965062235458 0.5336267315017873 0.5069746459037408 T T T
0.5598456229246597 0.8667035613930627 0.5072038359525034 T T T
0.8163943204743507 0.1523267231040685 0.5271389162904708 T T T
0.8164259015225861 0.4875261255306949 0.5271636385689942 T T T
0.8163058311585530 0.8200040948482068 0.5280050505868008 T T T
0.0743702793271269 0.1045817319453027 0.5478968410719732 T T T
0.0731024869419293 0.4392118411341105 0.5483481449897438 T T T
0.0730079728332775 0.7725827007869679 0.5483226904101536 T T T
0.3285912889367397 0.0591947222663244 0.5691501036365286 T T T
0.3283301545965527 0.3933555357976152 0.5691858687144011 T T T
0.3283817416117532 0.7266704599463820 0.5692833356740502 T T T
0.5854112599858953 0.0125796311675086 0.5891118088671162 T T T
0.5859622551688193 0.3473036955223177 0.5895004185588886 T T T
0.5865124601185518 0.6763606630349434 0.5896420937397278 T T T
0.8443548492235874 0.6282946340353772 0.6100465475735112 T T T
0.8451790696769951 0.2966739945843402 0.6076826917810356 T T T
0.8439210488461483 0.9666230304883604 0.6098758460925711 T T T
0.0993365194257504 0.5835770083318192 0.6327394488412729 T T T
0.0992495318293101 0.2504974515274376 0.6323922906040512 T T T
0.0983119802196507 0.9185824280326790 0.6325359346890280 T T T
0.3509467169071402 0.5401255353151894 0.6516691642652396 T T T
0.3530948509142237 0.2056814140899337 0.6518467603063732 T T T
0.3517495575475333 0.8741923633760262 0.6515501576783773 T T T
0.5977584940920614 0.5013576421693463 0.6745379369242273 T T T
0.6063615761109180 0.1606763517958818 0.6717520838014159 T T T
0.6068932894121212 0.8291925838334210 0.6718378128030943 T T T
0.8680532967619131 0.4473005147924422 0.6921069703008010 T T T
0.8651335671772643 0.1127913716493668 0.6918032558898248 T T T
0.8630588889669705 0.7828729673692800 0.6892420100357227 T T T
0.7415096130531958 0.3876428600832766 0.7313984054323855 T T T
0.7171309819812063 0.4048157190113620 0.7812136977089303 T T T
0.6042751579755599 0.4691782450405281 0.7885806108487351 T T T

COH/Cu(533) E_{ads} = −3.13 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F

0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0476423418904959	0.2929491136408762	0.4662425083547571	T	T	T
0.0479235381629832	0.6260705869385818	0.4660539282795589	T	T	T
0.0474553203808799	0.9600379492470192	0.4660819342749437	T	T	T
0.3040533025521270	0.2459725552913160	0.4868000467046606	T	T	T
0.3044044237405291	0.5791112298422257	0.4867499110406290	T	T	T
0.3040210446029933	0.9128104504495914	0.4867134381986965	T	T	T
0.5595991140733211	0.1999753772334074	0.5069941872657698	T	T	T
0.5591228170010984	0.5333866066111504	0.5068476746968663	T	T	T
0.5593587487583271	0.8666453658623093	0.5069131464200335	T	T	T
0.8159395341978394	0.1539105832084411	0.5270416853762677	T	T	T
0.8166871928627881	0.4850666887143595	0.5275673206000360	T	T	T
0.8165228833364924	0.8173470443515127	0.5269142679798425	T	T	T
0.0733276143734695	0.1031204866379533	0.5490570982142547	T	T	T
0.0734287464293246	0.4382716028336616	0.5489086555314898	T	T	T
0.0730130586316466	0.7710494110130249	0.5484621961750549	T	T	T
0.3278639339857860	0.0587539889533119	0.5690220266022977	T	T	T
0.3279689520947467	0.3922398187131882	0.5693394083719848	T	T	T
0.3271703818085053	0.7266317728627021	0.5692275629701523	T	T	T
0.5849882240214069	0.0108162611115305	0.5889020285417840	T	T	T
0.5841525913317824	0.3468049419207880	0.5891290270910926	T	T	T
0.5857992635380599	0.6773175526941556	0.5887070555454066	T	T	T
0.8446330170553339	0.6290520402355729	0.6091997291673260	T	T	T
0.8450460568405282	0.2934452145377578	0.6093545705980179	T	T	T
0.8382568129150735	0.9667588321298544	0.6062401600138920	T	T	T
0.1038747740276528	0.5769363817300248	0.6347105844624770	T	T	T
0.1011073644052925	0.2466189685414407	0.6326454980744577	T	T	T
0.1022487845869974	0.9115391100131824	0.6351242936786405	T	T	T
0.3581064903255310	0.5338741690854319	0.6520772819080357	T	T	T
0.3570415313891470	0.1980720997415704	0.6517192948139462	T	T	T
0.3570012784239228	0.8696584528786780	0.6515031512931613	T	T	T
0.6086926948976408	0.4918177864619568	0.6722398407126967	T	T	T
0.6069777379377861	0.1594056564481445	0.6717333414842143	T	T	T
0.6106342760120423	0.8242648416106402	0.6720930663098433	T	T	T
0.8613295595681351	0.4481842653615151	0.6892985489680542	T	T	T
0.8604331646668205	0.1152228295722783	0.6905387062053192	T	T	T
0.8631914890116119	0.7812042411329240	0.6901586147816919	T	T	T
0.0509764702888585	0.7910583814265857	0.6941631643846173	T	T	T
0.1459995972225396	0.7215343281623781	0.7368753448870500	T	T	T
0.0949882875660232	0.6964363178510884	0.7639573885959194	T	T	T

COH/Defected-Cu(533) E_{ads} = −3.13 eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H
59 1 1 1
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0469599083626449	0.2941995584366595	0.4660006808929964	T	T	T
0.0469973738745892	0.6266166879094754	0.4659148026777800	T	T	T
0.0474004451301937	0.9605178902731666	0.4658566966253161	T	T	T
0.3036108619447333	0.2465145926232069	0.4868677830364803	T	T	T
0.3043936582968811	0.5792934585918346	0.4864439951659136	T	T	T
0.3038766614828106	0.9130672132787083	0.4867215277961989	T	T	T
0.5594807918007874	0.1999688333939460	0.5068104375577107	T	T	T
0.5599383653587608	0.5332250483920618	0.5068016650352476	T	T	T
0.5589811917106928	0.8672163701468349	0.5074777130388597	T	T	T
0.8166013787639983	0.1527540915836738	0.5272290975870462	T	T	T
0.8152757548648069	0.4872663365148426	0.5274436339410329	T	T	T
0.8158383407454437	0.8194937524588823	0.5274865821339318	T	T	T
0.0724159649978589	0.1062143953088750	0.5481595364757936	T	T	T
0.0715726460092299	0.4393529111760941	0.5486088072886659	T	T	T
0.0736357313719438	0.7709430371084736	0.5474149132241806	T	T	T
0.3271793290141360	0.0596978842278091	0.5692023065877052	T	T	T
0.3284990357633646	0.3921296569833146	0.5689982835884919	T	T	T
0.3292565502711469	0.7247172500871386	0.5685491792812485	T	T	T
0.5850838772022158	0.0142339514434298	0.5898091342656215	T	T	T
0.5862820441697068	0.3436149835785187	0.5887535111639011	T	T	T
0.5859585540696273	0.6757643784592844	0.5897754896773435	T	T	T
0.8429495422268687	0.6270689602829194	0.6104436755455609	T	T	T
0.8434264416410855	0.2995829145656188	0.6098309069624008	T	T	T
0.8441340919038893	0.9642471152824896	0.6085525597579391	T	T	T
0.0984911060448681	0.5828915058419426	0.6319098161769929	T	T	T
0.0948735771428559	0.2519758452762346	0.6336040863865904	T	T	T
0.1001444025378504	0.9159007066860454	0.6309880891868360	T	T	T
0.3507484545908639	0.5398294685030578	0.6511533230804574	T	T	T
0.3496747528454662	0.2058105543222410	0.6517197705026092	T	T	T
0.3524010743990189	0.8713195831885869	0.6517103198706309	T	T	T

0.6074283692257652	0.4935255596712125	0.6735049322083242	T	T	T
0.5983354712810183	0.1639986452349902	0.6758395792488514	T	T	T
0.6070784773240661	0.8246020670924707	0.6705053730905348	T	T	T
0.8738371354151298	0.1106039569404018	0.6893592105289130	T	T	T
0.8603158883118311	0.7853302019296891	0.6876940037881525	T	T	T
0.6746892953781156	0.2667604933596266	0.7259754582795281	T	T	T
0.6382155895378716	0.3026753214510123	0.7751864755676081	T	T	T
0.7271771925222339	0.2828315077706733	0.7940354252514297	T	T	T

COH/Cu(533) E_{ads} = −3.11 eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H

60 1 1 1

Selective dynamics

Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0471833040990569	0.2943053870480852	0.4657992970577536	T	T	T
0.0473599797139480	0.6272232648949611	0.4659076638387590	T	T	T
0.0478614506863380	0.9601580323467604	0.4659587722024993	T	T	T
0.3042379761935208	0.2464422408407906	0.4867808538034156	T	T	T
0.3043072768048655	0.5798240508015648	0.4867318291310208	T	T	T
0.3044894349323181	0.9129122125895656	0.4867257835584977	T	T	T
0.5593357186431409	0.2006844749297281	0.5069541159167291	T	T	T
0.5597854079587983	0.5337506777048960	0.5069339815915034	T	T	T
0.5594171016122661	0.8674048917474211	0.5073440059340452	T	T	T
0.8164477360817054	0.1530993057646176	0.5271188321484805	T	T	T
0.8154259903912308	0.4875923111097752	0.5274752213961372	T	T	T
0.8159360424393269	0.8202729846539093	0.5274847990162831	T	T	T
0.0728267901831974	0.1065565421882499	0.5478408642429469	T	T	T
0.0724086507741935	0.4398653465906082	0.5481333113443875	T	T	T
0.0730481450833795	0.7719954130708100	0.5479734701794473	T	T	T

0.3274559031463962 0.0600363232228635 0.5691170594037418 T T T
0.3274609702514398 0.3936846297563483 0.5692142756174575 T T T
0.3283527972764795 0.7263941686729428 0.5689236328739540 T T T
0.5842018441977546 0.0153193059429666 0.5896696281469972 T T T
0.5856439987033204 0.3453769180533009 0.5889695614137774 T T T
0.5846778700084725 0.6775478356588809 0.5897875112685118 T T T
0.8424058492667988 0.6323626064627509 0.6091025961937371 T T T
0.8432491687449112 0.2966590454879926 0.6088452007755439 T T T
0.8430242923557358 0.9661660334131192 0.6089678777260983 T T T
0.0975576274437244 0.5855365208669163 0.6326397033205438 T T T
0.0978500093374908 0.2508863586874271 0.6324755108678224 T T T
0.0990105074942641 0.9172516224101823 0.6315949569038567 T T T
0.3502434145542832 0.5411247385265362 0.6511760678625577 T T T
0.3496570842114436 0.2071103365088423 0.6518435873717408 T T T
0.3513196896464236 0.8734971288018132 0.6518415227833690 T T T
0.6025163000192448 0.4974095263599590 0.6751292815530979 T T T
0.5992603440267797 0.1646928005738017 0.6744814403953397 T T T
0.6035036020696588 0.8295629566201509 0.6715945760086823 T T T
0.8606188002265976 0.4526076709576775 0.6889382871691369 T T T
0.8734654205948533 0.1081903913091546 0.6911003768397391 T T T
0.8593716373416229 0.7837593547736325 0.6891563403136671 T T T
0.6734116520274294 0.2641132772368517 0.7266677114717232 T T T
0.6423080677568676 0.2931084359712357 0.7761245424851810 T T T
0.5286426501910039 0.3580240302829927 0.7820848096027252 T T T

COH/Cu(533) E_{ads} = −3.11 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F

0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0474475080777995	0.2942419120085187	0.4659027840898186	T	T	T
0.0475616733944289	0.6276092472833925	0.4659965603852031	T	T	T
0.0476026468288832	0.9608213133237207	0.4659694998829885	T	T	T
0.3044734625503010	0.2464006713186845	0.4866471465398584	T	T	T
0.3041803544842229	0.5803975833391081	0.4865766235171148	T	T	T
0.3043535329651217	0.9138456996541541	0.4868991265388957	T	T	T
0.5598247704721454	0.2004996739847387	0.5065509383328803	T	T	T
0.5597534318232485	0.5338707433083704	0.5068247132966980	T	T	T
0.5596584519287660	0.8672383855636864	0.5069341619890859	T	T	T
0.8167732210128761	0.1532430897127977	0.5274736230544957	T	T	T
0.8165230912768855	0.4867616845533555	0.5274399830268964	T	T	T
0.8168214709306831	0.8199270103227765	0.5274980202000371	T	T	T
0.0732872310665018	0.1068812623032052	0.5480574409294361	T	T	T
0.0733238416149243	0.4398359429292052	0.5480740052731676	T	T	T
0.0728840685450574	0.7739434741549107	0.5483423438549031	T	T	T
0.3286941696348268	0.0621691237324406	0.5695423641655288	T	T	T
0.3293949366157300	0.3929060548036375	0.5686910703727883	T	T	T
0.3289377285854419	0.7260531835652869	0.5691012042411828	T	T	T
0.5850527930730924	0.0140770581772410	0.5886507210529386	T	T	T
0.5855153204256786	0.3445161710132113	0.5886233329695757	T	T	T
0.5852574065178141	0.6792599194032022	0.5887582216272398	T	T	T
0.8444378859970383	0.6306360928292795	0.6093019299674060	T	T	T
0.8439932543225285	0.2972479330415048	0.6092693222361357	T	T	T
0.8417680197154703	0.9654082143659762	0.6099408641908003	T	T	T
0.0999458461882368	0.5853544176527758	0.6316536612371677	T	T	T
0.1010996450769961	0.2510308867239331	0.6322450286523122	T	T	T
0.0995067966795882	0.9208586425793615	0.6317543027951332	T	T	T
0.3492997110219436	0.5492733675412051	0.6525668995708105	T	T	T
0.3521373860448910	0.2066535176433696	0.6545487649003684	T	T	T
0.3544074332687229	0.8738522699717544	0.6514826150079326	T	T	T
0.6098161580192861	0.4926322282755338	0.6715932584228168	T	T	T
0.6133534179703164	0.1536267535289637	0.6759984975714980	T	T	T
0.6106624788606897	0.8227560902729072	0.6712864444411780	T	T	T
0.8643636967821908	0.4461326314379785	0.6895299699472219	T	T	T
0.8662514080731967	0.1116942837512359	0.6897764261829031	T	T	T
0.8672515816771774	0.7759737308527145	0.6900243005649371	T	T	T
0.4043596066477217	0.3431118817556006	0.7060546017089021	T	T	T
0.3537144954364778	0.3849655355401035	0.7536730633784264	T	T	T
0.2445354525719363	0.5270561754784154	0.7554806312903048	T	T	T

COH/Cu(533) $E_{ads} = -3.10$ eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H

60 1 1 1

Selective dynamics

Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F

0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0478398788927926	0.2936961229674159	0.4658199506751917	T	T	T
0.0472937031397872	0.6274541343842512	0.4660111936639015	T	T	T
0.0478518553442871	0.9603782002167081	0.4658121366314819	T	T	T
0.3046934724489977	0.2463601086304753	0.4868362463611487	T	T	T
0.3044758037071662	0.5802255990899605	0.4867019387272469	T	T	T
0.3051544110254909	0.9125158993216577	0.4865231175458568	T	T	T
0.5599954524220401	0.2007901866786008	0.5071569235964265	T	T	T
0.5599316755148511	0.5338305763304437	0.5069749783404827	T	T	T
0.5600354083590269	0.8669127968765237	0.5071844730906229	T	T	T
0.8165376079442835	0.1526315473853467	0.5270555572160329	T	T	T
0.8165562219327311	0.4878821103696394	0.5270494250036541	T	T	T
0.8165371807018614	0.8204091391994581	0.5278737719610876	T	T	T
0.0746883869308739	0.1050499501180843	0.5477679425156489	T	T	T
0.0734103801836188	0.4395680173112709	0.5481923919248676	T	T	T
0.0732981460113497	0.7731185829084772	0.5481930169441493	T	T	T
0.3288698954335000	0.0597338515996961	0.5690400409941742	T	T	T
0.3286740285962026	0.3938261332032874	0.5690776810694119	T	T	T
0.3286572900134733	0.7271794591829416	0.5691979707433608	T	T	T
0.5857081471760733	0.0131016394432907	0.5890570429783273	T	T	T
0.5863456075403009	0.3478854399282972	0.5896772528050525	T	T	T
0.5867059189165444	0.6766351699674538	0.5897085984786238	T	T	T
0.8445651679899259	0.6289086886518084	0.6096950777692396	T	T	T
0.8454381169390202	0.2967710814213895	0.6074606710773034	T	T	T
0.8442924130940525	0.9667932046923997	0.6097163837076517	T	T	T
0.0997402978728639	0.5843175548689215	0.6325323497272357	T	T	T
0.0995243127842716	0.2512676306751345	0.6321593992877023	T	T	T
0.0986520333401628	0.9192173939234537	0.6323370855008159	T	T	T
0.3513385389531780	0.5407691030196103	0.6515048773547292	T	T	T
0.3532368116055500	0.2065110011326445	0.6516829887712430	T	T	T
0.3517183265973963	0.8751910210200895	0.6513692651751959	T	T	T
0.5977141616865959	0.5027037136752915	0.6751273730514782	T	T	T
0.6066191594572826	0.1611510292990417	0.6717028674566109	T	T	T
0.6070724834357155	0.8299583485661884	0.6716614569662837	T	T	T
0.8677720146340574	0.4474436554999642	0.6913075542582491	T	T	T
0.8658938462298289	0.1117818655715551	0.6916614377934486	T	T	T
0.8634277404840356	0.7824739626224468	0.6889868656215296	T	T	T
0.7433299635843673	0.3847705671250998	0.7314338462163077	T	T	T
0.7097033143818976	0.4137856890708905	0.7808285316049934	T	T	T
0.8097249410392245	0.3407404490199850	0.8003923579923542	T	T	T

COH/Defected-Cu(533) E_{ads} = −3.09 eV

1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
59 1 1 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0466492094757519 0.2950318015111399 0.4661928801031927 T T T
0.0470646838971366 0.6272019699635228 0.4659137742061075 T T T
0.0473748940408420 0.9611198719822971 0.4658009693328416 T T T
0.3028817671216158 0.2484611503292114 0.4869812988844963 T T T
0.3044120905603317 0.5796255196961956 0.4863181716553386 T T T
0.3036053541686522 0.9141165059819590 0.4868491354669783 T T T
0.5589152234653831 0.2016210809535742 0.5069290421721683 T T T
0.5594383863764207 0.5343433998925793 0.5072158339791231 T T T
0.5581160593179207 0.8694940795972932 0.5072673563205174 T T T
0.8159702589198076 0.1553376702583765 0.5268821293465525 T T T
0.8148082653444224 0.4899288232857649 0.5275745063001611 T T T
0.8152903061613417 0.8204435039631605 0.5272561665181735 T T T
0.0719844509382442 0.1080878005639060 0.5483343769912522 T T T
0.0707062296802823 0.4416505898723462 0.5491393886103196 T T T
0.0741447383692293 0.7718514031411452 0.5473226818944272 T T T
0.3257581980520855 0.0629475225330211 0.5694656618230358 T T T
0.3266883244472927 0.3954494999259485 0.5693998663931353 T T T
0.3282421020769749 0.7266477588457171 0.5686280037210383 T T T
0.5846148542550145 0.0164892501111941 0.5896699834075676 T T T
0.5858638348333001 0.3438877857084922 0.5895372268561722 T T T
0.5843181890819864 0.6815631653436182 0.5891846847430831 T T T
0.8414909580788504 0.6330171843023136 0.6117267168912688 T T T
0.8420680060473618 0.3040089319347256 0.6094202716006750 T T T
0.8449626363435813 0.9656845852876703 0.6071388240494336 T T T
0.0941630653923408 0.5886916773352551 0.6331276066952785 T T T
0.0911553697748226 0.2567160620226494 0.6347384626401152 T T T

0.0988343246459733 0.9189681437173426 0.6310866346707200 T T T
0.3497561413895442 0.5428646746925180 0.6514541986887167 T T T
0.3467591854371745 0.2110842242222604 0.6517090457236897 T T T
0.3498750146710455 0.8757564674697447 0.6519037459394315 T T T
0.6061307516575312 0.4981586645459091 0.6704431615127170 T T T
0.5950358914932070 0.1709659730404261 0.6757335163923652 T T T
0.6046245308739766 0.8290453935350469 0.6705116079327215 T T T
0.8714743011525785 0.1276405605613242 0.6888668035497462 T T T
0.8549596370468399 0.8006887830768560 0.6904576454954542 T T T
0.7477141637863992 0.0775941601066038 0.7307293383899180 T T T
0.7166907034318543 0.1004506499676708 0.7803766496206562 T T T
0.7782133314043520 0.1420632318941745 0.7975150460911407 T T T

COH/Cu(533) $E_{ads} = -3.07$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0473940889888811 0.2941518031015536 0.4659912627802822 T T T
0.0473976745067063 0.6275739941391313 0.4660899350566757 T T T
0.0474149093491535 0.9608396186834682 0.4660498370105514 T T T
0.3042369694989220 0.2464504194629374 0.4867716973356761 T T T
0.3040737480591879 0.5803827379147874 0.4867164663084111 T T T
0.3041701720226252 0.9136039979810723 0.4871300397634569 T T T
0.5594513344644566 0.2008208361802787 0.5066510806771862 T T T
0.5592735148446861 0.5341111362037094 0.5069550692882234 T T T
0.5593280016246127 0.8673004713839194 0.5070027888849676 T T T
0.8160449590433577 0.1536154145264996 0.5275899148170247 T T T
0.8160843716420942 0.4868815526962556 0.5275281721596705 T T T

0.8162435198724894 0.8201086791430912 0.5275781935469712 T T T
0.0727602486691887 0.1068095610988671 0.5481713407471754 T T T
0.0728535504292249 0.4397608338193725 0.5482401683514621 T T T
0.0725423926083921 0.7739049627343816 0.5483521619335440 T T T
0.3279563095114655 0.0621886396587325 0.5697471287552713 T T T
0.3287681987847861 0.3932271211662385 0.5690138974177458 T T T
0.3284476474193729 0.7252242904113357 0.5697181003837662 T T T
0.5841750298447843 0.0145055805699514 0.5886687168840821 T T T
0.5843147005081265 0.3452867556591794 0.5889151411642186 T T T
0.5846258583736043 0.6794745000996144 0.5888981078823484 T T T
0.8435129623441967 0.6308918974968755 0.6094335552161948 T T T
0.8433247199562960 0.2972505879535990 0.6094005204735798 T T T
0.8418072878306724 0.9650395147537091 0.6099265857307187 T T T
0.0989118519770646 0.5852816414400389 0.6316003550086768 T T T
0.0998637670615532 0.2508027579944717 0.6324324464487439 T T T
0.0991596515205963 0.9199337981012756 0.6318347979412613 T T T
0.3475730424335509 0.5480758246636522 0.6545062619012895 T T T
0.3503890310437535 0.2068709858354087 0.6547713765385622 T T T
0.3536171045783242 0.8731748562792347 0.6517874791602076 T T T
0.6087690632926629 0.4930674898464430 0.6718049952098842 T T T
0.6146921314406831 0.1525346925669482 0.6753000085186833 T T T
0.6093869967257356 0.8237586146499147 0.6714989091022031 T T T
0.8624749085599274 0.4472872508511657 0.6897299096694887 T T T
0.8659580512615437 0.1120966731187715 0.6899567644501823 T T T
0.8665295111250820 0.7757940306353032 0.6902032389266005 T T T
0.4073722206401403 0.3338028089874162 0.7067771229361733 T T T
0.3577288927226063 0.3739201006467584 0.7546828368625380 T T T
0.4470252331459399 0.2641368758504669 0.7767735760194133 T T T

COH/Cu(533) E_{ads} = −3.07 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F

0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0473300768649801	0.2946259655857907	0.4657024555888544	T	T	T
0.0473943718792747	0.6275812447978354	0.4658851352018442	T	T	T
0.0479582521494185	0.9605638190477529	0.4658947487322379	T	T	T
0.3043596880471441	0.2469489127099723	0.4867278932429260	T	T	T
0.3045149165567340	0.5804742912190833	0.4866698538962952	T	T	T
0.3046778824707125	0.9135400105732864	0.4867224749937312	T	T	T
0.5595352666000220	0.2012120527024586	0.5069989558810817	T	T	T
0.5601083083036142	0.5341386699989848	0.5069031139295247	T	T	T
0.5594998482798651	0.8681110518021298	0.5074422681323247	T	T	T
0.8166297298968335	0.1534023279821049	0.5270462010719010	T	T	T
0.8156568187411062	0.4878933831087767	0.5273918134600609	T	T	T
0.8159899934046444	0.8206930563226756	0.5274532807963122	T	T	T
0.0733420165688547	0.1075089165469399	0.5477415762393462	T	T	T
0.0726582036734161	0.4405706034942520	0.5480318365159168	T	T	T
0.0734294259300871	0.7729176225317564	0.5477946230725056	T	T	T
0.3277564839608514	0.0618663038418490	0.5691832366078696	T	T	T
0.3280695417445341	0.3948054108076719	0.5690634034303221	T	T	T
0.3292860970344929	0.7272809391495940	0.5688777345955175	T	T	T
0.5849461788587347	0.0169543708114106	0.5899551415739989	T	T	T
0.5863029547889513	0.3463070650284237	0.5891290809455639	T	T	T
0.5850141183447777	0.6791693270275884	0.5898151788365645	T	T	T
0.8428461239808827	0.6322896669777860	0.6089829484438700	T	T	T
0.8438404255242110	0.2968418785618254	0.6086442733706586	T	T	T
0.8435855114049893	0.9661672614297497	0.6088121038055292	T	T	T
0.0988151093652835	0.5866077461585609	0.6322186947239973	T	T	T
0.0980951542390875	0.2537080286231704	0.6327028756616622	T	T	T
0.1002492758440785	0.9183891877967932	0.6311221973147373	T	T	T
0.3509512904434496	0.5429167350859031	0.6510959471060856	T	T	T
0.3517515736736306	0.2093437291864459	0.6519985464702872	T	T	T
0.3508558358838292	0.8779462706390445	0.6516678848830745	T	T	T
0.6000130836957984	0.5041605798463363	0.6747985528126855	T	T	T
0.6028526109980870	0.1676384258260258	0.6759524379913711	T	T	T
0.6043413947853568	0.8331170281207571	0.6716766884809887	T	T	T
0.8594271653342047	0.4524557686303128	0.6888605791736484	T	T	T
0.8760328793697886	0.1036082840755296	0.6905006758258779	T	T	T
0.8619384156994814	0.7806348448130547	0.6888506884808994	T	T	T
0.6778847013936210	0.2784803723860578	0.7269016359791610	T	T	T
0.6384552333717716	0.3148329037516469	0.7758883688079438	T	T	T
0.7356921534411806	0.2208259656590402	0.7966314789173268	T	T	T

COH/Defected-Cu(533) E_{ads} = −3.06 eV

1.00000000000000		
10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H
59 1 1 1
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F

0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0472894240198372	0.2937926644529441	0.4660536930450760	T	T	T
0.0470885228383580	0.6269603396086225	0.4659811541092793	T	T	T
0.0476387925420099	0.9601429701122797	0.4657328319358243	T	T	T
0.3033791951318392	0.2467031403969884	0.4868571191629059	T	T	T
0.3040770303374316	0.5796508135147178	0.4864542503140612	T	T	T
0.3034129303315609	0.9134075478814125	0.4867896123430739	T	T	T
0.5590727315704598	0.1999457989590496	0.5064036439369204	T	T	T
0.5596223888523468	0.5347206957798321	0.5065277044403373	T	T	T
0.5587435153276630	0.8674762782963867	0.5074970992866454	T	T	T
0.8173011368379264	0.1517878333076226	0.5271355425649560	T	T	T
0.8155200141755472	0.4869506077968069	0.5275046100693004	T	T	T
0.8156128713505169	0.8195858544878902	0.5276817103138214	T	T	T
0.0722860681368545	0.1061853411070999	0.5482494703314060	T	T	T
0.0714713372020128	0.4395362862956418	0.5485181938512440	T	T	T
0.0725553534873669	0.7725169310568702	0.5478974895649813	T	T	T
0.3269274324890361	0.0600015075001323	0.5694110310774008	T	T	T
0.3281914025400852	0.3939301236785582	0.5690717363108391	T	T	T
0.3290202304662557	0.7242742865717418	0.5690344150957145	T	T	T
0.5839897482574017	0.0161707458750868	0.5893546148047832	T	T	T
0.5862057971170103	0.3449404384374617	0.5872040252966713	T	T	T
0.5856917923296336	0.6769205040949515	0.5897930235407713	T	T	T
0.8420825205898055	0.6266609446438878	0.6106620885458725	T	T	T
0.8427901073177679	0.3001845167811865	0.6101576986132855	T	T	T
0.8410211057398840	0.9654634593130638	0.6091175174614776	T	T	T
0.0966560737043949	0.5836539793902915	0.6315555163018090	T	T	T
0.0954046529996191	0.2522438540642327	0.6333215967300632	T	T	T
0.0988113238015202	0.9183087924104711	0.6312011710869712	T	T	T
0.3449407858380695	0.5438884178790957	0.6527701795329790	T	T	T
0.3506528511030993	0.2051796372615229	0.6517909932620611	T	T	T
0.3525974065463515	0.8728477751917936	0.6521500808138896	T	T	T
0.6163113874156068	0.4934168156947365	0.6733833071923954	T	T	T
0.6044931022797613	0.1636160087389058	0.6759624091615635	T	T	T
0.6080814826260692	0.8285122994708018	0.6703506088491338	T	T	T
0.8670023465346759	0.1083612886174095	0.6879047611852798	T	T	T
0.8606506738541668	0.7829420801832256	0.6883388552322671	T	T	T
0.4782746227987289	0.4536509744959716	0.7115151953421943	T	T	T
0.4376246590399688	0.4915043598529252	0.7601931921968514	T	T	T

0.3215803667478241	0.5641811592670578	0.7638125997587721	T	T	T

COH/Defected-Cu(533) E_{ads} = −3.05 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
59 1 1 1
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0470115714660295	0.2941681355070287	0.4660115035766026	T	T	T
0.0472762177242814	0.6270488704222785	0.4660239813745335	T	T	T
0.0471108644107190	0.9611241929637444	0.4659731188542295	T	T	T
0.3037558820022426	0.2465904103525460	0.4867702109799765	T	T	T
0.3040119530491836	0.5800572205002723	0.4864177314805076	T	T	T
0.3034727976375109	0.9139149145650762	0.4870028884453177	T	T	T
0.5596081552000172	0.2004142607663226	0.5064117006006654	T	T	T
0.5593900780009875	0.5338354464789532	0.5067994845402595	T	T	T
0.5587416767049191	0.8672672844642477	0.5069947368849910	T	T	T
0.8162847257335315	0.1534909690494857	0.5275671324885209	T	T	T
0.8159168134997401	0.4867592445594795	0.5274376461311618	T	T	T
0.8163269874656578	0.8194877089252230	0.5274914510426001	T	T	T
0.0720299410098235	0.1073000535970010	0.5483487918974674	T	T	T
0.0721229721315524	0.4395104125696676	0.5484288134389317	T	T	T
0.0729171593434614	0.7730715825944472	0.5479490167463368	T	T	T
0.3269648851136182	0.0626925272813352	0.5698355314726626	T	T	T
0.3290210640638875	0.3929105710728962	0.5688091131524260	T	T	T
0.3286284391241523	0.7249094057669296	0.5693329843462038	T	T	T
0.5841329933001873	0.0141461365617772	0.5882769196456508	T	T	T
0.5848716894557668	0.3443792614341845	0.5884775089160215	T	T	T
0.5854186436276407	0.6783353773542373	0.5888146753897630	T	T	T
0.8433297234781563	0.6272139252807420	0.6104225368898497	T	T	T

0.8431492976261907 0.3013212607947651 0.6105349028216764 T T T
0.8420462198289940 0.9644762028307170 0.6094160834682114 T T T
0.0984616596743706 0.5843121120166330 0.6311806654681575 T T T
0.0959671674395892 0.2536564682414522 0.6333884584208249 T T T
0.0987599332891733 0.9214016122156821 0.6312552397528179 T T T
0.3462003870640018 0.5500359939040322 0.6542549999315312 T T T
0.3504005563524260 0.2078025432259309 0.6545872964559933 T T T
0.3529956557812000 0.8739880415644024 0.6517817532990904 T T T
0.6103953801280042 0.4927954238551138 0.6700943396774832 T T T
0.6142732535524758 0.1528438074432614 0.6752269066086924 T T T
0.6110606010354616 0.8212716695303399 0.6697352358209940 T T T
0.8656230286506599 0.1113804617104606 0.6883964352970082 T T T
0.8656660434051204 0.7768709429968297 0.6887710915385767 T T T
0.4070119248341300 0.3371671303589920 0.7066642086868882 T T T
0.3577329223191299 0.3772801849262706 0.7546244745921342 T T T
0.4435570670231712 0.2584572184097951 0.7762003544607552 T T T

COH/Cu(533) $E_{ads} = -3.05$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0470520333995539 0.2941408286210776 0.4659962800910774 T T T
0.0472398688301913 0.6273931435824353 0.4659622911665523 T T T
0.0477373376031689 0.9601504361983045 0.4657658119136713 T T T
0.3038793874111477 0.2463512099916479 0.4868113346005123 T T T
0.3037519986775660 0.5799234395580126 0.4865481037628962 T T T
0.3034018566117198 0.9136076447249893 0.4867889824348500 T T T
0.5585829877402970 0.1999052506057746 0.5065702419442337 T T T

0.5590189844514594	0.5346031365401709	0.5065981529925022	T	T	T
0.5589355611919665	0.8673292181126078	0.5073547591480957	T	T	T
0.8167645022429928	0.1520987602625173	0.5271627039192450	T	T	T
0.8149862596653920	0.4870811910335197	0.5275635914797971	T	T	T
0.8154784097502945	0.8199374018472607	0.5274684694186670	T	T	T
0.0717807453693693	0.1067763039717896	0.5481569280353450	T	T	T
0.0721557751216293	0.4396841524521015	0.5480869381760933	T	T	T
0.0720743473974393	0.7733053749529647	0.5480975082569874	T	T	T
0.3273133171219312	0.0601753563586044	0.5692643756016593	T	T	T
0.3276977895415314	0.3943548990399880	0.5692018490069322	T	T	T
0.3277059132221181	0.7257589017204888	0.5689288056489441	T	T	T
0.5837478202683929	0.0146585578434823	0.5896546395274019	T	T	T
0.5852800698365208	0.3446169248167701	0.5874817995290789	T	T	T
0.5835393493431695	0.6775536815811637	0.5896624963451198	T	T	T
0.8424735832636905	0.6301158728752699	0.6091698547156806	T	T	T
0.8402677874742723	0.2982139875166006	0.6094324782432183	T	T	T
0.8408077590747991	0.9649849712631768	0.6093801333264794	T	T	T
0.0980428583652536	0.5844060555839822	0.6317928133756311	T	T	T
0.0989489897185906	0.2507879815082174	0.6323469142811815	T	T	T
0.0976142165630231	0.9196794629791190	0.6315886655233603	T	T	T
0.3456562965002819	0.5461916456772207	0.6521749933642818	T	T	T
0.3524895048455510	0.2046182595833342	0.6520324911047588	T	T	T
0.3517750903572328	0.8749575842241449	0.6519643705001448	T	T	T
0.6057366640935937	0.4942934092213471	0.6757974620013846	T	T	T
0.6098640063042443	0.1533205886813008	0.6757137022312166	T	T	T
0.6081345597953862	0.8241414277915469	0.6716219969544593	T	T	T
0.8625644454756836	0.4455966858308369	0.6894631422914475	T	T	T
0.8671800009761247	0.1080800117101865	0.6892597813700709	T	T	T
0.8649778152901921	0.7753927432638974	0.6896180551460829	T	T	T
0.4731258351747020	0.4294460816348737	0.7121102888061233	T	T	T
0.4276082869845402	0.4665520482303328	0.7602888106810285	T	T	T
0.3132723625001518	0.5954515388820892	0.7628222310932303	T	T	T

COH/Cu(533) E_{ads} = −3.02 eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H

60 1 1 1

Selective dynamics

Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F

0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0473689787260623	0.2942937378777512	0.4659799008021798	T	T	T
0.0475487898998407	0.6275836324647617	0.4659153692617687	T	T	T
0.0479251254287878	0.9603983552911627	0.4657555082545248	T	T	T
0.3043290509870011	0.2468470345085610	0.4869377201863178	T	T	T
0.3042084260662450	0.5801836000376946	0.4866625062588882	T	T	T
0.3037852678558245	0.9137848813460092	0.4868808203541731	T	T	T
0.5589107001537353	0.2006579764682582	0.5066573571282418	T	T	T
0.5593092839087971	0.5353010361048105	0.5066556563169616	T	T	T
0.5593376448057421	0.8678657023347399	0.5072430642011221	T	T	T
0.8170769940483859	0.1529872383545021	0.5271689159021429	T	T	T
0.8155948613479126	0.4877581467614778	0.5275193806958588	T	T	T
0.8160754358636136	0.8204847796587676	0.5273874367425433	T	T	T
0.0723907911183720	0.1073917901188293	0.5481161013651410	T	T	T
0.0728640186870772	0.4404345052595021	0.5480419603816802	T	T	T
0.0726532965520652	0.7740154412877809	0.5480287737793919	T	T	T
0.3279541587608274	0.0610592882974960	0.5692967962016686	T	T	T
0.3283298422520848	0.3960176016526933	0.5696659864857920	T	T	T
0.3284167479971608	0.7263095177650414	0.5693316294402549	T	T	T
0.5842323989829314	0.0159180666709422	0.5894847822395062	T	T	T
0.5854834646937433	0.3462958148556129	0.5876508912780418	T	T	T
0.5840380347833348	0.6794802668866071	0.5895096520116840	T	T	T
0.8431334205450133	0.6318439967909809	0.6091278408453599	T	T	T
0.8408962985602830	0.3000509447731935	0.6093200372947194	T	T	T
0.8412671434700727	0.9665567952040505	0.6092177331589728	T	T	T
0.0985621156774284	0.5861564071346544	0.6317399658665841	T	T	T
0.0992305552869312	0.2525563763721568	0.6322020807364858	T	T	T
0.0978008758646497	0.9213793507720790	0.6313938100934444	T	T	T
0.3449711455471803	0.5496707792069826	0.6539320030126350	T	T	T
0.3526791071216070	0.2067138503418613	0.6520312501158266	T	T	T
0.3517979891707518	0.8776144012595609	0.6520915850454518	T	T	T
0.6063967906472779	0.4980736232507165	0.6749663374995796	T	T	T
0.6097306434281529	0.1559651320425509	0.6753190271027248	T	T	T
0.6085583555328041	0.8270889210431167	0.6715786720052564	T	T	T
0.8631340207139894	0.4481555486812545	0.6894370235293734	T	T	T
0.8664529755544176	0.1116129224034827	0.6889797630416007	T	T	T
0.8649781936529634	0.7784147476167362	0.6895754262793726	T	T	T
0.4780819203181645	0.4299348386527813	0.7127451047993929	T	T	T
0.4341901243959073	0.4736795308027336	0.7611136587807511	T	T	T
0.5175839548666786	0.3494905321296642	0.7821902579022930	T	T	T

COH/Cu(533) E_{ads} = −2.98 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics

Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0466648528734236	0.2943363114718974	0.4661420744507976	T	T	T
0.0469299485222133	0.6271207484546643	0.4660877449385245	T	T	T
0.0467156745941539	0.9604399955396331	0.4660645150424106	T	T	T
0.3027737663424976	0.2459030708919318	0.4864552825339808	T	T	T
0.3029213811785397	0.5807609096743495	0.4864796944748701	T	T	T
0.3030456129368916	0.9135523908236839	0.4869423105056836	T	T	T
0.5590654327913838	0.1997957023534863	0.5065013764045034	T	T	T
0.5581586434396045	0.5339084347024908	0.5067454843008485	T	T	T
0.5585730160145534	0.8666959879022843	0.5066738337171979	T	T	T
0.8145565959208708	0.1535544121540578	0.5274944944010439	T	T	T
0.8150497417951412	0.4863856661917061	0.5274161033373087	T	T	T
0.8148690796283303	0.8196653652348317	0.5273979460886170	T	T	T
0.0708872366411232	0.1061260107591152	0.5480898216885564	T	T	T
0.0713610371739777	0.4408785399040253	0.5489715472365677	T	T	T
0.0707235830052507	0.7720230396020683	0.5488174373117651	T	T	T
0.3256580864887872	0.0615247067866262	0.5693705421116991	T	T	T
0.3263247080162352	0.3930513711845358	0.5675547660140290	T	T	T
0.3254738325581506	0.7260995691526514	0.5690351787274013	T	T	T
0.5805707950179231	0.0142764795970699	0.5885165030468064	T	T	T
0.5805787468169744	0.3470608970917628	0.5887809419057485	T	T	T
0.5823311769414772	0.6792311059996272	0.5885371220591180	T	T	T
0.8407972823970098	0.6308933715339763	0.6090888324875163	T	T	T
0.8412093369855322	0.2967586894095798	0.6092984857624817	T	T	T
0.8390982402810740	0.9652384654145354	0.6090011973415195	T	T	T
0.0939045307659100	0.5877586476722559	0.6355257478046616	T	T	T
0.0965979437263833	0.2494481565584961	0.6322628645815055	T	T	T
0.0956620032237265	0.9207600960263773	0.6321157312749531	T	T	T
0.3507955980838504	0.5439831779721398	0.6533388764129620	T	T	T
0.3542954641117203	0.1956096268036746	0.6542702136770440	T	T	T
0.3512152253182724	0.8709361086708464	0.6513160140395409	T	T	T
0.6052650769796813	0.4933450972213105	0.6715894233046716	T	T	T
0.6030395549331694	0.1622399333134348	0.6721767375458574	T	T	T
0.6045141054609047	0.8234440508951349	0.6714836081792680	T	T	T

0.8581435126278771 0.4482403074985805 0.6895893726222353 T T T
0.8569792849747300 0.1150890646075529 0.6897472249135417 T T T
0.8490902689510756 0.7897618368490336 0.6897040300226606 T T T
0.2389900790833141 0.4596936684201728 0.6936756859864033 T T T
0.2090444120790722 0.4908033191921883 0.7428472818517976 T T T
0.1050489162723793 0.6385842763854008 0.7486976297746248 T T T

COH/Cu(533) $E_{ads} = -2.96$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0471629370974103 0.2943975046079642 0.4660783072694363 T T T
0.0473683490436708 0.6273618695481711 0.4660720267029307 T T T
0.0476568308839668 0.9600934859511446 0.4661474222553540 T T T
0.3036290111225293 0.2464585678823113 0.4865226080497080 T T T
0.3037501240512196 0.5812396451236546 0.4864713910683848 T T T
0.3040552987603249 0.9139773095381202 0.4869823491779231 T T T
0.5606083135706631 0.1997372515969921 0.5065453495090271 T T T
0.5596256994035695 0.5340700302577113 0.5066282228717954 T T T
0.5598426580759155 0.8668295195152917 0.5068792570382505 T T T
0.8172453423814170 0.1527457286235595 0.5274826971981945 T T T
0.8167316261230653 0.4863031029596624 0.5275184833472740 T T T
0.8163592454508966 0.8199778799539647 0.5275715252294457 T T T
0.0734357515823994 0.1056948488958237 0.5480960961998500 T T T
0.0731127946543258 0.4410252474819563 0.5489027552211605 T T T
0.0732224169995143 0.7711712911853957 0.5490632980852217 T T T
0.3277557207929162 0.0625169333816834 0.5694663442614981 T T T
0.3285786746753219 0.3939814507823405 0.5676279446249921 T T T

0.3282746866548843	0.7264509266922450	0.5691190673833896	T	T	T
0.5825211939607268	0.0156784607805863	0.5887205887753834	T	T	T
0.5846302055425804	0.3468050501545088	0.5884037049337505	T	T	T
0.5847324794781915	0.6800034307096393	0.5886503493602382	T	T	T
0.8423498627302416	0.6321185578220820	0.6091594752044535	T	T	T
0.8445492238683248	0.2966480280557267	0.6092744751986140	T	T	T
0.8427665787067254	0.9646917056251356	0.6092141544120531	T	T	T
0.0959319659266608	0.5860903105432724	0.6354739015149536	T	T	T
0.0995333142726864	0.2485560206291374	0.6322080655674929	T	T	T
0.0999152177074691	0.9191279267874173	0.6322277679150948	T	T	T
0.3580957252894343	0.5414300477396584	0.6531432308353780	T	T	T
0.3549163456658030	0.2017524835820878	0.6543725114782812	T	T	T
0.3552572471137903	0.8723952683610604	0.6515221720563330	T	T	T
0.6096252047758736	0.4948347113785279	0.6717669164334411	T	T	T
0.6083464215395946	0.1615259692307632	0.6720315130821614	T	T	T
0.6076360459056209	0.8271909834788611	0.6718351015744879	T	T	T
0.8614002993711612	0.4497940961360231	0.6896219855187506	T	T	T
0.8606631515349359	0.1176334493563652	0.6895566427002852	T	T	T
0.8556433461621159	0.7881994418200747	0.6903714962406056	T	T	T
0.2369326672314119	0.4780911614931206	0.6932815451108688	T	T	T
0.2067069655834805	0.5031152706840328	0.7429019115537017	T	T	T
0.3049548419990188	0.4548705842095789	0.7612136079241015	T	T	T

COH/Defected-Cu(533) E_{ads} = −2.94 eV
1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H
59 1 1 1
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0464699154157557	0.2937837985058138	0.4661738602707572	T	T	T

0.0470282611415200 0.6261692900408420 0.4662500601189237 T T T
0.0472841278337199 0.9599654535328312 0.4657420455789705 T T T
0.3028308643633864 0.2466662497054841 0.4867907347994276 T T T
0.3036384554415505 0.5790321795144493 0.4863962737706373 T T T
0.3035010488650087 0.9128587245702278 0.4866092030803983 T T T
0.5590917001474125 0.1998699107968420 0.5065479327621816 T T T
0.5589557201755184 0.5335539139401675 0.5068265058458579 T T T
0.5574478318013902 0.8679456870311668 0.5069442271679563 T T T
0.8163252663944576 0.1516082476481699 0.5270548608516634 T T T
0.8145634506830319 0.4881066908726979 0.5272414755024712 T T T
0.8152710042255364 0.8183910861083206 0.5271604518323088 T T T
0.0717431659973684 0.1046547959721948 0.5485356962984653 T T T
0.0712435699233467 0.4364662236727739 0.5492832563608161 T T T
0.0728987343977892 0.7709028930280866 0.5479652904494188 T T T
0.3241175467512321 0.0612247625739570 0.5694861296555729 T T T
0.3277079979926540 0.3910015359813812 0.5686917796612363 T T T
0.3273228490352835 0.7251408215558257 0.5686485612160013 T T T
0.5842805734167911 0.0119376228187775 0.5885154730295383 T T T
0.5848022149460235 0.3442845226899891 0.5882476925730558 T T T
0.5808244336250823 0.6829885892328917 0.5892568719273399 T T T
0.8429236653857117 0.6260934944401484 0.6105918987175585 T T T
0.8379039643665109 0.3049798668502959 0.6074664414084623 T T T
0.8438600073101057 0.9612532758222514 0.6079534240312938 T T T
0.1008929625033872 0.5754294458964395 0.6318579386012146 T T T
0.0910694503422320 0.2558237198306159 0.6381201335424507 T T T
0.1053986142417500 0.8997078373000349 0.6324257571927987 T T T
0.3576780387575056 0.5295176305066320 0.6513622653666928 T T T
0.3557702288750235 0.2029835947642482 0.6516514804057252 T T T
0.3488802363267922 0.8742604327291801 0.6536736576593185 T T T
0.6085353297208300 0.4942633994213139 0.6701086543762642 T T T
0.6126769218105963 0.1589608577056723 0.6716904613040242 T T T
0.6086916609912407 0.8254194457774418 0.6704494677988819 T T T
0.8702927431960461 0.1195111726271350 0.6869979511492801 T T T
0.8628620681831407 0.7864204619752755 0.6879115435068996 T T T
0.0829173282746325 0.0792960125451145 0.6905095164841200 T T T
0.1327858195183822 0.0647892229907328 0.7386214469716634 T T T
0.0862750459961674 0.0138553165399244 0.7610035325030324 T T T

COH/Defected-Cu(533) E_{ads} = −2.87 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
59 1 1 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F

0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0475305732471369	0.2935194943614619	0.4659621001131029	T	T	T
0.0472978269242503	0.6266582790852269	0.4659827222668440	T	T	T
0.0474057887832302	0.9602764624869877	0.4658788651559505	T	T	T
0.3040506892294133	0.2460868750418612	0.4868604339974922	T	T	T
0.3047107655957149	0.5794503250750793	0.4865176595589418	T	T	T
0.3045647096223405	0.9125830183966883	0.4866586769455026	T	T	T
0.5601224471023727	0.1999049931030967	0.5071652084897593	T	T	T
0.5600462672722344	0.5328455482349455	0.5067990589755311	T	T	T
0.5594148936200583	0.8664900893494121	0.5071550130666864	T	T	T
0.8168196416326410	0.1519197997734594	0.5273100253261731	T	T	T
0.8162523941412587	0.4867064173844966	0.5272440868704464	T	T	T
0.8165540411986854	0.8189892807825956	0.5275615667419586	T	T	T
0.0739040837131526	0.1044991047167017	0.5481100768422920	T	T	T
0.0723559676100933	0.4387418682229836	0.5486106932911241	T	T	T
0.0740728099580537	0.7709973102160248	0.5477765700568682	T	T	T
0.3277626926346997	0.0595470141960135	0.5693083176032090	T	T	T
0.3291293262908610	0.3922066667738378	0.5688218874383608	T	T	T
0.3296560795832804	0.7247128021719078	0.5689345784740993	T	T	T
0.5857495853413326	0.0108785333899917	0.5888957772337946	T	T	T
0.5870632360770713	0.3455665293504993	0.5896967708546583	T	T	T
0.5869353599537703	0.6756961612989159	0.5893984343747789	T	T	T
0.8440679234767146	0.6258517499179916	0.6105151086728640	T	T	T
0.8454811261065913	0.2975821096520761	0.6089485429273651	T	T	T
0.8451014438309485	0.9634971742854503	0.6091717651252821	T	T	T
0.1001464546061115	0.5825263644904553	0.6320014623296686	T	T	T
0.0956493046643629	0.2529173915273617	0.6333774516177400	T	T	T
0.1001870997636303	0.9165220960037246	0.6318085606624138	T	T	T
0.3536109011161344	0.5383509423666126	0.6514411934024622	T	T	T
0.3516946169395112	0.2061606737293360	0.6517165137227181	T	T	T
0.3512947776930204	0.8743742162135888	0.6516280977956086	T	T	T
0.6031056236563899	0.5043572376773469	0.6739497646392607	T	T	T
0.6056221720236792	0.1581466877871023	0.6712656983270548	T	T	T
0.6093353046779058	0.8250844547154088	0.6709835626944738	T	T	T
0.8691851757240272	0.1096520875977092	0.6902414203187632	T	T	T
0.8637063838527865	0.7827544561946311	0.6881633965885925	T	T	T
0.7451670468285414	0.3723445994077537	0.7284934178152085	T	T	T
0.7555872419783398	0.4330726656916610	0.7737476210153815	T	T	T
0.8539379289640650	0.3106403165678344	0.7910561720948479	T	T	T

COH/Cu(533) $E_{ads} = -2.82$ eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000

0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0475179590369876 0.2933117442630463 0.4659361758630420 T T T
0.0474938636561704 0.6266136721664047 0.4658921129235001 T T T
0.0470269417783212 0.9603880143945055 0.4659729590330659 T T T
0.3041341147545326 0.2458596143951105 0.4866566878537740 T T T
0.3038667515619556 0.5796515490949113 0.4868404862603414 T T T
0.3040158512762651 0.9124815157238846 0.4867222183166774 T T T
0.5594254138246978 0.1997420165078854 0.5069197543609462 T T T
0.5594883851728438 0.5328736396829896 0.5070568763014770 T T T
0.5597790046730886 0.8659446738119927 0.5069540991633876 T T T
0.8163506360661491 0.1518628004246687 0.5277364008113162 T T T
0.8164519626421980 0.4847610813090438 0.5272742256969662 T T T
0.8163654966585058 0.8194902726546427 0.5272642770178730 T T T
0.0726919946915703 0.1047774984559806 0.5482146035428489 T T T
0.0730606659422557 0.4381572330732872 0.5481589416311269 T T T
0.0728410276668571 0.7718235235744861 0.5483179598947443 T T T
0.3282525706576260 0.0586914060517961 0.5690323589999041 T T T
0.3282029611000235 0.3917405353866394 0.5691914115541661 T T T
0.3277628419390649 0.7257560854752254 0.5693918973590688 T T T
0.5856635044106994 0.0104882141221583 0.5889745624488806 T T T
0.5851132290040498 0.3443019753942385 0.5889445386190317 T T T
0.5855601952294169 0.6772086804017088 0.5890678786389537 T T T
0.8430473837831390 0.6293245708642495 0.6087243656526086 T T T
0.8434785580983102 0.2971107915121536 0.6097951594548904 T T T
0.8434576673613822 0.9599613399496187 0.6100510811196882 T T T
0.0993606714457447 0.5827613415293340 0.6321185096523761 T T T
0.0998218399953719 0.2484131267612076 0.6319868201116859 T T T
0.0988416164461513 0.9159951860791147 0.6327492694607263 T T T
0.3524136609802673 0.5379038428823407 0.6521411155552277 T T T
0.3520761882144849 0.2054039115552093 0.6518985232252861 T T T

0.3520207744921418	0.8712311312709480	0.6521549318926552	T	T	T
0.6064917992139504	0.4931514888486029	0.6715851815567034	T	T	T
0.6064836378554617	0.1591132045480096	0.6715487868302741	T	T	T
0.6036043169122013	0.8285224763976889	0.6710605721958757	T	T	T
0.8660400307421584	0.4358339856001333	0.6920063566841327	T	T	T
0.8601790374674948	0.1146648693205919	0.6896959257388983	T	T	T
0.8653937271633920	0.7839693428230768	0.6928715284724140	T	T	T
0.9229413157347973	0.5610944914105974	0.7393496305067235	T	T	T
0.9930007201174650	0.5057666630115214	0.7835977149604989	T	T	T
0.0168505487773919	0.3654177437708470	0.7954220419259038	T	T	T

COH/Cu(111) $E_{ads} = -3.24$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
3.8289832201000000 6.6319934786000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu C O H
45 1 1 1
Selective dynamics
Direct

0.8888888887999968	0.2222222223999992	0.3170124957488483	F	F	F
0.2222222221000010	0.2222222223999992	0.3170124957488483	F	F	F
0.5555555553999980	0.2222222223999992	0.3170124957488483	F	F	F
0.8888888890000004	0.5555555553000033	0.3170124957488483	F	F	F
0.2222222222999974	0.5555555553000033	0.3170124957488483	F	F	F
0.5555555556000016	0.5555555553000033	0.3170124957488483	F	F	F
0.8888888891999969	0.8888888882000003	0.3170124957488483	F	F	F
0.2222222225000010	0.8888888882000003	0.3170124957488483	F	F	F
0.5555555557999980	0.8888888882000003	0.3170124957488483	F	F	F
0.0000000000000000	0.0000000000000000	0.3975777759823913	F	F	F
0.3333333332999970	0.0000000000000000	0.3975777759823913	F	F	F
0.6666666666000012	0.0000000000000000	0.3975777759823913	F	F	F
0.0000000002103135	0.3333333328999970	0.3975777759823913	F	F	F
0.3333333335000006	0.3333333328999970	0.3975777759823913	F	F	F
0.6666666668999994	0.3333333328999970	0.3975777759823913	F	F	F
0.9999999996666986	0.6666666672999995	0.3975777759823913	F	F	F
0.3333333329999988	0.6666666672999995	0.3975777759823913	F	F	F
0.6666666663000029	0.6666666672999995	0.3975777759823913	F	F	F
0.1111111113999996	0.1111111104999978	0.4771948603999974	F	F	F
0.4444444447999985	0.1111111104999978	0.4771948603999974	F	F	F
0.7777777781000026	0.1111111104999978	0.4771948603999974	F	F	F
0.1111111108999978	0.4444444449000002	0.4771948603999974	F	F	F
0.4444444442000020	0.4444444449000002	0.4771948603999974	F	F	F
0.7777777774999990	0.4444444449000002	0.4771948603999974	F	F	F
0.1111111111000014	0.7777777777999972	0.4771948603999974	F	F	F
0.4444444443999984	0.7777777777999972	0.4771948603999974	F	F	F
0.7777777777000026	0.7777777777999972	0.4771948603999974	F	F	F
0.8911019588025724	0.2228497915564489	0.5574877725384795	T	T	T
0.2222079633069214	0.2234219193231155	0.5566105094767835	T	T	T
0.5556167554244453	0.2223787371653927	0.5569769069154304	T	T	T
0.8906157135053974	0.5550520103614929	0.5565739987979512	T	T	T
0.2221628568679321	0.5550722022059631	0.5565770170902269	T	T	T
0.5568309118814128	0.5547281878279264	0.5568511695130951	T	T	T
0.8909734597644743	0.8866491277414354	0.5573617758755560	T	T	T
0.2228994227009906	0.8889866905676982	0.5568396590071387	T	T	T
0.5566139119242877	0.8891075904084076	0.5568493454628012	T	T	T
0.0012843273656244	0.9993706564225846	0.6373388060365670	T	T	T

0.3353560758929319	0.9984165941837446	0.6371755268903954	T	T	T
0.6695845427840155	0.9989844974568740	0.6371576065364550	T	T	T
0.9962606120823025	0.3331137602981471	0.6406913153414351	T	T	T
0.3447167965673401	0.3290985317182376	0.6394665311581775	T	T	T
0.6692432119552265	0.3321165051355237	0.6371825341653050	T	T	T
0.9988236110481239	0.6689907863049172	0.6404296386772899	T	T	T
0.3355028457211944	0.6677090083693642	0.6370734708671577	T	T	T
0.6644318084480076	0.6683854594240799	0.6371593198376218	T	T	T
0.1231502609875648	0.4356743735161857	0.6876013846455393	T	T	T
0.1192544497635097	0.4395807149607620	0.7399571505450808	T	T	T
0.2538831754340904	0.3990937856363246	0.7534276100793775	T	T	T

COH/Cu(100) $E_{ads} = -3.42$ eV

1.00000000000000

7.6579664403000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.6579664403000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.5000000000000000

Cu C O H

45 1 1 1

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.3173193249345303	F	F	F
0.3333333332999970	0.0000000000000000	0.3173193249345303	F	F	F
0.6666666666000012	0.0000000000000000	0.3173193249345303	F	F	F
0.0000000000000000	0.3333333332999970	0.3173193249345303	F	F	F
0.3333333332999970	0.3333333332999970	0.3173193249345303	F	F	F
0.6666666666000012	0.3333333332999970	0.3173193249345303	F	F	F
0.0000000000000000	0.6666666666000012	0.3173193249345303	F	F	F
0.3333333332999970	0.6666666666000012	0.3173193249345303	F	F	F
0.6666666666000012	0.6666666666000012	0.3173193249345303	F	F	F
0.1666666667000030	0.1666666667000030	0.3854655552433357	F	F	F
0.5000000000000000	0.1666666667000030	0.3854655552433357	F	F	F
0.8333333332999970	0.1666666667000030	0.3854655552433357	F	F	F
0.1666666667000030	0.5000000000000000	0.3854655552433357	F	F	F
0.5000000000000000	0.5000000000000000	0.3854655552433357	F	F	F
0.8333333332999970	0.5000000000000000	0.3854655552433357	F	F	F
0.1666666667000030	0.8333333332999970	0.3854655552433357	F	F	F
0.5000000000000000	0.8333333332999970	0.3854655552433357	F	F	F
0.8333333332999970	0.8333333332999970	0.3854655552433357	F	F	F
0.0000000000000000	0.0000000000000000	0.4552941175999976	F	F	F
0.3333333332999970	0.0000000000000000	0.4552941175999976	F	F	F
0.6666666666000012	0.0000000000000000	0.4552941175999976	F	F	F
0.0000000000000000	0.3333333332999970	0.4552941175999976	F	F	F
0.3333333332999970	0.3333333332999970	0.4552941175999976	F	F	F
0.6666666666000012	0.3333333332999970	0.4552941175999976	F	F	F
0.0000000000000000	0.6666666666000012	0.4552941175999976	F	F	F
0.3333333332999970	0.6666666666000012	0.4552941175999976	F	F	F
0.6666666666000012	0.6666666666000012	0.4552941175999976	F	F	F
0.1660377763967915	0.1679356306541990	0.5251482625716122	T	T	T
0.4985607087184007	0.1679157821371717	0.5255117795343693	T	T	T
0.8347638754962787	0.1676132862858921	0.5256443975840170	T	T	T
0.1664979766488770	0.5000039881823923	0.5210350001806461	T	T	T
0.4990432928101995	0.5002111553089179	0.5248317983471296	T	T	T
0.8348450532679621	0.4995013717481100	0.5251251742286840	T	T	T
0.1667383169135306	0.8315512928559983	0.5252503710886387	T	T	T
0.4990392716942864	0.8321727875435911	0.5254820028553056	T	T	T
0.8354102134386494	0.8312339781501947	0.5258073396205631	T	T	T

0.0002359689989149 0.9992680370830982 0.5930440319549035 T T T
0.3334961496758311 0.0006602648233027 0.5929417437125295 T T T
0.6666663144016383 0.9996934928876584 0.5933318126284348 T T T
0.0000102386525072 0.3335919444273756 0.5961094258670272 T T T
0.3313702448055480 0.3357662246556501 0.5950741767779206 T T T
0.6658561018711850 0.3329118146153007 0.5929427412986428 T T T
0.0025505106626156 0.6631793607910481 0.5964401610328807 T T T
0.3340024528058692 0.6658970458767328 0.5956934360669166 T T T
0.6673083773380455 0.6661703643604895 0.5929484197686108 T T T
0.1680105809662535 0.4992456309167608 0.6332454133948815 T T T
0.1663773309665117 0.5022313976429800 0.6869735179692000 T T T
0.2656339121387035 0.4351385022767857 0.7002128230702027 T T T

COH/Cu(100) $E_{ads} = -2.89$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu C O H
45 1 1 1
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.3173193249345303 F F F
0.3333333332999970 0.0000000000000000 0.3173193249345303 F F F
0.6666666666000012 0.0000000000000000 0.3173193249345303 F F F
0.0000000000000000 0.3333333332999970 0.3173193249345303 F F F
0.3333333332999970 0.3333333332999970 0.3173193249345303 F F F
0.6666666666000012 0.3333333332999970 0.3173193249345303 F F F
0.0000000000000000 0.6666666666000012 0.3173193249345303 F F F
0.3333333332999970 0.6666666666000012 0.3173193249345303 F F F
0.6666666666000012 0.6666666666000012 0.3173193249345303 F F F
0.1666666667000030 0.1666666667000030 0.3854655552433357 F F F
0.5000000000000000 0.1666666667000030 0.3854655552433357 F F F
0.8333333332999970 0.1666666667000030 0.3854655552433357 F F F
0.1666666667000030 0.5000000000000000 0.3854655552433357 F F F
0.5000000000000000 0.5000000000000000 0.3854655552433357 F F F
0.8333333332999970 0.5000000000000000 0.3854655552433357 F F F
0.1666666667000030 0.8333333332999970 0.3854655552433357 F F F
0.5000000000000000 0.8333333332999970 0.3854655552433357 F F F
0.8333333332999970 0.8333333332999970 0.3854655552433357 F F F
0.0000000000000000 0.0000000000000000 0.4552941175999976 F F F
0.3333333332999970 0.0000000000000000 0.4552941175999976 F F F
0.6666666666000012 0.0000000000000000 0.4552941175999976 F F F
0.0000000000000000 0.3333333332999970 0.4552941175999976 F F F
0.3333333332999970 0.3333333332999970 0.4552941175999976 F F F
0.6666666666000012 0.3333333332999970 0.4552941175999976 F F F
0.0000000000000000 0.6666666666000012 0.4552941175999976 F F F
0.3333333332999970 0.6666666666000012 0.4552941175999976 F F F
0.6666666666000012 0.6666666666000012 0.4552941175999976 F F F
0.1674893589573543 0.1683319135006158 0.5252557232582191 T T T
0.4995323754953347 0.1675076967700875 0.5244906253081609 T T T
0.8313239439980435 0.1684321148808010 0.5252904422932474 T T T
0.1673377224314336 0.4979706837234161 0.5250732277108696 T T T
0.4996303166902010 0.4993727763993903 0.5238106982720652 T T T
0.8315369036658922 0.4979605386273107 0.5251123367965320 T T T
0.1662467185115446 0.8329757042535917 0.5250877541744288 T T T
0.4998517069475241 0.8325113625092655 0.5253248270009863 T T T

0.8334614718453892 0.8331347449987874 0.5250544947093090 T T T
0.9995817730712702 0.0002184813726345 0.5931229876506166 T T T
0.3322903219052407 0.9977935399185611 0.5929297494743082 T T T
0.6670545417337763 0.9980900194054314 0.5929917578256791 T T T
0.9982859062226836 0.3334548238785970 0.5933213068370762 T T T
0.3224116447649337 0.3323435689997183 0.5973223709109803 T T T
0.6736904061847966 0.3325581581254156 0.5975171900278795 T T T
0.9995560043621765 0.6662603842697621 0.5930335163940725 T T T
0.3322797764097629 0.6662601284620209 0.5932949814316046 T T T
0.6672971156596077 0.6665721271686706 0.5932697661605886 T T T
0.4970102226445334 0.3576015986956804 0.6481699180031768 T T T
0.4906701955284305 0.3686839293520521 0.6996609934017144 T T T
0.6088648534653700 0.3701443328555740 0.7144633598545482 T T T

COH/Cu(211) $E_{ads} = -3.12$ eV
1.00000000000000
6.2527034153000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.3164343000000009
Cu C O H
45 1 1 1
Selective dynamics
Direct
0.0061862950247047 0.1666666667000030 0.3120745335338029 F F F
0.0061862950247047 0.5000000000000000 0.3120745335338029 F F F
0.0061862950247047 0.8333333332999970 0.3120745335338029 F F F
0.3355456677560653 0.0000000000000000 0.3354619372229379 F F F
0.3355456677560653 0.3333333332999970 0.3354619372229379 F F F
0.3355456677560653 0.6666666666000012 0.3354619372229379 F F F
0.6630854692850079 0.1666666667000030 0.3607350091654666 F F F
0.6630854692850079 0.5000000000000000 0.3607350091654666 F F F
0.6630854692850079 0.8333333332999970 0.3607350091654666 F F F
0.9944057463905267 0.0000000000000000 0.3915351276171819 F F F
0.9944057463905267 0.3333333332999970 0.3915351276171819 F F F
0.9944057463905267 0.6666666666000012 0.3915351276171819 F F F
0.3330656692422309 0.1666666667000030 0.4179888222780335 F F F
0.3330656692422309 0.5000000000000000 0.4179888222780335 F F F
0.3330656692422309 0.8333333332999970 0.4179888222780335 F F F
0.6656564241704075 0.0000000000000000 0.4448469552356400 F F F
0.6656564241704075 0.3333333332999970 0.4448469552356400 F F F
0.6656564241704075 0.6666666666000012 0.4448469552356400 F F F
0.0003515212697778 0.1666666667000030 0.4732099031121066 F F F
0.0003515212697778 0.5000000000000000 0.4732099031121066 F F F
0.0003515212697778 0.8333333332999970 0.4732099031121066 F F F
0.3333333329999988 0.0000000000000000 0.5000000000000000 F F F
0.3333333329999988 0.3333333332999970 0.5000000000000000 F F F
0.3333333329999988 0.6666666666000012 0.5000000000000000 F F F
0.6663151448302216 0.1666666667000030 0.5267900968878934 F F F
0.6663151448302216 0.5000000000000000 0.5267900968878934 F F F
0.6663151448302216 0.8333333332999970 0.5267900968878934 F F F
0.0001428718186811 0.0007517479355891 0.5551102274295029 T T T
0.0020310898855091 0.3336347249625046 0.5549564004145801 T T T
0.0004536918918137 0.6666961616969994 0.5551638268720434 T T T
0.3323869838815570 0.1692021298217158 0.5830262526534652 T T T
0.3317865480793615 0.4985969962284514 0.5827267615212532 T T T
0.3311456295106750 0.8341860774779771 0.5819677405016508 T T T
0.6686324596230068 0.0017450318452305 0.6088687885116018 T T T

0.6707092286731307 0.3328574541991934 0.6072930531185549 T T T
0.6675852457668484 0.6658851747673222 0.6085279137614520 T T T
0.9963764354973522 0.1675388954774713 0.6392286100467914 T T T
0.9935798207522188 0.5013299592957926 0.6393801194580999 T T T
0.9975456900182023 0.8342331941995378 0.6391810087332834 T T T
0.3255379672563163 0.9989448076206821 0.6643552157180608 T T T
0.3152055340473555 0.3357168048636262 0.6679430534412126 T T T
0.3242876372149620 0.6696011223306567 0.6640962264591063 T T T
0.6594044968562582 0.1602395523146341 0.6907560732451931 T T T
0.6531575536218565 0.5034608887920845 0.6897045284924387 T T T
0.6580171957329736 0.8323826542451457 0.6880134947616533 T T T
0.5021325350617594 0.3277612255330435 0.7285256140415178 T T T
0.4394221483201656 0.3301791030317737 0.7770499557021542 T T T
0.3584512885981465 0.4369316396792648 0.7840469786715998 T T T

COH/Cu(211) $E_{ads} = -2.89$ eV
1.00000000000000
6.2527034153000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.3164343000000009
Cu C O H
45 1 1 1
Selective dynamics
Direct
0.0061862950247047 0.1666666667000030 0.3120745335338029 F F F
0.0061862950247047 0.5000000000000000 0.3120745335338029 F F F
0.0061862950247047 0.8333333332999970 0.3120745335338029 F F F
0.3355456677560653 0.0000000000000000 0.3354619372229379 F F F
0.3355456677560653 0.3333333332999970 0.3354619372229379 F F F
0.3355456677560653 0.6666666666000012 0.3354619372229379 F F F
0.6630854692850079 0.1666666667000030 0.3607350091654666 F F F
0.6630854692850079 0.5000000000000000 0.3607350091654666 F F F
0.6630854692850079 0.8333333332999970 0.3607350091654666 F F F
0.9944057463905267 0.0000000000000000 0.3915351276171819 F F F
0.9944057463905267 0.3333333332999970 0.3915351276171819 F F F
0.9944057463905267 0.6666666666000012 0.3915351276171819 F F F
0.3330656692422309 0.1666666667000030 0.4179888222780335 F F F
0.3330656692422309 0.5000000000000000 0.4179888222780335 F F F
0.3330656692422309 0.8333333332999970 0.4179888222780335 F F F
0.6656564241704075 0.0000000000000000 0.4448469552356400 F F F
0.6656564241704075 0.3333333332999970 0.4448469552356400 F F F
0.6656564241704075 0.6666666666000012 0.4448469552356400 F F F
0.0003515212697778 0.1666666667000030 0.4732099031121066 F F F
0.0003515212697778 0.5000000000000000 0.4732099031121066 F F F
0.0003515212697778 0.8333333332999970 0.4732099031121066 F F F
0.3333333329999988 0.0000000000000000 0.5000000000000000 F F F
0.3333333329999988 0.3333333332999970 0.5000000000000000 F F F
0.3333333329999988 0.6666666666000012 0.5000000000000000 F F F
0.6663151448302216 0.1666666667000030 0.5267900968878934 F F F
0.6663151448302216 0.5000000000000000 0.5267900968878934 F F F
0.6663151448302216 0.8333333332999970 0.5267900968878934 F F F
0.9998009099166730 0.9994498387764505 0.5550832448518813 T T T
0.0007854831491556 0.3331564790378098 0.5551723974699182 T T T
0.9996844169437392 0.6666750580459121 0.5551215373701895 T T T
0.3333778451349969 0.1667766747843675 0.5823187659479835 T T T
0.3332241890621359 0.4990796496896684 0.5823269852843738 T T T
0.3321574585568373 0.8328447734012605 0.5819675773003512 T T T

0.6691347461996815	0.0006888357682888	0.6090284229981409	T	T	T
0.6696884800638861	0.3327466848722577	0.6081999149985616	T	T	T
0.6690735169910470	0.6643364419885797	0.6091246165323710	T	T	T
0.9999424022452315	0.1650109564828816	0.6385482318293286	T	T	T
0.9998281862406364	0.5005024962720648	0.6387079115401336	T	T	T
0.9999612773637516	0.8326973060718089	0.6394384477752194	T	T	T
0.3289615486921539	0.9988406312657760	0.6641967125472379	T	T	T
0.3252021946457029	0.3325617701910408	0.6643732470611652	T	T	T
0.3290797314980456	0.6659463743286838	0.6643101316507931	T	T	T
0.6630065393202084	0.1574485607375108	0.6909447732492959	T	T	T
0.6630131072704974	0.5059835051636280	0.6912689550218822	T	T	T
0.6576665327569764	0.8318644872402715	0.6886091535901930	T	T	T
0.6651094269367249	0.3306646308765009	0.7408175103562684	T	T	T
0.6749283513257716	0.3224013475298223	0.7905532890961386	T	T	T
0.6808147464426522	0.4398207560862067	0.8054800809684931	T	T	T

11.5 *CHO Adsorption

CHO/R-Cu_3/Cu(533) $E_{ads} = -2.98$ eV

1.00000000000000					
10.3878408006999994	0.0000000000000000	0.0000000000000000			
4.5828709415000004	6.0103788927000004	0.0000000000000000			
0.0000000000000000	0.0000000000000000	26.5000000000000000			
Cu C O H					
63 1 1 1					
Selective dynamics					
Direct					
0.0032853599999996	0.9972806999999975	0.3042624500000031	F	F	F
0.0028217400000017	0.3308767700000033	0.3042691500000032	F	F	F
0.0026800899999984	0.6645640400000019	0.3042978000000005	F	F	F
0.2572489900000008	0.6186597399999982	0.3218759499999990	F	F	F
0.2571973700000001	0.2857762699999995	0.3217927099999969	F	F	F
0.2571614599999990	0.9524293899999989	0.3219123699999997	F	F	F
0.5099116399999986	0.5747781399999994	0.3415763200000015	F	F	F
0.5095861200000016	0.2417833900000019	0.3416938299999970	F	F	F
0.5096986000000001	0.9088501900000026	0.3416314700000029	F	F	F
0.7627858999999972	0.5310134699999978	0.3609394899999998	F	F	F
0.7629538699999969	0.1970798500000015	0.3608490599999996	F	F	F
0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F
0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0464705242807957	0.2952167498367426	0.4663049638521086	T	T	T
0.0462416245537639	0.6286908707431912	0.4663961872360391	T	T	T
0.0466864103944261	0.9618465178714867	0.4662428306207514	T	T	T
0.3024779291364136	0.2484608047382203	0.4869005509041179	T	T	T
0.3032542553488548	0.5809237014627185	0.4867884684511475	T	T	T

0.3032282581109374 0.9152862481749425 0.4868482156797162 T T T
0.5588209121763910 0.2015316134857207 0.5069952266036712 T T T
0.5592615645177851 0.5349979036580248 0.5064150936619274 T T T
0.5584096084938331 0.8692235644440122 0.5068514362497141 T T T
0.8162094665250574 0.1542558453358157 0.5274762136560723 T T T
0.8153512443525718 0.4883847343215988 0.5276181938828903 T T T
0.8145462655319673 0.8220776928764766 0.5278398801304901 T T T
0.0716408835230453 0.1090897267755745 0.5485728333762822 T T T
0.0703761056374165 0.4431645296745471 0.5487728640571964 T T T
0.0716851693630479 0.7749455528519396 0.5483887158529606 T T T
0.3265522345447339 0.0653922282201938 0.5694452841201438 T T T
0.3276056985226266 0.3938358911946309 0.5689653447769951 T T T
0.3281513052773807 0.7287343341970027 0.5681323415267167 T T T
0.5830493893265356 0.0147445048849764 0.5898464701618102 T T T
0.5858710795899290 0.3469896716615315 0.5884868828652213 T T T
0.5843028964373872 0.6821751988278112 0.5884980319550631 T T T
0.8390198786952050 0.6364752818235794 0.6105606256261120 T T T
0.8411606325989558 0.3010416203554455 0.6099859990300708 T T T
0.8400936780977812 0.9681152336704044 0.6095255718226527 T T T
0.0978849512789524 0.5846467123149113 0.6315705587961488 T T T
0.0967770887066835 0.2558750270527739 0.6328163064522212 T T T
0.0975334488858136 0.9237109610469343 0.6312338005589732 T T T
0.3543095566937338 0.5437342983996249 0.6483805931478885 T T T
0.3513355062105319 0.2087449572864532 0.6549124909261465 T T T
0.3513488555335068 0.8785432803892635 0.6494097972376809 T T T
0.6086338719720354 0.4929375721995033 0.6722756545060362 T T T
0.6085382247738786 0.1603299311372007 0.6730878609188307 T T T
0.6033786777496037 0.8324797173262845 0.6758170711641491 T T T
0.8600042562815103 0.4519296709930383 0.6908897543292913 T T T
0.8655236390763207 0.1131869643078341 0.6914238172298761 T T T
0.8645598557404033 0.7822688979988083 0.6913912549011246 T T T
0.4420588733644336 0.7853332933909684 0.7345654411659875 T T T
0.3778913660846709 0.3908354599951250 0.7299256329386015 T T T
0.1207413242388106 0.7392843953807640 0.7123818025916951 T T T
0.2530934352151296 0.6628388416529766 0.7764698168140238 T T T
0.3227677442827855 0.7517198140210810 0.7854467782141569 T T T
0.1935219710610186 0.6557427958918585 0.8106222700483251 T T T

CHO/R-Cu_3/Cu(533) E_{ads} = −2.43 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
63 1 1 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F
0.2571614599999990 0.9524293899999989 0.3219123699999997 F F F
0.5099116399999986 0.5747781399999994 0.3415763200000015 F F F
0.5095861200000016 0.2417833900000019 0.3416938299999970 F F F
0.5096986000000001 0.9088501900000026 0.3416314700000029 F F F
0.7627858999999972 0.5310134699999978 0.3609394899999998 F F F

0.7629538699999969	0.1970798500000015	0.3608490599999996	F	F	F
0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F
0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0475132255849360	0.2940980208123847	0.4664735839865273	T	T	T
0.0472668397589615	0.6274819968303404	0.4666665373201084	T	T	T
0.0476144835586965	0.9604621414204288	0.4661739978803965	T	T	T
0.3038821856534426	0.2469430641123793	0.4875311482882410	T	T	T
0.3044919347952515	0.5797546944684626	0.4872591256081833	T	T	T
0.3049079701493937	0.9130399414244934	0.4871756309524997	T	T	T
0.5594123095450527	0.2006867145880094	0.5066602557476045	T	T	T
0.5605743563602203	0.5332434093936129	0.5063605081396574	T	T	T
0.5592749319957520	0.8679578818404394	0.5066744388009568	T	T	T
0.8181026285813715	0.1514706567725028	0.5273321990233626	T	T	T
0.8175844380554551	0.4866596954533549	0.5274604809905057	T	T	T
0.8170195752014280	0.8192156710981138	0.5276376160615470	T	T	T
0.0753380864494986	0.1046611058543689	0.5484324274700541	T	T	T
0.0739081589962964	0.4388643681507389	0.5495358688042771	T	T	T
0.0743787313703379	0.7717398151424746	0.5487348777360950	T	T	T
0.3281049761428250	0.0602517054027913	0.5705981333565973	T	T	T
0.3278478415084223	0.3940489975557355	0.5703252028674584	T	T	T
0.3310136496498544	0.7249604762104411	0.5696271280313496	T	T	T
0.5859455119909498	0.0128192489450001	0.5884029884394550	T	T	T
0.5865350380765477	0.3435636385566170	0.5874941897917623	T	T	T
0.5861274403300953	0.6807570909715253	0.5876697941363958	T	T	T
0.8462288561805025	0.6296626495314328	0.6104933160840673	T	T	T
0.8479864188792234	0.2950850206087949	0.6087516903764012	T	T	T
0.8451893245515052	0.9624663149765524	0.6097395869463824	T	T	T
0.0997456570660233	0.5846133870627597	0.6349801526079233	T	T	T
0.0996682911499818	0.2513777805291255	0.6351609048061277	T	T	T
0.1003317363685952	0.9177976333505597	0.6309412903562190	T	T	T
0.3552894284926680	0.5367076796008732	0.6531549632199614	T	T	T
0.3543415287486908	0.2059761474224189	0.6530992367710553	T	T	T
0.3553293286253094	0.8727676623431222	0.6544536725814041	T	T	T
0.6140768947509230	0.4875180748297723	0.6655496576427140	T	T	T
0.6110704237445646	0.1554894366237960	0.6710935743328577	T	T	T
0.6092468320345006	0.8325745147798500	0.6707914987864498	T	T	T
0.8580470842769117	0.4535314673985553	0.6924231441429427	T	T	T
0.8705151431129394	0.1074760147010281	0.6924401483891387	T	T	T
0.8621506421493947	0.7834968011153407	0.6927159170393296	T	T	T
0.5782277603069730	0.6759752545278630	0.7432976097443813	T	T	T
0.5969868077815335	0.3490008509428861	0.7447759498176652	T	T	T
0.1793122045973377	0.8447248247487593	0.7162939807283593	T	T	T
0.4451636501847602	0.6252270950940257	0.7889164765143732	T	T	T
0.2934144365004840	0.7460834995745884	0.7808503710683823	T	T	T
0.4748235351824164	0.6010694268929129	0.8300757973068187	T	T	T

CHO/Cu_3/Cu(533) E_{ads} = −2.06 eV

1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
63 1 1 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F
0.2571614599999990 0.9524293899999989 0.3219123699999997 F F F
0.5099116399999986 0.5747781399999994 0.3415763200000015 F F F
0.5095861200000016 0.2417833900000019 0.3416938299999970 F F F
0.5096986000000001 0.9088501900000026 0.3416314700000029 F F F
0.7627858999999972 0.5310134699999978 0.3609394899999998 F F F
0.7629538699999969 0.1970798500000015 0.3608490599999996 F F F
0.7629705100000024 0.8638077299999978 0.3608832600000014 F F F
0.0188077500000006 0.4844866199999984 0.3845455499999986 F F F
0.0188649600000019 0.1508076399999965 0.3844206699999972 F F F
0.0189457299999987 0.8174492599999965 0.3845321800000008 F F F
0.2777182000000025 0.4350678200000004 0.4051130599999979 F F F
0.2779364200000032 0.1018241299999971 0.4049400600000013 F F F
0.2778532499999997 0.7683188099999967 0.4050370400000034 F F F
0.5346647900000008 0.3873898000000011 0.4243529600000002 F F F
0.5347255300000029 0.0542446099999978 0.4245416400000011 F F F
0.5343893300000033 0.7214487199999979 0.4243017399999971 F F F
0.7896143700000025 0.3418778500000030 0.4451831499999983 F F F
0.7893677400000030 0.0085227100000012 0.4452920299999974 F F F
0.7895473399999986 0.6754118300000016 0.4453449800000016 F F F
0.0463735579346221 0.2933706764809401 0.4664796767876283 T T T
0.0460060187668674 0.6281533108578614 0.4666429113436266 T T T
0.0459646479187938 0.9607965110456789 0.4663232333782759 T T T
0.3024722278921104 0.2466267037837326 0.4867635414931897 T T T
0.3026428446630263 0.5799367988486068 0.4872621068334624 T T T
0.3022988907714250 0.9131475131337652 0.4869627753803130 T T T
0.5581432341872627 0.2001155155250203 0.5065859285895584 T T T
0.5584122109908094 0.5333867074837499 0.5062480419529649 T T T
0.5587016494458013 0.8657986801012356 0.5065211008138775 T T T
0.8153882277803604 0.1523579084312487 0.5278419387612487 T T T
0.8151828533169692 0.4851331369928786 0.5273789188466793 T T T
0.8147964009015425 0.8202566607481003 0.5275254045128150 T T T
0.0704790251498082 0.1046763496898251 0.5491575939620077 T T T
0.0704504111451030 0.4396946535768080 0.5485313264214611 T T T
0.0711127124661530 0.7735781797082666 0.5492772159010570 T T T
0.3263145911389813 0.0591993955997978 0.5684399837497907 T T T
0.3261062849100327 0.3922739042809269 0.5692417434421557 T T T
0.3260771858092326 0.7255643343394169 0.5694229581166326 T T T
0.5830546862093371 0.0105750682734254 0.5881187513601205 T T T
0.5837172606618921 0.3448555819297283 0.5880030570800159 T T T
0.5841042810997124 0.6760943399971211 0.5881698799895503 T T T
0.8398210291879593 0.6318988750105419 0.6093692126044559 T T T
0.8418755169564491 0.2968134298743763 0.6109080373076168 T T T
0.8426106397901094 0.9611501428361109 0.6106072696186260 T T T
0.0951390752481487 0.5846412499966718 0.6325420465257849 T T T
0.0968026328919365 0.2507077967061875 0.6316872444993322 T T T

0.0962867003616807 0.9169351013173639 0.6358371355465806 T T T
0.3481444415673636 0.5355852536763521 0.6516439262460523 T T T
0.3481511064245737 0.2071939569106931 0.6516951627594807 T T T
0.3464541082251387 0.8793339154616504 0.6501619845583306 T T T
0.6046413404538242 0.4938945293855497 0.6697739466550274 T T T
0.6049472797930520 0.1507499942473487 0.6690674362614644 T T T
0.5986753356160222 0.8301083296841369 0.6704923097606752 T T T
0.8711029605312248 0.4458533047328999 0.6917685409748984 T T T
0.8573177850152476 0.1152613111613832 0.6919824819686156 T T T
0.8593208322642027 0.7801709901574156 0.6940684025846835 T T T
0.6273073543885985 0.6223016567035415 0.7516053869601862 T T T
0.6096322960047189 0.3109502084537397 0.7455939333717225 T T T
0.3704416355714812 0.6974395091201799 0.7272739903064007 T T T
0.8983941554222454 0.5959779341314189 0.7542651155847935 T T T
0.7945573701349318 0.6253676189208335 0.7858389496815334 T T T
0.0203594672486602 0.5203944501547682 0.7709565719468614 T T T

CHO/Cu_3/Cu(533) $E_{ads} = -1.99$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
63 1 1 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F
0.2571614599999990 0.9524293899999989 0.3219123699999997 F F F
0.5099116399999986 0.5747781399999994 0.3415763200000015 F F F
0.5095861200000016 0.2417833900000019 0.3416938299999970 F F F
0.5096986000000001 0.9088501900000026 0.3416314700000029 F F F
0.7627858999999972 0.5310134699999978 0.3609394899999998 F F F
0.7629538699999969 0.1970798500000015 0.3608490599999996 F F F
0.7629705100000024 0.8638077299999978 0.3608832600000014 F F F
0.0188077500000006 0.4844866199999984 0.3845455499999986 F F F
0.0188649600000019 0.1508076399999965 0.3844206699999972 F F F
0.0189457299999987 0.8174492599999965 0.3845321800000008 F F F
0.2777182000000025 0.4350678200000004 0.4051130599999979 F F F
0.2779364200000032 0.1018241299999971 0.4049400600000013 F F F
0.2778532499999997 0.7683188099999967 0.4050370400000034 F F F
0.5346647900000008 0.3873898000000011 0.4243529600000002 F F F
0.5347255300000029 0.0542446099999978 0.4245416400000011 F F F
0.5343893300000033 0.7214487199999979 0.4243017399999971 F F F
0.7896143700000025 0.3418778500000030 0.4451831499999983 F F F
0.7893677400000030 0.0085227100000012 0.4452920299999974 F F F
0.7895473399999986 0.6754118300000016 0.4453449800000016 F F F
0.0468058080610945 0.2945770756191308 0.4663051221972125 T T T
0.0463779098231498 0.6288003656154615 0.4666762633361543 T T T
0.0467980945724591 0.9613096511307901 0.4664937053020992 T T T
0.3033021739980128 0.2475574483708911 0.4871175103528529 T T T
0.3028988359738989 0.5814329133697314 0.4871286110477655 T T T
0.3035065000162618 0.9145141750689376 0.4869847454201022 T T T
0.5583147954492134 0.2020385458655909 0.5069116727106078 T T T

0.5591301873121708	0.5348267747718154	0.5063401620634522	T	T	T
0.5589130198971333	0.8684525940378549	0.5064819077589746	T	T	T
0.8159567108553532	0.1535183003668266	0.5274865682676690	T	T	T
0.8161636439308211	0.4873022978013140	0.5273875407452664	T	T	T
0.8152338497692710	0.8218472193769628	0.5277568635042584	T	T	T
0.0724507581225780	0.1067720461629094	0.5488607754634458	T	T	T
0.0718447817836889	0.4410887091716091	0.5486635395936190	T	T	T
0.0718296936097289	0.7749373364720853	0.5495137341815521	T	T	T
0.3276845540254314	0.0613295874336899	0.5692770707110384	T	T	T
0.3257406876044229	0.3961907584311888	0.5695068849734852	T	T	T
0.3278057874989315	0.7281935055578188	0.5690829665512922	T	T	T
0.5833136713909965	0.0152484251649980	0.5887348966323174	T	T	T
0.5846054178202209	0.3480254486175554	0.5882415866504189	T	T	T
0.5850307679910145	0.6804983351129437	0.5878788468384499	T	T	T
0.8423486361260757	0.6335938721777978	0.6096206764967746	T	T	T
0.8434896161517003	0.2977194075505523	0.6094527848623343	T	T	T
0.8423252213845274	0.9657946412924474	0.6104258776766898	T	T	T
0.0944378521076956	0.5888216766612970	0.6343918906801278	T	T	T
0.0978691897335366	0.2536525665057781	0.6324346102978708	T	T	T
0.0986861099483463	0.9196761849999220	0.6345285844098072	T	T	T
0.3499162996431480	0.5393759334124013	0.6508629834109669	T	T	T
0.3498937078768094	0.2102442347529418	0.6521061936579216	T	T	T
0.3506376042750290	0.8802782481494233	0.6512238863287010	T	T	T
0.6077174567441119	0.4966492744119222	0.6703701803413367	T	T	T
0.6035068139647350	0.1635801739436502	0.6713989281097454	T	T	T
0.6036891224914029	0.8349785794278546	0.6710412535869423	T	T	T
0.8646395790626258	0.4496156252751362	0.6898706195767872	T	T	T
0.8602211658152257	0.1160298996992566	0.6913445402070337	T	T	T
0.8537058084343911	0.7898600368448783	0.6926622750068248	T	T	T
0.6355006725635945	0.6560992621477482	0.7488751012691068	T	T	T
0.6221929315896659	0.3090493459403021	0.7507771768873681	T	T	T
0.3733794931890273	0.6899527230672504	0.7267827828500728	T	T	T
0.6137103772028709	0.4223244189669586	0.8164767867139986	T	T	T
0.6310601148409560	0.5723708721886354	0.8209125885563680	T	T	T
0.5983615334672550	0.3644723483529262	0.8533600176917560	T	T	T

CHO/Defected-Cu(533) E_{ads} = −1.97 eV
1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H
59 1 1 1
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F

0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0467427012786530	0.2935179114195847	0.4660099211283040	T	T	T
0.0468059016319486	0.6267078183070538	0.4658659079160543	T	T	T
0.0462976794322714	0.9608006872199368	0.4659342261341664	T	T	T
0.3035386966868572	0.2460091110042484	0.4866040264415190	T	T	T
0.3033438394823378	0.5795518667960522	0.4865402948791058	T	T	T
0.3030199701773242	0.9130058440156787	0.4866272534052385	T	T	T
0.5587505275746452	0.2002476659548620	0.5073891114564049	T	T	T
0.5589946858021051	0.5322989746802165	0.5066252218713458	T	T	T
0.5585543435371889	0.8666153783658714	0.5067029603417978	T	T	T
0.8148625398340243	0.1510372627437420	0.5282781753202102	T	T	T
0.8152072844941785	0.4844040708340742	0.5272955196251417	T	T	T
0.8149883920746035	0.8198863984202589	0.5272994720225768	T	T	T
0.0711081445543229	0.1052599623276080	0.5484116091819899	T	T	T
0.0715546578551312	0.4387284165115446	0.5482998202352078	T	T	T
0.0711458432046612	0.7724412403381322	0.5479774667351620	T	T	T
0.3263703858888221	0.0598417984474153	0.5688581816053713	T	T	T
0.3265608877854547	0.3938273192630177	0.5688624514134233	T	T	T
0.3271299940141787	0.7253993037469613	0.5688672268594317	T	T	T
0.5829834011051176	0.0116956081759767	0.5891728792251385	T	T	T
0.5844039947499979	0.3475282457750595	0.5898174802149825	T	T	T
0.5842595646369091	0.6769804583406156	0.5882087287989961	T	T	T
0.8402490784330183	0.6270137893347325	0.6088041830989894	T	T	T
0.8431037684558547	0.2959330995392691	0.6103484746127421	T	T	T
0.8419219980118626	0.9563922548221129	0.6108030049158302	T	T	T
0.0958491705209283	0.5844956120936331	0.6322987160125706	T	T	T
0.0930668497776423	0.2539177549410425	0.6323773797586796	T	T	T
0.0970199559376539	0.9163290860778588	0.6320224762356403	T	T	T
0.3525186451954951	0.5396878619257279	0.6516532007260949	T	T	T
0.3466371496101743	0.2120409425642507	0.6513450270915015	T	T	T
0.3456800860788718	0.8759162125527169	0.6510436955079086	T	T	T
0.6171382727212134	0.4961813015547705	0.6745030984257951	T	T	T
0.6039537161045132	0.1633373372602236	0.6710982769645426	T	T	T
0.5923260371814081	0.8365174284382704	0.6705306728449401	T	T	T
0.8602593300516830	0.1038712670500246	0.6887723259983574	T	T	T
0.8593974006191090	0.7630349205576792	0.6909928745131140	T	T	T
0.6800169333274084	0.6182004230495579	0.7305646194674935	T	T	T
0.8003802837984253	0.6156528225909170	0.7408674924255649	T	T	T
0.6154263036444618	0.6193795226276748	0.7643865735638258	T	T	T

CHO/Cu_3/Cu(533) $E_{ads} = -1.95$ eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H

63 1 1 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F
0.2571614599999990 0.9524293899999989 0.3219123699999997 F F F
0.5099116399999986 0.5747781399999994 0.3415763200000015 F F F
0.5095861200000016 0.2417833900000019 0.3416938299999970 F F F
0.5096986000000001 0.9088501900000026 0.3416314700000029 F F F
0.7627858999999972 0.5310134699999978 0.3609394899999998 F F F
0.7629538699999969 0.1970798500000015 0.3608490599999996 F F F
0.7629705100000024 0.8638077299999978 0.3608832600000014 F F F
0.0188077500000006 0.4844866199999984 0.3845455499999986 F F F
0.0188649600000019 0.1508076399999965 0.3844206699999972 F F F
0.0189457299999987 0.8174492599999965 0.3845321800000008 F F F
0.2777182000000025 0.4350678200000004 0.4051130599999979 F F F
0.2779364200000032 0.1018241299999971 0.4049400600000013 F F F
0.2778532499999997 0.7683188099999967 0.4050370400000034 F F F
0.5346647900000008 0.3873898000000011 0.4243529600000002 F F F
0.5347255300000029 0.0542446099999978 0.4245416400000011 F F F
0.5343893300000033 0.7214487199999979 0.4243017399999971 F F F
0.7896143700000025 0.3418778500000030 0.4451831499999983 F F F
0.7893677400000030 0.0085227100000012 0.4452920299999974 F F F
0.7895473399999986 0.6754118300000016 0.4453449800000016 F F F
0.0469337414372575 0.2935700274152566 0.4663346640520487 T T T
0.0458353446138062 0.6286808699490933 0.4664797702872931 T T T
0.0461854021930606 0.9607201712678375 0.4662248124860895 T T T
0.3027337620197770 0.2476618617364323 0.4867913165195219 T T T
0.3027796822301951 0.5798782105092926 0.4873730098471825 T T T
0.3029928307443726 0.9124754150950949 0.4867653735303463 T T T
0.5578948924861251 0.2001422035029208 0.5066490255582821 T T T
0.5588610945028307 0.5330813494527931 0.5061257287759986 T T T
0.5594244863337039 0.8653214184010167 0.5062679955519371 T T T
0.8161320875582589 0.1512033718280179 0.5277496880743300 T T T
0.8165950699873221 0.4854569908402837 0.5274377073733447 T T T
0.8149740524292710 0.8200775417072279 0.5278042937901120 T T T
0.0721753896819095 0.1036681397298338 0.5484882445657675 T T T
0.0708981920371130 0.4412853103380883 0.5483510850942821 T T T
0.0712945872579240 0.7736613743238223 0.5492389429838411 T T T
0.3274973159969221 0.0598731839336395 0.5676107261443804 T T T
0.3262761024242522 0.3937548176149122 0.5703503006019233 T T T
0.3264944662804083 0.7244439266217455 0.5696222831210846 T T T
0.5833977662415180 0.0087766027848488 0.5879993655946549 T T T
0.5837806414715487 0.3441627155997722 0.5872858760360060 T T T
0.5856206983877073 0.6761032593090732 0.5876376711556262 T T T
0.8409562212074206 0.6325203589144337 0.6111722415797942 T T T
0.8435523266581839 0.2961575358886250 0.6096923283329971 T T T
0.8439872499662116 0.9602560974732270 0.6110940756526020 T T T
0.0966583159383205 0.5849734167069016 0.6334281155333770 T T T
0.0996716261206032 0.2506377380918394 0.6300730754648995 T T T
0.0957026824475946 0.9196941097276650 0.6357131831260787 T T T
0.3475820016273019 0.5406239307564675 0.6551992449326676 T T T
0.3493064697344508 0.2073620680346835 0.6521894309476579 T T T
0.3476331182664225 0.8812643659176089 0.6484499637167431 T T T
0.6041883712013885 0.4923036385737021 0.6671634570231006 T T T

0.6058127260878337	0.1485754680679179	0.6677832379450521	T	T	T
0.6018460474914278	0.8257856752659904	0.6721505519480218	T	T	T
0.8845576891229570	0.4267139556639137	0.6908890939145778	T	T	T
0.8528247277363690	0.1236056017321872	0.6923053829095807	T	T	T
0.8633696269876694	0.7870953281183617	0.6946338241691450	T	T	T
0.6720619767185667	0.5683825142159620	0.7487708630248591	T	T	T
0.5913701107603657	0.3225740714947136	0.7435956825927974	T	T	T
0.3902427855241939	0.7197851056412148	0.7287781468185628	T	T	T
0.8832181480620918	0.5104107991514653	0.7659972949490523	T	T	T
0.9097345083989339	0.6531606796540359	0.7654536527583744	T	T	T
0.9535566107484570	0.3774200233960556	0.7951728438953793	T	T	T

CHO/Defected-Cu(533) $E_{ads} = -1.94$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
59 1 1 1
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0474386501093136	0.2939435521037979	0.4659679832435799	T	T	T
0.0469410742391716	0.6270163142358882	0.4658165353253167	T	T	T
0.0472059631487056	0.9606511890873435	0.4658988859802662	T	T	T
0.3041113625183769	0.2464770950369441	0.4867895591195577	T	T	T
0.3045466027527226	0.5794733261173377	0.4864746129108397	T	T	T
0.3042427575985229	0.9127707407712080	0.4866374507997833	T	T	T
0.5601871637597782	0.1998566140881621	0.5070753444362666	T	T	T
0.5602808522529656	0.5325211543553934	0.5067014208694545	T	T	T
0.5596833210027157	0.8665153858890875	0.5068325816572283	T	T	T
0.8170086950836293	0.1516648355329124	0.5274878093333868	T	T	T
0.8167985075767206	0.4853579518152884	0.5274796199486005	T	T	T
0.8168063171407312	0.8197941875078314	0.5279756531299498	T	T	T

0.0730525668083928	0.1056632175828511	0.5482311285640620	T	T	T
0.0727944954579485	0.4389394064772389	0.5485509131077251	T	T	T
0.0735390869780730	0.7714255135998371	0.5477301484605377	T	T	T
0.3283245663874013	0.0591773362067229	0.5690234559299512	T	T	T
0.3291322336940965	0.3921673800095107	0.5688848959569270	T	T	T
0.3295039824092711	0.7246234210051696	0.5688691310270499	T	T	T
0.5861733406177265	0.0101481185744063	0.5886794779828435	T	T	T
0.5868468823831563	0.3452904855495333	0.5894468756809488	T	T	T
0.5869258431923186	0.6752464687139934	0.5888248141499233	T	T	T
0.8436956841984653	0.6247052582972117	0.6101352323910518	T	T	T
0.8442314525005870	0.2971025961413218	0.6105180681776048	T	T	T
0.8455710476797833	0.9640731909621394	0.6104770981509304	T	T	T
0.0996164095251757	0.5821527264174549	0.6320653405840702	T	T	T
0.0960372273451640	0.2528372115289272	0.6329243556495499	T	T	T
0.1007271073796971	0.9161273616193313	0.6314296064320502	T	T	T
0.3521021803790916	0.5376406029568486	0.6514804952903788	T	T	T
0.3525601513838694	0.2050661807742316	0.6517074439849253	T	T	T
0.3505277527512405	0.8751150477985661	0.6511207972024948	T	T	T
0.6030247157549837	0.4989546138621748	0.6725829846525713	T	T	T
0.6076950809586705	0.1562860559362207	0.6708685202593685	T	T	T
0.6090128922070832	0.8226243607705896	0.6705563977909534	T	T	T
0.8753977630506071	0.0993779132977934	0.6911898285506339	T	T	T
0.8622114618076395	0.7764611159660006	0.6882731703906728	T	T	T
0.6640192013546837	0.4645924056376742	0.7424217687257340	T	T	T
0.7985527742418768	0.2900711867844166	0.7547648244341403	T	T	T
0.5891073436092853	0.5801130999241195	0.7740061839367911	T	T	T

CHO/Defected-Cu(533) $E_{ads} = -1.85$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
59 1 1 1
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F

0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0469215088478023 0.2941350605949040 0.4661223777363901 T T T
0.0469188054597751 0.6272325576243460 0.4658201146668262 T T T
0.0468457690949649 0.9608487337694527 0.4659143470837037 T T T
0.3033753109562625 0.2469253612434059 0.4867490452377581 T T T
0.3038252550154965 0.5797737042508757 0.4865535457351911 T T T
0.3031600074979437 0.9137348267582084 0.4866481552257298 T T T
0.5588459537258288 0.2007592987137699 0.5066366902674133 T T T
0.5592921037229885 0.5339598208798648 0.5068670405806870 T T T
0.5587797443448821 0.8668755645382689 0.5071075340755087 T T T
0.8156108229322498 0.1528572813599709 0.5274160814564581 T T T
0.8154565956080830 0.4870337637007793 0.5274803702297177 T T T
0.8156585965004979 0.8199516586018163 0.5274976495722896 T T T
0.0723874848259101 0.1056942408795720 0.5483894316325930 T T T
0.0713581867757540 0.4400844699164992 0.5484863205126231 T T T
0.0726494594722027 0.7722785869046476 0.5479006320448363 T T T
0.3265617391000362 0.0606490152847456 0.5690425888449440 T T T
0.3270760547830065 0.3938492127200064 0.5689550818202207 T T T
0.3273937447468924 0.7268359133762132 0.5689971478487692 T T T
0.5839746916729425 0.0131564295776059 0.5884205751750073 T T T
0.5842858015718306 0.3464408401777774 0.5888259548642836 T T T
0.5854149881496298 0.6772764181981330 0.5895746188816560 T T T
0.8421571225935551 0.6273436963262071 0.6104324718472895 T T T
0.8433948112606515 0.2993847083324468 0.6091864367056701 T T T
0.8438069342278283 0.9635620996343519 0.6093231294983781 T T T
0.0975295521333521 0.5838906135299311 0.6321986580945733 T T T
0.0954728067755894 0.2524993615366569 0.6328677146733312 T T T
0.0969432433128503 0.9191415500467954 0.6327782335613819 T T T
0.3508855631435779 0.5406540582656376 0.6514823846870215 T T T
0.3492936879226960 0.2083729396253418 0.6517525693933024 T T T
0.3516852771240124 0.8724704957464269 0.6517793007626125 T T T
0.6078470366865503 0.4948525194108555 0.6730096898528544 T T T
0.6034647139128211 0.1609129383517640 0.6709275822120802 T T T
0.6048403152775563 0.8308220256761913 0.6703247946511155 T T T
0.8554767804625740 0.1253385026554454 0.6895576950877569 T T T
0.8607075501470263 0.7835182404776546 0.6884898978579628 T T T
0.7610066532176774 0.4037039905013273 0.7351742144849283 T T T
0.7199226950821185 0.3960206133303998 0.7775637473656403 T T T
0.8336055479158091 0.4690522815450677 0.7282550220167892 T T T

CHO/Defected-Cu(533) E_{ads} = −1.83 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
59 1 1 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F

0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0471568776316115	0.2938757182096735	0.4659710680304048	T	T	T
0.0468316911825495	0.6272198614103535	0.4658610994839532	T	T	T
0.0469356630524185	0.9607279025200721	0.4658912872396381	T	T	T
0.3037729723713865	0.2465518142448361	0.4867095930764854	T	T	T
0.3042396666442373	0.5792566901521149	0.4864797957472276	T	T	T
0.3035967663098739	0.9132146305502288	0.4865516476801345	T	T	T
0.5595192170452874	0.1999711457664157	0.5071072013843282	T	T	T
0.5596444203795302	0.5332121146837505	0.5068658012251462	T	T	T
0.5589963247155927	0.8670042624981826	0.5069523989763990	T	T	T
0.8159422839728497	0.1527561308283596	0.5275216551992773	T	T	T
0.8159891276808889	0.4862015723709626	0.5275270194441389	T	T	T
0.8154596424757640	0.8201462910507409	0.5275131157332139	T	T	T
0.0723334656066145	0.1061240134147373	0.5483155229471528	T	T	T
0.0721640352800986	0.4391451680823211	0.5483791510182778	T	T	T
0.0731111096321277	0.7718577326906827	0.5477998740123876	T	T	T
0.3273011465174366	0.0600354440176965	0.5690739593305529	T	T	T
0.3284404668048084	0.3923423583303738	0.5689026049191492	T	T	T
0.3283911353265217	0.7255465501680233	0.5687374078772581	T	T	T
0.5848930831518636	0.0101084627220616	0.5894304876125347	T	T	T
0.5850889595374137	0.3465906091816232	0.5893143961433923	T	T	T
0.5858331452732924	0.6776960630479066	0.5888650806193638	T	T	T
0.8431770925223163	0.6268487764548127	0.6100734510669336	T	T	T
0.8433858365965371	0.2992990317956959	0.6099812668896734	T	T	T
0.8437860613802923	0.9627765650799830	0.6088742367541884	T	T	T
0.0989185574338608	0.5823521716625532	0.6319940866266510	T	T	T
0.0948155514571961	0.2537123488616482	0.6333157484890110	T	T	T
0.0991442007612806	0.9174315257983743	0.6319173181564147	T	T	T
0.3522141874690981	0.5385827755234958	0.6513842436146290	T	T	T
0.3516830638522273	0.2060159962849934	0.6515133529589288	T	T	T
0.3498193235393547	0.8744185417325798	0.6508903709383969	T	T	T
0.6072621124962387	0.4967960805900981	0.6728278507990829	T	T	T
0.6062606324899379	0.1602845386802650	0.6714730256547267	T	T	T
0.6074553547831707	0.8215258988325090	0.6728397024066538	T	T	T
0.8619528814020910	0.1121605086522119	0.6882249165633445	T	T	T
0.8616083713632927	0.7828367446104851	0.6881735191018181	T	T	T
0.6815876479511146	0.5964005719757469	0.7322552544482568	T	T	T
0.6062326731035081	0.6600082900687007	0.7717602820531426	T	T	T
0.8186522784021018	0.4810075180519378	0.7323711697500647	T	T	T

CHO/Defected-Cu(533) $E_{ads} = -1.83$ eV

1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
59 1 1 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0467191886187166 0.2944789455105834 0.4660138676054189 T T T
0.0462460552631185 0.6273331558628570 0.4658335150383479 T T T
0.0469796569473715 0.9609389467022353 0.4658238280811631 T T T
0.3031119507984812 0.2472802470019957 0.4868799529406687 T T T
0.3039131588064876 0.5794686984158659 0.4862839180096188 T T T
0.3036606008849390 0.9133501634416135 0.4865750401411830 T T T
0.5591130613280484 0.2000434707160466 0.5067213301401807 T T T
0.5596226852532951 0.5337162633569719 0.5066139151644720 T T T
0.5587045595312787 0.8674439146226547 0.5075585117730412 T T T
0.8164393236202798 0.1524042799093834 0.5274813892894699 T T T
0.8152333152060933 0.4865865140237275 0.5277477048939687 T T T
0.8150384587261428 0.8206884120402762 0.5280484919450359 T T T
0.0716237605531305 0.1073556293710780 0.5480803676347392 T T T
0.0706648944022916 0.4405762130701447 0.5486295207431411 T T T
0.0721843416815133 0.7720264186281156 0.5473945575176771 T T T
0.3264718074170503 0.0608241322044023 0.5691777614239655 T T T
0.3272373504682733 0.3933726958757759 0.5689923619433728 T T T
0.3284193505500852 0.7256052038661878 0.5683062898886746 T T T
0.5842018092399073 0.0152449342203269 0.5897878053362433 T T T
0.5855662153793944 0.3442683521729819 0.5881217861261305 T T T
0.5853916103945807 0.6759772246424021 0.5896099943193533 T T T
0.8409458320312808 0.6269452087414535 0.6103963101037309 T T T
0.8420922674824425 0.2983664525299190 0.6113331998741742 T T T
0.8426320292627523 0.9663726753367996 0.6102889323831846 T T T
0.0964477600997995 0.5848103144970693 0.6321881947962069 T T T
0.0938144197118689 0.2541551830036468 0.6333595737795221 T T T

0.0999243463665067	0.9172691535553597	0.6301988836645407	T	T	T
0.3472553675906198	0.5425682235166605	0.6506388086872406	T	T	T
0.3494564096406378	0.2081686413361012	0.6520154491374512	T	T	T
0.3496008986915058	0.8755526871130641	0.6515205724973825	T	T	T
0.6003620858509890	0.4967249315733966	0.6717416311180244	T	T	T
0.6014990827537261	0.1696583129122402	0.6748607217338716	T	T	T
0.6039684245780634	0.8285725489591158	0.6704462546621883	T	T	T
0.8887253898997471	0.0890422675307647	0.6913236054395355	T	T	T
0.8580922735555987	0.7776871557715879	0.6878413766056326	T	T	T
0.6147764151566051	0.3400635096913689	0.7357260437445632	T	T	T
0.7560006674229598	0.2288236142828666	0.7547915276880914	T	T	T
0.5136851553425643	0.4219559095540575	0.7633901359954365	T	T	T

CHO/Cu(533) $E_{ads} = -1.81$ eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H

60 1 1 1

Selective dynamics

Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0469789510273131	0.2946026081335765	0.4658947181108659	T	T	T
0.0467901203344488	0.6281548534991162	0.4659152082686405	T	T	T
0.0470813508538050	0.9610753918164820	0.4659593206666123	T	T	T
0.3036210488188350	0.2473850666651319	0.4867052647390508	T	T	T
0.3035854424138559	0.5806969763752592	0.4866378298112390	T	T	T
0.3037163266461994	0.9141243463369972	0.4866340018309242	T	T	T
0.5594236582284685	0.2009038344214703	0.5068530987317376	T	T	T
0.5592194747839807	0.5342379536570349	0.5069475819840346	T	T	T
0.5593276945284706	0.8676915507589787	0.5069610305520256	T	T	T
0.8161205742268224	0.1541801173839572	0.5276026564452179	T	T	T
0.8158587342832681	0.4874237144854085	0.5276325115669150	T	T	T

0.8160871886863431	0.8197000239918188	0.5279773101130332	T	T	T
0.0723029885550809	0.1071491923952468	0.5481572624120781	T	T	T
0.0718479572257160	0.4410765385093191	0.5481526069434112	T	T	T
0.0722771974384519	0.7736325032671576	0.5482582943465421	T	T	T
0.3274935755756148	0.0612034106724639	0.5689990714699679	T	T	T
0.3271163185974426	0.3948082005740882	0.5690664344994550	T	T	T
0.3269990577497733	0.7282465219536457	0.5690185474715265	T	T	T
0.5844598253241693	0.0138582229391490	0.5887882445569361	T	T	T
0.5847256933154219	0.3468499362699060	0.5887950570436168	T	T	T
0.5845096578314779	0.6801160430689239	0.5887837313242218	T	T	T
0.8432905193848822	0.6287192284480654	0.6104989995445215	T	T	T
0.8431960675399777	0.2988068036811563	0.6104155787224199	T	T	T
0.8429861215422041	0.9671895291308819	0.6096508920625020	T	T	T
0.0983181484050531	0.5860669587186292	0.6325530847639822	T	T	T
0.0991862137955631	0.2514954407173930	0.6318355382496359	T	T	T
0.0976353709075223	0.9197567076008440	0.6324855427179057	T	T	T
0.3508403818301895	0.5420462505481111	0.6520483640322222	T	T	T
0.3509296857259619	0.2082069086228433	0.6518766079143892	T	T	T
0.3512278381408138	0.8750674606607769	0.6517477747403766	T	T	T
0.6043046675671728	0.4973582964597082	0.6707198848921279	T	T	T
0.6033234398704240	0.1644137785466638	0.6712881975808759	T	T	T
0.6051331818213304	0.8297389426132845	0.6713185293697616	T	T	T
0.8671220145939961	0.4525533087862670	0.6925814572330589	T	T	T
0.8603691916414759	0.1112968580735798	0.6924209196873662	T	T	T
0.8591952391135296	0.7859522828324826	0.6892882076792402	T	T	T
0.8805592421433274	0.1891868868539638	0.7593956411005564	T	T	T
0.8972930309285557	0.3375785305160460	0.7657929738926180	T	T	T
0.8817453798634881	0.1068959915905582	0.7946476132933392	T	T	T

CHO/Defected-Cu(533) E_{ads} = −1.79 eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H

59 1 1 1

Selective dynamics

Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F

0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0470350535581829 0.2943265442526197 0.4662119429681297 T T T
0.0470746263181923 0.6270303559143642 0.4658525710318742 T T T
0.0470337022377976 0.9610480901956322 0.4659563786713008 T T T
0.3035595690766613 0.2471426883488874 0.4867963085623188 T T T
0.3041330070598391 0.5799209012288813 0.4866089973320271 T T T
0.3034609403686872 0.9135977612804140 0.4867175959184635 T T T
0.5593046760931415 0.2006696393849978 0.5067217418402876 T T T
0.5596033529982307 0.5340467118746233 0.5067939396490715 T T T
0.5588910623889802 0.8672554955717118 0.5070444903701343 T T T
0.8160828037685519 0.1529077243411621 0.5274199950687759 T T T
0.8156421851099154 0.4873280107485058 0.5274638930985347 T T T
0.8161061039883961 0.8200604241233549 0.5275906663283507 T T T
0.0726403377378517 0.1057754748449398 0.5485005346642566 T T T
0.0716759441318331 0.4402629852353783 0.5487024281596575 T T T
0.0731004970358811 0.7722225497613167 0.5478466768928385 T T T
0.3267907074682910 0.0608707309568999 0.5690523763967477 T T T
0.3279271793462186 0.3935258004970947 0.5689610098125755 T T T
0.3280140013361432 0.7265429217566250 0.5690445199296050 T T T
0.5846040938315795 0.0127057985248982 0.5884020257727087 T T T
0.5850940934039528 0.3467032399208136 0.5887646564261715 T T T
0.5855439946965788 0.6775763958023049 0.5894348872642325 T T T
0.8425530793813323 0.6275740482564842 0.6105448277438228 T T T
0.8438889781178887 0.2997211438890091 0.6093178974659281 T T T
0.8444006017923797 0.9639167000477684 0.6093931249485749 T T T
0.0982715574286885 0.5840000688245226 0.6321966181053043 T T T
0.0956239329169293 0.2528681055588891 0.6330466805891177 T T T
0.0973038153897576 0.9192191768220326 0.6327398368562029 T T T
0.3516034998195110 0.5405649995726236 0.6514015980289258 T T T
0.3503249218973039 0.2080172499376687 0.6517237886519140 T T T
0.3520858847282895 0.8725124930425849 0.6517254801061512 T T T
0.6096071199477961 0.4963816175689999 0.6731017041128879 T T T
0.6042491784348982 0.1603011917687667 0.6707104623750837 T T T
0.6057876521562093 0.8294288964459113 0.6704217108428239 T T T
0.8537561750273142 0.1254196189477241 0.6895942504123980 T T T
0.8607909254833856 0.7850401293374603 0.6885198458681927 T T T
0.7241715667822390 0.3891276038740372 0.7416096234173253 T T T
0.8343921176578135 0.3918883454019237 0.7570777357937928 T T T
0.6370790065234431 0.4031952548807851 0.7693737743477769 T T T

CHO/Cu_3/Cu(533) E_{ads} = −1.78 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
63 1 1 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F

0.2571973700000001	0.2857762699999995	0.3217927099999969	F	F	F
0.2571614599999990	0.9524293899999989	0.3219123699999997	F	F	F
0.5099116399999986	0.5747781399999994	0.3415763200000015	F	F	F
0.5095861200000016	0.2417833900000019	0.3416938299999970	F	F	F
0.5096986000000001	0.9088501900000026	0.3416314700000029	F	F	F
0.7627858999999972	0.5310134699999978	0.3609394899999998	F	F	F
0.7629538699999969	0.1970798500000015	0.3608490599999996	F	F	F
0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F
0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0464497192320068	0.2940585137360707	0.4664056206184449	T	T	T
0.0458746818356707	0.6281795436626247	0.4665260696771917	T	T	T
0.0465764538352292	0.9606742908994371	0.4664282261147272	T	T	T
0.3025848154050854	0.2472354271494177	0.4870652716892771	T	T	T
0.3028051337643187	0.5799755040708650	0.4869322093399969	T	T	T
0.3025440696434972	0.9137181751517591	0.4869632603168759	T	T	T
0.5578704542348599	0.2005056726497481	0.5064151771223622	T	T	T
0.5586546306846283	0.5338039031158274	0.5062678100633977	T	T	T
0.5584460079860265	0.8668747721818616	0.5067208033929899	T	T	T
0.8157910318447983	0.1522135198445121	0.5273558059936966	T	T	T
0.8152357580315548	0.4864066383600300	0.5275314737430473	T	T	T
0.8146827488835240	0.8200313120260839	0.5277104489807654	T	T	T
0.0713026097081529	0.1056229223479159	0.5490409123571975	T	T	T
0.0706426260797152	0.4402586368285091	0.5487049831468102	T	T	T
0.0717446258937336	0.7726550605805192	0.5490603818934204	T	T	T
0.3262137363886900	0.0602527528031084	0.5688548521239070	T	T	T
0.3255650741123609	0.3938297932885693	0.5694831374549845	T	T	T
0.3267498697478674	0.7258112487648637	0.5689631822902579	T	T	T
0.5825213756821747	0.0128982264378391	0.5884012978299403	T	T	T
0.5837791694189550	0.3450209923018800	0.5874639641018909	T	T	T
0.5837186905276510	0.6783094033495990	0.5883191640444504	T	T	T
0.8413751165542216	0.6309318757695462	0.6100434421883667	T	T	T
0.8418734683708483	0.2962023476407854	0.6097761490115023	T	T	T
0.8426612291095000	0.9630543313507942	0.6097701071599706	T	T	T
0.0949528683981191	0.5853460225480951	0.6338146914230353	T	T	T
0.0966960477723955	0.2517274339904069	0.6326365076985840	T	T	T
0.0977220868475393	0.9170805196714933	0.6344063959946040	T	T	T
0.3483742585844313	0.5370249632089285	0.6513000397183315	T	T	T
0.3492648282932934	0.2066804309870598	0.6519675462844837	T	T	T
0.3487577259951432	0.8783841777516078	0.6507327045765124	T	T	T
0.6046177463173196	0.4935399518845178	0.6693471870024632	T	T	T
0.6042756467824615	0.1559282944066032	0.6697786666310914	T	T	T
0.6039500780481464	0.8298453029796873	0.6712502947999436	T	T	T
0.8629833573397603	0.4475393174376011	0.6907531221006936	T	T	T
0.8612018076407085	0.1124259043519228	0.6914550660859249	T	T	T
0.8568180904310660	0.7847107848387136	0.6917611482184590	T	T	T
0.6274586018300456	0.6329442141294079	0.7497100864313542	T	T	T
0.6175419273777173	0.3098645886124501	0.7463001364348220	T	T	T

0.3697259336917120 0.6914037142974836 0.7275510107026665 T T T
0.6459030937064373 0.7119982211209778 0.8166456778125023 T T T
0.5957085123512459 0.8962833726610940 0.8303372936872022 T T T
0.7089481312072341 0.5710823139268753 0.8447307133847876 T T T

CHO/Cu(533) $E_{ads} = -1.75$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0469379022388392 0.2944163437100780 0.4659775198120111 T T T
0.0464720755508425 0.6281193940102682 0.4658078730118030 T T T
0.0469655505116549 0.9610046683173070 0.4659330770708249 T T T
0.3028397199731481 0.2479135626204128 0.4866514575478753 T T T
0.3029729381955303 0.5808367718305976 0.4866219474099924 T T T
0.3032137543005791 0.9141103145897213 0.4866205504507928 T T T
0.5579856658462019 0.2018721459801920 0.5067250811886406 T T T
0.5583324126742368 0.5347732387212379 0.5066913516714951 T T T
0.5581456194076683 0.8682789675116658 0.5067310115832186 T T T
0.8146808856127071 0.1539792089461111 0.5271758825595565 T T T
0.8145286352590883 0.4885312629332466 0.5271698326416727 T T T
0.8142812965145033 0.8214491250134438 0.5277303774675797 T T T
0.0709366383003374 0.1079011644789169 0.5479695925909130 T T T
0.0700802585344474 0.4426077371701801 0.5480701105517273 T T T
0.0705147228379045 0.7741935891445937 0.5479922908890753 T T T
0.3253708759048927 0.0626011202431144 0.5688574098429980 T T T
0.3249735463967181 0.3960758609962365 0.5690130777584788 T T T
0.3258053411216678 0.7287417886224899 0.5688084382805075 T T T
0.5821729171168841 0.0151617983216922 0.5885687502714463 T T T

0.5825295278528644	0.3475682918179665	0.5884811775216555	T	T	T
0.5825407482831858	0.6819237928669069	0.5885193049278382	T	T	T
0.8409656342199743	0.6307755269132967	0.6098866479883318	T	T	T
0.8408136630206348	0.2995369244441325	0.6083171114362863	T	T	T
0.8411471990206876	0.9675322380857412	0.6097361524084298	T	T	T
0.0958753711820851	0.5873245127777958	0.6326505305592314	T	T	T
0.0963495218376724	0.2542702873176175	0.6317452515138683	T	T	T
0.0964322667974974	0.9193397357857019	0.6314636483853492	T	T	T
0.3484270660439890	0.5428675897348363	0.6517828308985679	T	T	T
0.3488934487096131	0.2095350244238978	0.6517639646201416	T	T	T
0.3483577590437068	0.8772056853762383	0.6514634599213823	T	T	T
0.5996175974990587	0.5004677462764572	0.6701172450759665	T	T	T
0.6027111367586492	0.1644050869793305	0.6711943552661432	T	T	T
0.6028538728713442	0.8311200637792266	0.6712668401435761	T	T	T
0.8581607865927668	0.4465744916928248	0.6912797820460831	T	T	T
0.8573392765697423	0.1227231747699608	0.6910443153098239	T	T	T
0.8568501577949628	0.7859360125095614	0.6892180090707303	T	T	T
0.9235874732139202	0.2254387865650188	0.7511680961574319	T	T	T
0.8431053200043563	0.3022659992555116	0.7895004476313837	T	T	T
0.0596425886608010	0.1050470065225419	0.7534290462225965	T	T	T

CHO/Defected-Cu(533) $E_{ads} = -1.74$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
59 1 1 1
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0467885822690574	0.2944142777264238	0.4660700930908789	T	T	T
0.0466766609837707	0.6272567764246245	0.4658501454091768	T	T	T
0.0467145622992582	0.9610825414224862	0.4658970208194223	T	T	T

0.3030791738320610	0.2473048206902212	0.4867053677485024	T	T	T
0.3038125333129730	0.5798436773596327	0.4865232591228164	T	T	T
0.3032090640689903	0.9135478309138312	0.4865964451244770	T	T	T
0.5589797600586239	0.2004693779854166	0.5068675862707013	T	T	T
0.5591921081014926	0.5338771598866413	0.5066304843860320	T	T	T
0.5582762762553852	0.8676919956995499	0.5068883042430333	T	T	T
0.8156291717335011	0.1529797220854969	0.5274350483611557	T	T	T
0.8152666706500039	0.4872610332024776	0.5274275208464986	T	T	T
0.8151994862569842	0.8206429265549938	0.5276264863070272	T	T	T
0.0718807078806013	0.1064051889270632	0.5483184542701546	T	T	T
0.0708321993104587	0.4406638108803362	0.5486477200785040	T	T	T
0.0723049374906086	0.7726944714690946	0.5477970118775385	T	T	T
0.3258694863227310	0.0615076098541716	0.5689076883569346	T	T	T
0.3272293814949853	0.3936295107444118	0.5688100344101330	T	T	T
0.3274858045875635	0.7267201497311899	0.5688882992717001	T	T	T
0.5837026217498696	0.0125755965397400	0.5887343430477764	T	T	T
0.5844839768768368	0.3474390504904804	0.5889109196955573	T	T	T
0.5847203919489214	0.6781559764222673	0.5889152564280492	T	T	T
0.8413242173712853	0.6283054720530202	0.6105309751553980	T	T	T
0.8429033695659403	0.3003852745203289	0.6095515639700709	T	T	T
0.8431899181504759	0.9638988374631350	0.6092729356366698	T	T	T
0.0974751707907228	0.5842721900843048	0.6321142504774009	T	T	T
0.0940796210278477	0.2544019644401144	0.6330953558517728	T	T	T
0.0972353373091777	0.9195969363209381	0.6323912453553359	T	T	T
0.3506948809368249	0.5405717493129104	0.6509946644781394	T	T	T
0.3496151454090694	0.2086930299186801	0.6516470721531785	T	T	T
0.3500360546899352	0.8749570131376257	0.6513114108159973	T	T	T
0.6079451987706955	0.4974976421597277	0.6726370842743664	T	T	T
0.6043471999740045	0.1612244844289370	0.6710304934709983	T	T	T
0.6042267628271223	0.8293469662992907	0.6707069676643435	T	T	T
0.8564476838833235	0.1203416572987382	0.6884487185439411	T	T	T
0.8596857902735293	0.7848588252530886	0.6886194674951319	T	T	T
0.6587871324944885	0.5060402091844614	0.7433645919122683	T	T	T
0.7685280938285338	0.5000554907147787	0.7619056612493993	T	T	T
0.5639415680945997	0.5258051653672738	0.7685575691928135	T	T	T

CHO/Cu(533) $E_{ads} = -1.73$ eV

1.00000000000000		
10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H
60 1 1 1
Selective dynamics
Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F

0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0470708347317618	0.2939207861925360	0.4659795961402276	T	T	T
0.0466509267860412	0.6277524889536067	0.4659232667366418	T	T	T
0.0471022344765083	0.9606400150816029	0.4659877416687245	T	T	T
0.3032313227248563	0.2470565930445129	0.4866891504912096	T	T	T
0.3031865568818664	0.5803869363873838	0.4866706464955404	T	T	T
0.3035493987010583	0.9135007043831155	0.4866558797470080	T	T	T
0.5584812755830901	0.2013420781556969	0.5067789722040161	T	T	T
0.5587288119929390	0.5340568753918193	0.5067289448536078	T	T	T
0.5587465705597706	0.8673894627064305	0.5067701339759875	T	T	T
0.8152675428398208	0.1531086493416499	0.5273145190488794	T	T	T
0.8152388710161290	0.4876011263091963	0.5272646187566307	T	T	T
0.8148914719473253	0.8207511072701726	0.5278961225601013	T	T	T
0.0719064517740329	0.1064991956886373	0.5480392718510144	T	T	T
0.0709087360155963	0.4412162947201211	0.5481459716821995	T	T	T
0.0711969261595057	0.7732824065197101	0.5482063106115155	T	T	T
0.3264704749748969	0.0609923591032506	0.5689364801407633	T	T	T
0.3259488865606567	0.3947449388408644	0.5690001861208259	T	T	T
0.3267055649306461	0.7274503133269098	0.5689514710185837	T	T	T
0.5834325522307563	0.0137902378688026	0.5886616617992073	T	T	T
0.5838358005988433	0.3461722534419320	0.5886288843361043	T	T	T
0.5839152118748764	0.6804083403771097	0.5885559298484829	T	T	T
0.8425586992774770	0.6289246043148380	0.6101263720675859	T	T	T
0.8427064815258321	0.2976475590465124	0.6085658601977384	T	T	T
0.8424796582077284	0.9664350622639665	0.6101226616819385	T	T	T
0.0971793312500379	0.5855805488363398	0.6326637474765539	T	T	T
0.0973962193289913	0.2523664465071502	0.6318705498153616	T	T	T
0.0972255188296184	0.9184691625793723	0.6318513795494687	T	T	T
0.3501832405382129	0.5407984106341026	0.6517419885350890	T	T	T
0.3506146164952934	0.2075519198811265	0.6516975745313768	T	T	T
0.3500082107204777	0.8753603857228854	0.6515219014428434	T	T	T
0.6015327414031268	0.4986784468550856	0.6700104352456860	T	T	T
0.6044073116510622	0.1627512940277071	0.6715214534510271	T	T	T
0.6046387518345888	0.8293984483687245	0.6715276655286604	T	T	T
0.8581367630161556	0.4469122373906087	0.6919149181080092	T	T	T
0.8582603141886275	0.1225099098304154	0.6919240136660827	T	T	T
0.8582087305007585	0.7849193118553902	0.6894683735352430	T	T	T
0.8762176802990700	0.2685695446520323	0.7553419740953038	T	T	T
0.0105598425614406	0.1632537443311377	0.7745995575224565	T	T	T
0.7660799839705135	0.3565647285260153	0.7798678006359192	T	T	T

CHO/Cu(533) $E_{ads} = -1.73$ eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H
60 1 1 1
Selective dynamics
Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0474645310889583	0.2940282673024308	0.4659532939703072	T	T	T
0.0472149090518426	0.6275130438805537	0.4658478361570347	T	T	T
0.0472276719150582	0.9604944635569345	0.4659310008571829	T	T	T
0.3039271867451202	0.2471504825152888	0.4867046284116801	T	T	T
0.3037543637976212	0.5805771136498324	0.4868706936891847	T	T	T
0.3037876551095235	0.9133822482270888	0.4866153599981287	T	T	T
0.5592913207193408	0.2013458908357078	0.5068507232525233	T	T	T
0.5589049206640740	0.5353073470677348	0.5070969265369747	T	T	T
0.5594104922790667	0.8671954083879341	0.5072201979690045	T	T	T
0.8159329966530080	0.1546928864705150	0.5274701160201574	T	T	T
0.8158444748663468	0.4877714445478188	0.5273482550223912	T	T	T
0.8163121011560135	0.8198633560361771	0.5277086042823805	T	T	T
0.0726653055780191	0.1059327262319583	0.5481122212408716	T	T	T
0.0724211095534804	0.4405466368211366	0.5480368544948687	T	T	T
0.0727175876582578	0.7730275834573334	0.5483414555461071	T	T	T
0.3277025848793372	0.0604472014084257	0.5687746421830299	T	T	T
0.3273583842026596	0.3945670775204549	0.5691772650279115	T	T	T
0.3262419170497585	0.7290758660058296	0.5695208555982768	T	T	T
0.5844808520683147	0.0141776461683040	0.5885094075678022	T	T	T
0.5844076140048748	0.3491837659718640	0.5890930946605135	T	T	T
0.5849262517770740	0.6779007604406477	0.5900211177496250	T	T	T
0.8433217422388443	0.6303986547201607	0.6099489279992296	T	T	T
0.8432664996153616	0.3015076679466622	0.6094858925112713	T	T	T
0.8427652739583669	0.9679222360605934	0.6088034182380472	T	T	T
0.0980864023707691	0.5852289640638699	0.6326286436247381	T	T	T
0.1001165261386139	0.2498574464680028	0.6313750745408744	T	T	T
0.0944276140178385	0.9223658848808470	0.6335260991216878	T	T	T
0.3494255944446159	0.5431298735962636	0.6518308141167442	T	T	T
0.3505085406612146	0.2081768889368039	0.6518067079920233	T	T	T
0.3520287258530540	0.8729456824774667	0.6519785128905088	T	T	T

0.6028751559128925	0.4984335463663482	0.6760214569544695	T	T	T
0.6015829932045509	0.1633262707868672	0.6707409107591634	T	T	T
0.6053202701690353	0.8311104371824263	0.6709053050808456	T	T	T
0.8765776622878310	0.4539468828348032	0.6917406861993185	T	T	T
0.8501749308434081	0.1251424892335319	0.6901185648532675	T	T	T
0.8600580363540608	0.7920698228091831	0.6889062190182619	T	T	T
0.7138471389868967	0.3687519574539430	0.7444223370316955	T	T	T
0.8119727906914609	0.4042482806644153	0.7601849995623570	T	T	T
0.6450988117210829	0.3549106783758286	0.7742093570596367	T	T	T

CHO/Defected-Cu(533) $E_{ads} = -1.70$ eV
1.00000000000000
10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H
59 1 1 1
Selective dynamics
Direct
0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0468109029517416	0.2939609739558149	0.4661033733081570	T	T	T
0.0469382251395375	0.6270776790841908	0.4659283857866924	T	T	T
0.0469358906465195	0.9608069395300016	0.4660716135480928	T	T	T
0.3032265839855799	0.2467202254702141	0.4867515539984938	T	T	T
0.3039101282382695	0.5796892805323840	0.4865201735341517	T	T	T
0.3030688848197775	0.9137168913581135	0.4867581502921540	T	T	T
0.5592999323756372	0.2001366032298141	0.5066654128066094	T	T	T
0.5593183526855267	0.5334413515023158	0.5067593487895946	T	T	T
0.5587024980733205	0.8671535226032764	0.5071055743068731	T	T	T
0.8160097604500470	0.1530411915855817	0.5275013251605838	T	T	T
0.8153999712385587	0.4868069108607638	0.5276789984873241	T	T	T
0.8158650584850580	0.8189504318118302	0.5274299711543310	T	T	T
0.0715055045424185	0.1068036956445978	0.5486730483557711	T	T	T
0.0712717334976853	0.4396915738802763	0.5484926137269320	T	T	T

0.0728710593882084	0.7717355448391844	0.5478425722272903	T	T	T
0.3265688455659995	0.0604483362463503	0.5691364028529386	T	T	T
0.3277431435360859	0.3928155775338552	0.5688796278447528	T	T	T
0.3275614647232075	0.7261747580520201	0.5688425077004544	T	T	T
0.5847232378179650	0.0119646907160035	0.5885762016425631	T	T	T
0.5853124437441907	0.3447084591149615	0.5885745287457649	T	T	T
0.5854747503496321	0.6774436672474059	0.5890658814494975	T	T	T
0.8428093764899397	0.6261398352242891	0.6107447039581908	T	T	T
0.8432936494997243	0.2982860334793457	0.6110907717807879	T	T	T
0.8441397193784960	0.9633483858959717	0.6090894754087937	T	T	T
0.0984090140151064	0.5828508469033847	0.6320221935263320	T	T	T
0.0955336829297157	0.2525230838740983	0.6331887254816345	T	T	T
0.0973261851993499	0.9182052377518968	0.6320369674793795	T	T	T
0.3511444875700185	0.5397578312378770	0.6516538887794345	T	T	T
0.3506234694261887	0.2063367775420454	0.6518061201293446	T	T	T
0.3510271821233075	0.8728432531440202	0.6518011338993506	T	T	T
0.6069328357274864	0.4942668658389771	0.6704240450418893	T	T	T
0.6039794144907338	0.1606122015000752	0.6708995683667801	T	T	T
0.6063935490784118	0.8258948645167532	0.6703729739606260	T	T	T
0.8564184278744353	0.1155877565755707	0.6915436019542825	T	T	T
0.8597034033308706	0.7816489820172605	0.6883450965324900	T	T	T
0.8551562740109310	0.1369296578391106	0.7642662509672546	T	T	T
0.9725799321612180	0.1042345080038856	0.7841261143523391	T	T	T
0.7513138168913777	0.1750711003799820	0.7875953583927425	T	T	T

CHO/Defected-Cu(533) $E_{ads} = -1.69$ eV
1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H
59 1 1 1
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F

0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0468204299654618	0.2939091248269367	0.4660707573226116	T	T	T
0.0468896117106670	0.6272241631542251	0.4659874080795343	T	T	T
0.0468302511436870	0.9608093062304799	0.4661047661017028	T	T	T
0.3032794400678149	0.2468057560185287	0.4866691999247077	T	T	T
0.3037895434476790	0.5798886161665576	0.4865199999747229	T	T	T
0.3029891424650531	0.9138517565264309	0.4867119097139761	T	T	T
0.5593988133062511	0.2002045548094922	0.5066575566639451	T	T	T
0.5593288042447451	0.5335038694818101	0.5067307987014210	T	T	T
0.5588552628428849	0.8671035927979477	0.5070764377733338	T	T	T
0.8160391214577838	0.1530997292266013	0.5275613766435221	T	T	T
0.8156307956372304	0.4867367251938485	0.5276481388391437	T	T	T
0.8159793715501956	0.8189312176530987	0.5274650060639452	T	T	T
0.0715513587341651	0.1067647163273524	0.5487179847851010	T	T	T
0.0714415169176626	0.4396971580529405	0.5484584427353367	T	T	T
0.0728962132820138	0.7719375454638968	0.5480282528533154	T	T	T
0.3266893793687606	0.0605719970713509	0.5689805841098772	T	T	T
0.3277770501597559	0.3929711311000774	0.5688190713557475	T	T	T
0.3275222492476187	0.7264888001822423	0.5687978597086325	T	T	T
0.5845821591730943	0.0121170866355489	0.5885597156130299	T	T	T
0.5851557080162790	0.3449471304163099	0.5886338650082946	T	T	T
0.5855318350867349	0.6774712492693270	0.5889946169159778	T	T	T
0.8427263175305775	0.6263115178802872	0.6107606681155088	T	T	T
0.8430691250633576	0.2987781250790862	0.6110772367573095	T	T	T
0.8437342609218231	0.9635834580634427	0.6091063773344015	T	T	T
0.0982435025007010	0.5831447665219217	0.6320866124691504	T	T	T
0.0954236741997699	0.2528265497740415	0.6330822248300657	T	T	T
0.0971269409155122	0.9187059601894382	0.6323063310628554	T	T	T
0.3506967558630964	0.5404186117790345	0.6515859221145063	T	T	T
0.3500975446541223	0.2067376778078581	0.6517006987196593	T	T	T
0.3507225158880676	0.8734814446142390	0.6516463494764719	T	T	T
0.6062960936511020	0.4950307764090403	0.6704165188727939	T	T	T
0.6029735567012977	0.1610262526116974	0.6708961109739455	T	T	T
0.6060058954358857	0.8262012140777852	0.6702906415636987	T	T	T
0.8554766018456015	0.1157579476154010	0.6910428769489202	T	T	T
0.8595868762847468	0.7814362803617184	0.6883515574975924	T	T	T
0.8617868188459052	0.1426590310298393	0.7631755011096866	T	T	T
0.7693058502709132	0.1812853884402335	0.7964797045406529	T	T	T
0.9807778825603140	0.1100360805341672	0.7724345579818712	T	T	T

CHO/Cu(533) $E_{ads} = -1.69$ eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H

60 1 1 1

Selective dynamics

Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F

0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0472921542645468	0.2940405386139841	0.4660159506805164	T	T	T
0.0469924760174547	0.6276006793381335	0.4659262424642673	T	T	T
0.0469943966998283	0.9609260525295803	0.4659363062796610	T	T	T
0.3037693779185301	0.2469432638023148	0.4867515315051258	T	T	T
0.3035403760995766	0.5802937637913944	0.4866823877532021	T	T	T
0.3037297491234597	0.9135247655098588	0.4866761708135960	T	T	T
0.5589406017967016	0.2009581787617654	0.5069168007677880	T	T	T
0.5589820064503007	0.5342350030734667	0.5068716876546568	T	T	T
0.5590089783892721	0.8672637137285482	0.5068882194098561	T	T	T
0.8155546334337461	0.1534219631933539	0.5275881625160148	T	T	T
0.8157050125572446	0.4868602810329933	0.5272773080209002	T	T	T
0.8153642290102242	0.8207460791118365	0.5275467257836349	T	T	T
0.0721905312733237	0.1063959837685104	0.5481308746882051	T	T	T
0.0720267750435473	0.4403770869175666	0.5481082398493423	T	T	T
0.0717461850133390	0.7736362359752951	0.5481413812492592	T	T	T
0.3270047767193911	0.0608632763471029	0.5690743522668386	T	T	T
0.3267758971469418	0.3944619536179200	0.5691154186114168	T	T	T
0.3269410501342104	0.7274962605014170	0.5690088646978415	T	T	T
0.5840858128401335	0.0134185198006140	0.5887824064580388	T	T	T
0.5841091054807683	0.3465732929386039	0.5887944827097907	T	T	T
0.5844662656942561	0.6796894556790319	0.5888587692566639	T	T	T
0.8430806888549586	0.6293319947448091	0.6094787505629945	T	T	T
0.8431232450910263	0.2990242681517407	0.6095154846310084	T	T	T
0.8429612442320580	0.9642503483340918	0.6096803887834037	T	T	T
0.0979253037261331	0.5851678412309043	0.6324344283463843	T	T	T
0.0974947848668215	0.2522663544770530	0.6321523747963124	T	T	T
0.0981401113682129	0.9186234286638327	0.6323120079718826	T	T	T
0.3508394307550441	0.5409104317853239	0.6517939292055839	T	T	T
0.3507812926262801	0.2079196734491394	0.6517905155904182	T	T	T
0.3510099600519231	0.8743760687422720	0.6517939873901205	T	T	T
0.6038137418657066	0.4960916176096957	0.6711043080092129	T	T	T
0.6044937998410900	0.1632177607413924	0.6718454561209002	T	T	T
0.6039952038484446	0.8309096237585293	0.6711026659680196	T	T	T
0.8581337298246402	0.4518230884017997	0.6924893252359529	T	T	T
0.8594375557281982	0.1174964379343948	0.6898115647113027	T	T	T
0.8588581853567655	0.7844142494183227	0.6897807295645962	T	T	T
0.8685439659680515	0.4486279628193725	0.7657915422800290	T	T	T
0.9970107590044602	0.3540396511837764	0.7872265142877937	T	T	T
0.7528028754511941	0.5351824322688036	0.7875415104113086	T	T	T

CHO/Cu(533) $E_{ads} = -1.68$ eV

1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0472447629721192 0.2941630523570919 0.4660440626176826 T T T
0.0469964189159620 0.6276670870861146 0.4659638570970282 T T T
0.0469316847058834 0.9610869609198966 0.4659765638345428 T T T
0.3036094750656453 0.2471161188283333 0.4867677687583841 T T T
0.3034758106618544 0.5804071405024989 0.4866773823438029 T T T
0.3035641320677878 0.9137061902044264 0.4866924826401555 T T T
0.5588904437878189 0.2011236463934089 0.5069378052998584 T T T
0.5588870084423085 0.5344288611710042 0.5068764211288056 T T T
0.5588943870050217 0.8674673337968883 0.5068669707399303 T T T
0.8153065754825668 0.1536707203380901 0.5275164390507834 T T T
0.8155963760337734 0.4870477653358670 0.5272480794633835 T T T
0.8152913024376734 0.8210148513305281 0.5274899615085978 T T T
0.0720662058815692 0.1068026871999671 0.5481812303942435 T T T
0.0719022907830320 0.4405641454839372 0.5481570054980620 T T T
0.0716930274648782 0.7738956956394234 0.5481401742921141 T T T
0.3266599141813377 0.0612617177511941 0.5690078923587955 T T T
0.3265166107344290 0.3948322233363601 0.5690680545060881 T T T
0.3266950014422618 0.7277946339855433 0.5689993472916984 T T T
0.5836103634096884 0.0138831999311910 0.5887149933322101 T T T
0.5835921489392274 0.3471614843234830 0.5887928936666910 T T T
0.5841387918423691 0.6801198410320082 0.5888804242477708 T T T
0.8426336963875160 0.6297910519884823 0.6095316633665708 T T T
0.8425701203717966 0.2993487381318201 0.6094253289386624 T T T
0.8425768565755610 0.9646491446635649 0.6096258569713895 T T T
0.0975005633655140 0.5856568824192878 0.6324392554113060 T T T
0.0969433874519088 0.2529887882833989 0.6323528926073275 T T T

0.0975611253084898 0.9193154876214994 0.6323649869855004 T T T
0.3500168153690955 0.5416323901021933 0.6518230942175630 T T T
0.3501407180236430 0.2086848945443049 0.6517541970496749 T T T
0.3503422686356532 0.8751490778812361 0.6517293744159690 T T T
0.6025173671772713 0.4972140781557781 0.6710765759448803 T T T
0.6037877121330848 0.1637049083558635 0.6716516973465122 T T T
0.6030032704255414 0.8321343115965244 0.6711106726859803 T T T
0.8565456499337755 0.4528309548382768 0.6921393847743462 T T T
0.8584897441200524 0.1182556024626100 0.6896582473485900 T T T
0.8588370693363466 0.7842627862356113 0.6896604609053966 T T T
0.8781693029007069 0.4282805581947349 0.7649506989697110 T T T
0.7770393186276233 0.5132909101748221 0.7976442421564846 T T T
0.0108603255774906 0.3143887985509879 0.7747781125959839 T T T

CHO/Cu(533) $E_{ads} = -1.67$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0466841649517759 0.2947498929105812 0.4658886177536160 T T T
0.0465995025223833 0.6278223102923122 0.4658573241268334 T T T
0.0470939055691092 0.9609954865001253 0.4657559250172524 T T T
0.3034890329867233 0.2473685628017133 0.4867354496701133 T T T
0.3034583420713680 0.5805250969068695 0.4865471290090220 T T T
0.3035347830281483 0.9138763094520701 0.4866365667087783 T T T
0.5584795690462635 0.2012343709923140 0.5067713059360669 T T T
0.5585758165466751 0.5351531828531076 0.5067645513349350 T T T
0.5587473653469254 0.8678319348160086 0.5073720827823173 T T T
0.8153937931714107 0.1540486773683631 0.5273287222487933 T T T

0.8147178906287076 0.4873583920445569 0.5277752836916967 T T T
0.8148611454855830 0.8216870354491698 0.5277609537037428 T T T
0.0712626963976099 0.1077164159580196 0.5478557064964684 T T T
0.0712503165982988 0.4409986192292727 0.5481403407571248 T T T
0.0711901467804999 0.7742479533742110 0.5477558445187126 T T T
0.3264950620025221 0.0613076922646615 0.5690547279164727 T T T
0.3264012091068693 0.3948994274094715 0.5690125508232678 T T T
0.3267114556052061 0.7281500967391134 0.5688221610021668 T T T
0.5832070238020560 0.0164174678470185 0.5895474189062442 T T T
0.5839659489035545 0.3469803222858643 0.5883154383029937 T T T
0.5834647345322255 0.6785140846586982 0.5896792296854749 T T T
0.8406364759470669 0.6331154896088853 0.6088177893240644 T T T
0.8410565604950859 0.2967056099663665 0.6102012908940101 T T T
0.8409437891582948 0.9687728079567578 0.6101345003395598 T T T
0.0964714139842030 0.5868991416919269 0.6321915888340327 T T T
0.0967279510493445 0.2527032505291613 0.6322597134755733 T T T
0.0977918573155090 0.9194154915147348 0.6314024262195465 T T T
0.3466996621613135 0.5448494018096056 0.6507104822208361 T T T
0.3491159172901754 0.2087311439730499 0.6516849493125304 T T T
0.3497131253575937 0.8760936565116019 0.6518262498135157 T T T
0.5991011417408207 0.4968254634005583 0.6738599235332909 T T T
0.5988919637170632 0.1707425772960040 0.6736898130179318 T T T
0.6025367744628547 0.8313198516532558 0.6717642834732147 T T T
0.8588690367107982 0.4546384294435287 0.6886223487294493 T T T
0.8827806110394975 0.0980434859071093 0.6925680578974208 T T T
0.8588825200678479 0.7811547343803705 0.6885591651222844 T T T
0.6049875422104216 0.3247180079534059 0.7364714184206125 T T T
0.7437581228249069 0.2131289429043813 0.7571524685512481 T T T
0.5003732182745322 0.4115735919877010 0.7628385932397203 T T T

CHO/Defected-Cu(533) E_{ads} = −1.64 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
59 1 1 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F

0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0467007710528035 0.2947975953643204 0.4660524397669124 T T T
0.0467415581929390 0.6279752415997623 0.4658756389523650 T T T
0.0464435190347010 0.9621183043758470 0.4658840226762111 T T T
0.3030459316643986 0.2480397656850513 0.4867258626392511 T T T
0.3035981975747706 0.5812663651119923 0.4864442641756651 T T T
0.3024776181354888 0.9152839915501193 0.4868080944592220 T T T
0.5584868052663278 0.2027572194251516 0.5070825184561343 T T T
0.5581519556958343 0.5352232965294420 0.5069218386832131 T T T
0.5577977825891555 0.8687198380701754 0.5074025513714007 T T T
0.8145885504750958 0.1552102553831841 0.5274494146790364 T T T
0.8141459597442720 0.4880364340058412 0.5275639046822163 T T T
0.8143247049857566 0.8212228497714701 0.5270868447189336 T T T
0.0695106192504388 0.1102953236381838 0.5487241011485172 T T T
0.0700495743496658 0.4423800254010623 0.5483207618576676 T T T
0.0717043552287317 0.7748323337387606 0.5474558327759235 T T T
0.3245816545316065 0.0648254941840023 0.5690809302426335 T T T
0.3266783442215720 0.3965650475888434 0.5686858717259429 T T T
0.3252395929923291 0.7304628894002744 0.5688903272719502 T T T
0.5826340670062160 0.0182214591943325 0.5891603313355495 T T T
0.5841837154565745 0.3487908026072150 0.5901374553838937 T T T
0.5828233756058240 0.6801480863295283 0.5893890870520931 T T T
0.8392304713381319 0.6289290940855936 0.6095743128996599 T T T
0.8405195046944660 0.3010206775179821 0.6115016553583690 T T T
0.8421080441391288 0.9636767221468058 0.6080455897880193 T T T
0.0969390354169867 0.5872570196834733 0.6315023405550499 T T T
0.0915966603674599 0.2597971215593943 0.6336222563789560 T T T
0.0942089663015693 0.9241149574259238 0.6323940134921310 T T T
0.3480181703283214 0.5455630009128555 0.6508122649913624 T T T
0.3492379952754187 0.2135092975626259 0.6518811884786812 T T T
0.3451866795467344 0.8836963454976605 0.6511915359529025 T T T
0.6014222156782290 0.5128650584590163 0.6719546150863176 T T T
0.6047340013676804 0.1628429749124738 0.6755949396755295 T T T
0.6017795543315343 0.8368763229158056 0.6695385500419624 T T T
0.8611378618138636 0.0979002976503023 0.6896281150238253 T T T
0.8628684557858503 0.7685889644076725 0.6870748077317281 T T T
0.6746583997550354 0.2367430095667143 0.7410230102181207 T T T
0.6186531946042909 0.4374659375712162 0.7481838835759697 T T T
0.6835060031182163 0.1452799455245267 0.7754225614791814 T T T

CHO/Cu(533) E_{ads} = −1.64 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F

0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0474446022137787	0.2941777659926640	0.4661109649941737	T	T	T
0.0473837087027507	0.6268507123084853	0.4660530048479886	T	T	T
0.0475590856215568	0.9598423124524309	0.4659481982681753	T	T	T
0.3036662815554780	0.2462549071304573	0.4868568586639493	T	T	T
0.3038346899822287	0.5788895717711944	0.4868233046570496	T	T	T
0.3042955126975910	0.9127051729246441	0.4867723530230331	T	T	T
0.5590854859643060	0.1995218386156436	0.5071400489456496	T	T	T
0.5596044739844971	0.5322254309643440	0.5067532272884655	T	T	T
0.5598565451467397	0.8659056734009336	0.5068912285272766	T	T	T
0.8163805200159256	0.1519212546154098	0.5273408091506852	T	T	T
0.8168587021963633	0.4843931791774105	0.5278645174087676	T	T	T
0.8167956804435668	0.8179490727940969	0.5274425272683589	T	T	T
0.0725116355152960	0.1057685585637993	0.5476453756963990	T	T	T
0.0731972983495167	0.4397450891397609	0.5493769962618075	T	T	T
0.0726763414014805	0.7702260301535877	0.5487246392604345	T	T	T
0.3282233943484450	0.0583350940093446	0.5690636530269442	T	T	T
0.3261505801383447	0.3928733526603380	0.5699212584177910	T	T	T
0.3288591560389670	0.7239196666706458	0.5686656024210720	T	T	T
0.5861957467580401	0.0088506682033329	0.5887045572811258	T	T	T
0.5842014288027245	0.3442820431050467	0.5887352499642351	T	T	T
0.5856807528058375	0.6758612263783786	0.5886292600726206	T	T	T
0.8446002964207312	0.6274500123590890	0.6091114603528668	T	T	T
0.8446167702553972	0.2910958852556499	0.6101369583876820	T	T	T
0.8426519690720471	0.9633864305349104	0.6090685943736984	T	T	T
0.1020184663896848	0.5827365741697880	0.6381205096623830	T	T	T
0.1011987145071456	0.2455846352863257	0.6319950180488744	T	T	T
0.1021873400282774	0.9165697948624050	0.6298063982685057	T	T	T
0.3551936343981716	0.5364217642715261	0.6525639685990655	T	T	T
0.3577488700677643	0.1973224016562997	0.6511918530387717	T	T	T
0.3559121481690566	0.8673475130824476	0.6515784912945131	T	T	T
0.6100949531869707	0.4861156712111580	0.6717788976255705	T	T	T
0.6093090941322300	0.1560665795666198	0.6712976714854636	T	T	T
0.6063942902959987	0.8242833585684514	0.6721428505101660	T	T	T
0.8606607711206362	0.4461236791956013	0.6892762047391666	T	T	T
0.8688778584681081	0.1122650398830751	0.6926089647506610	T	T	T
0.8575619175259693	0.7728868681235843	0.6903376355530887	T	T	T
0.0873470649331894	0.6522744183019000	0.7132271116606405	T	T	T

0.0291729945820409	0.8363270913020935	0.7358708121835893	T	T	T
0.1644533075612723	0.5017269004347905	0.7371222456269514	T	T	T

CHO/Defected-Cu(533) E_{ads} = −1.59 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
59 1 1 1
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0470173084543930	0.2943366286388525	0.4660428970398840	T	T	T
0.0470620638079922	0.6270810849339625	0.4660390111893946	T	T	T
0.0469915442494582	0.9612320825760676	0.4658017946938529	T	T	T
0.3034215222754568	0.2475010482250113	0.4867199074732440	T	T	T
0.3037486915080336	0.5806390669059098	0.4865903316387943	T	T	T
0.3031648407974856	0.9138162362338917	0.4869049752642525	T	T	T
0.5595210974560629	0.2019867179248749	0.5068253925172428	T	T	T
0.5594190898894098	0.5348962241502662	0.5067138674070151	T	T	T
0.5589026005561735	0.8670740547068547	0.5069499292472273	T	T	T
0.8164095684268560	0.1536440369545389	0.5274358297356301	T	T	T
0.8159506284888778	0.4870240690509391	0.5275201826871339	T	T	T
0.8162485286259624	0.8197122989104102	0.5275291312820087	T	T	T
0.0714526592225582	0.1075832721044065	0.5484238231957690	T	T	T
0.0715258144115651	0.4405400896722540	0.5486793307601872	T	T	T
0.0721849624392945	0.7737165762488942	0.5478245775531647	T	T	T
0.3268842331211061	0.0615820364094049	0.5686667167985036	T	T	T
0.3279578459509125	0.3952885573099962	0.5689555121683512	T	T	T
0.3291059446641640	0.7246804664393949	0.5693731041911221	T	T	T
0.5841011160779033	0.0160209470170258	0.5880004171101234	T	T	T
0.5856871322108290	0.3489267694347120	0.5890906555530506	T	T	T
0.5862530209640511	0.6778309401850038	0.5894967674948788	T	T	T

0.8427221338180004	0.6277143443812037	0.6104849611553576	T	T	T
0.8435072115719464	0.3000839758885618	0.6108125562708437	T	T	T
0.8411244965103180	0.9664461513985856	0.6091501486220636	T	T	T
0.0980653679704346	0.5850261148836111	0.6320904454022909	T	T	T
0.0943898195204511	0.2545728323692060	0.6334116980254478	T	T	T
0.1024426403823142	0.9149659302844597	0.6312033165526785	T	T	T
0.3526420886478903	0.5371670265289552	0.6545569438241969	T	T	T
0.3487774940135466	0.2070477726462556	0.6506647457770498	T	T	T
0.3522473286875183	0.8758210849668657	0.6506906024450458	T	T	T
0.6195521628794083	0.4996107706755666	0.6729480909845833	T	T	T
0.6019745305101054	0.1663548439622957	0.6733045430638853	T	T	T
0.6067141517328949	0.8338790839126489	0.6694732965564114	T	T	T
0.8711083000529669	0.1031357185093640	0.6877980980618190	T	T	T
0.8587164279776047	0.7852613056858289	0.6882467118915301	T	T	T
0.4646919592367738	0.4044776816273341	0.7259511721624818	T	T	T
0.5235391757990087	0.4972813365544653	0.7432422721474197	T	T	T
0.3929986502575034	0.3832433291189190	0.7530163175793447	T	T	T

CHO/Cu(533) $E_{ads} = -1.55$ eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O H

60 1 1 1

Selective dynamics

Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0477570937387739	0.2935531152752517	0.4657471731768013	T	T	T
0.0478781844148273	0.6267862483676012	0.4658681932088413	T	T	T
0.0478251200189703	0.9600711610659758	0.4657833177291693	T	T	T
0.3053977049958831	0.2445846226054869	0.4865813597762738	T	T	T
0.3055244092941436	0.5791979026693852	0.4866115738333647	T	T	T
0.3053451251396098	0.9122114860933337	0.4871898861073376	T	T	T

0.5614249481872804 0.1989515424381594 0.5070361109205592 T T T
0.5602960563159485 0.5328421117125046 0.5071658903069149 T T T
0.5604178988336912 0.8663665426497857 0.5072655274206710 T T T
0.8175079164169219 0.1517597746956483 0.5277548456857346 T T T
0.8173246815935116 0.4858106850379897 0.5276316619527393 T T T
0.8172839301119339 0.8187028726871901 0.5275881332185008 T T T
0.0750144603286955 0.1042352801532118 0.5476649557296653 T T T
0.0750396108564360 0.4360980996342008 0.5477252404722535 T T T
0.0753434230346457 0.7716999442307824 0.5475807914300717 T T T
0.3304179053518439 0.0593703134515664 0.5701902273498689 T T T
0.3328445534394859 0.3892249812264765 0.5682943531021323 T T T
0.3311207753458447 0.7225579412669987 0.5700719424289318 T T T
0.5854074802425870 0.0124507831170391 0.5895137615369137 T T T
0.5856326902507760 0.3443258632109902 0.5897275050857687 T T T
0.5869929681832744 0.6778011031953497 0.5892599789028736 T T T
0.8469373241477101 0.6290094807966682 0.6098826129791988 T T T
0.8457274961030521 0.2954196012832213 0.6090468915869209 T T T
0.8485951512898353 0.9583512475684799 0.6096315054374060 T T T
0.1048675507771222 0.5791549337017017 0.6279392347006834 T T T
0.1014263755007931 0.2464741123377294 0.6319766356725722 T T T
0.1028783770731465 0.9168022711842028 0.6316323399263482 T T T
0.3505468495898185 0.5368868740121897 0.6562483502889833 T T T
0.3507509746253774 0.2107383184086018 0.6561633771508326 T T T
0.3568218210866263 0.8702536820234883 0.6526629014517553 T T T
0.6074305018184276 0.4921121926835141 0.6720937969740390 T T T
0.6217549346095552 0.1451163966912290 0.6715420203102695 T T T
0.6135229428960685 0.8249548152139994 0.6719823821271973 T T T
0.8614846985058051 0.4464056829125127 0.6892367821158842 T T T
0.8658107032542333 0.1159598278710448 0.6893058294352414 T T T
0.8846218485577921 0.7623501566246915 0.6926307437034183 T T T
0.2476046777505019 0.4616842649515220 0.7134657748800635 T T T
0.1054892457262042 0.5793227672002033 0.7309654361877023 T T T
0.3430109699667341 0.3804986785388920 0.7433280444083721 T T T

CHO/Cu(533) $E_{ads} = -1.53$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F

0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0477484573362252	0.2935703468384782	0.4657814492864943	T	T	T
0.0477148842212587	0.6267993550715840	0.4658870857026499	T	T	T
0.0472974178904438	0.9605700510182053	0.4658632926624056	T	T	T
0.3047395161407231	0.2464170210875379	0.4869200795246296	T	T	T
0.3045090707050939	0.5796615305502677	0.4869827545759767	T	T	T
0.3046720628019113	0.9119130322530113	0.4867866779273541	T	T	T
0.5599666713967957	0.1999457977711109	0.5069908606392877	T	T	T
0.5597793559084669	0.5333151225426885	0.5069121004516692	T	T	T
0.5601254894601151	0.8660760253067956	0.5070937739165905	T	T	T
0.8159590625240868	0.1531675115103029	0.5276624750181260	T	T	T
0.8170252945490600	0.4854253781398220	0.5274277910015563	T	T	T
0.8168135932357062	0.8188539822940700	0.5275625971926725	T	T	T
0.0733326384259740	0.1050409582087768	0.5478304206211126	T	T	T
0.0738798209840108	0.4378532036050924	0.5479859339621695	T	T	T
0.0734495166271132	0.7719878253379120	0.5478778418759991	T	T	T
0.3293204118772948	0.0580592362945164	0.5686065936919513	T	T	T
0.3293253524172312	0.3932446519891142	0.5698055595572555	T	T	T
0.3295034419892760	0.7240874668530378	0.5699485739291245	T	T	T
0.5861094528347960	0.0114868717248504	0.5889051692868121	T	T	T
0.5843553260570979	0.3468914897175841	0.5897054893458101	T	T	T
0.5870215165944723	0.6751558213396845	0.5894355375504328	T	T	T
0.8452398179542041	0.6278240408737802	0.6092696029246831	T	T	T
0.8431138983361803	0.2970355845155714	0.6095070575104344	T	T	T
0.8453278613187611	0.9622337340837437	0.6091553096195943	T	T	T
0.0998695632160634	0.5814800456912689	0.6318323785713539	T	T	T
0.1018902767455243	0.2471997523246909	0.6318783604976194	T	T	T
0.1003009620677147	0.9171655639446770	0.6314815479927343	T	T	T
0.3482108172083184	0.5393710313901384	0.6537138803435131	T	T	T
0.3557768814608161	0.2012130129383927	0.6512693873191241	T	T	T
0.3559384329064511	0.8722248906176098	0.6509699722698504	T	T	T
0.6095570825412873	0.4920612615525017	0.6757764081282284	T	T	T
0.6129217575272750	0.1536623420444097	0.6714796298176030	T	T	T
0.6106418391889514	0.8245311376867017	0.6717399441814040	T	T	T
0.8681708861853586	0.4439599761453211	0.6895041342262360	T	T	T
0.8679387551774530	0.1084369296578397	0.6893627411645673	T	T	T
0.8653326351364340	0.7779576285194681	0.6897701117440596	T	T	T
0.4965423178950654	0.5211925508181642	0.7376104954956827	T	T	T
0.3614566828994470	0.5632448271167347	0.7384303953134267	T	T	T
0.5528147963704252	0.5079557979889624	0.7747459909487195	T	T	T

CHO/Cu(533) $E_{ads} = -1.51$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1

Selective dynamics
Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0471522469131241	0.2944893856175225	0.4658100636231822	T	T	T
0.0474135268435887	0.6278145368618239	0.4658841645705999	T	T	T
0.0472770149011125	0.9612439425307051	0.4658376934694605	T	T	T
0.3041091566363961	0.2473636637060923	0.4865654602920570	T	T	T
0.3038250360384262	0.5809732771026258	0.4867884863705280	T	T	T
0.3036827721840254	0.9139082688471902	0.4869042005233734	T	T	T
0.5595620973000807	0.2021846313248796	0.5069742591924770	T	T	T
0.5593856271179365	0.5352965995917841	0.5068635106410553	T	T	T
0.5597110098188470	0.8672694529579653	0.5069254489135143	T	T	T
0.8160661115965495	0.1546711844015160	0.5275671316037561	T	T	T
0.8159963501834004	0.4876977634253100	0.5276541052994732	T	T	T
0.8164763512121224	0.8207928138493056	0.5273817464574970	T	T	T
0.0718968346886268	0.1078474052144483	0.5482211450336245	T	T	T
0.0728403535877380	0.4408519575064946	0.5480098235686173	T	T	T
0.0720767225382715	0.7746491386567042	0.5480930983777479	T	T	T
0.3283813040400224	0.0613851464436538	0.5684329233229868	T	T	T
0.3281998708336293	0.3951922768012351	0.5689960520296254	T	T	T
0.3285169402858035	0.7263687196907086	0.5694339369822236	T	T	T
0.5852956096344938	0.0156106081739280	0.5886510556400029	T	T	T
0.5850812310223591	0.3492661650960001	0.5894456022892144	T	T	T
0.5849362561837257	0.6800590064290168	0.5894428222755267	T	T	T
0.8440943832283678	0.6328765240058383	0.6091012944833727	T	T	T
0.8423567895207765	0.2998097380837490	0.6100064363528985	T	T	T
0.8414316289599426	0.9680594290155917	0.6095887697129498	T	T	T
0.0994265988241657	0.5854297835467867	0.6323859364758916	T	T	T
0.1000223200726420	0.2513184730504103	0.6317505654258837	T	T	T
0.1016601020056935	0.9162850235156109	0.6317427075326674	T	T	T
0.3523128078228394	0.5383622329810313	0.6530055636570599	T	T	T
0.3518606392882118	0.2057318742547402	0.6505890558822822	T	T	T
0.3530381544538060	0.8757776278335536	0.6507361669259462	T	T	T
0.6098269402270232	0.5019239933422861	0.6741114660609409	T	T	T
0.6035728766000469	0.1652105746907212	0.6742502186238919	T	T	T

0.6090351166688224 0.8295465403489588 0.6711001216122913 T T T
0.8671611124532810 0.4497753217245640 0.6894888065382831 T T T
0.8690405371751153 0.1115180328904985 0.6891374194656193 T T T
0.8613329256418620 0.7862441777850127 0.6894168676764454 T T T
0.4774211486084123 0.3713071262064295 0.7310098820457006 T T T
0.5042872355322099 0.5004582748626559 0.7476674081868843 T T T
0.4067149706970959 0.3386241438966109 0.7555891997725617 T T T

CHO/Cu(533) E_{ads} = −1.51 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0477166225503397 0.2938046042383574 0.4657539321584985 T T T
0.0476985178753026 0.6274084219924144 0.4659165970482455 T T T
0.0472771256449839 0.9611116510669331 0.4659965971189876 T T T
0.3045592810580603 0.2471842599119424 0.4869114978063965 T T T
0.3039784991439239 0.5801971129648005 0.4869307654264699 T T T
0.3044806188570026 0.9130723412621089 0.4871577066109829 T T T
0.5595332827358704 0.2009333151149142 0.5068425575866398 T T T
0.5595497829618321 0.5336094057227992 0.5069991513002495 T T T
0.5597240277379943 0.8667901048233243 0.5066593151458029 T T T
0.8156565470738633 0.1539309706786561 0.5277254761207151 T T T
0.8171956109302797 0.4858252939920972 0.5273976782823482 T T T
0.8170638409857846 0.8197176059542952 0.5273809411611237 T T T
0.0739962185885454 0.1061801677902101 0.5479890231227370 T T T
0.0740445149169598 0.4392397033761939 0.5478306571580361 T T T
0.0726742359419590 0.7741124437286054 0.5482124656123790 T T T
0.3295716999443562 0.0615429307219234 0.5694849060520170 T T T

0.3294559484445693 0.3935477109718903 0.5701525636511560 T T T
0.3284967627972350 0.7256266258301433 0.5698139684392689 T T T
0.5862208753073623 0.0117912484153346 0.5882494029654266 T T T
0.5837840170261291 0.3457329360585851 0.5898149385976384 T T T
0.5855972158358254 0.6787852274376106 0.5884183351295278 T T T
0.8454914042312049 0.6290336245062538 0.6090237099537444 T T T
0.8453726858163139 0.2957572481178431 0.6090712038441803 T T T
0.8419017198391283 0.9649441523393077 0.6097469891783092 T T T
0.0993857213159966 0.5854950118643119 0.6310100598832572 T T T
0.1034346143308035 0.2506979008004815 0.6321876526035350 T T T
0.0981533500653589 0.9223438571702205 0.6319928857874382 T T T
0.3484008036306361 0.5530536336961075 0.6537523219854139 T T T
0.3572508428824789 0.2029864576823937 0.6545984489214453 T T T
0.3552828730794440 0.8742385990731550 0.6514804688481274 T T T
0.6115984698715995 0.4925280306054162 0.6709005004416644 T T T
0.6063043571422480 0.1553000373178557 0.6749513943670055 T T T
0.6133479533328282 0.8177775056873737 0.6707416998523041 T T T
0.8674788340217972 0.4419095431847485 0.6894725712699766 T T T
0.8606696917430344 0.1140783001818610 0.6895124016976567 T T T
0.8657867633196542 0.7768037679704368 0.6896371482463457 T T T
0.4173441579366252 0.2767072920461168 0.7243195740725135 T T T
0.3362671950981478 0.4810677633670444 0.7330496618665913 T T T
0.4294624559514502 0.1704391656833279 0.7559288557935280 T T T

CHO/Cu(533) $E_{ads} = -1.51$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F

0.0477991616594866 0.2935720563744347 0.4658572054517864 T T T
0.0477136274860430 0.6269271483659141 0.4658616767215963 T T T
0.0476025088420797 0.9603893044340882 0.4658788303274445 T T T
0.3048229115639911 0.2460039001947892 0.4867963024494880 T T T
0.3046593163327770 0.5796559066539700 0.4868765447686529 T T T
0.3049266890232015 0.9123454799103240 0.4867354632943309 T T T
0.5602182249938367 0.2000091389555584 0.5070456262762500 T T T
0.5601488933694730 0.5333378666878152 0.5070106690479692 T T T
0.5603997231888441 0.8661605963857720 0.5071877195362348 T T T
0.8169250380471063 0.1526544401498254 0.5275663140807206 T T T
0.8172100430274067 0.4855705123813986 0.5275434250629280 T T T
0.8171074114651593 0.8190920822857217 0.5276093173474987 T T T
0.0738966346634050 0.1049383240184923 0.5480381897874820 T T T
0.0741591913657941 0.4381278232067141 0.5480517702959979 T T T
0.0740274558022126 0.7718577248875711 0.5480883189377949 T T T
0.3298308593019212 0.0579952060523778 0.5690475473948481 T T T
0.3297155652118075 0.3920124585498509 0.5691132372495115 T T T
0.3297446359571458 0.7254549368786851 0.5694114553418036 T T T
0.5864740638249037 0.0115710757080079 0.5890161743775204 T T T
0.5867998895826073 0.3461602400077617 0.5897059530518656 T T T
0.5871943860996788 0.6756326574201388 0.5897263946408391 T T T
0.8457257171076882 0.6284526321853169 0.6092145248655999 T T T
0.8439810543306626 0.2967066851211372 0.6095440736934226 T T T
0.8459478862403272 0.9624053640127224 0.6092633462287116 T T T
0.1017883204819887 0.5815071639651994 0.6322161606882568 T T T
0.1028170110766664 0.2471888847131627 0.6318746080021264 T T T
0.1016282576314328 0.9158360864556510 0.6323874944237364 T T T
0.3539997162333715 0.5369667354738872 0.6512822895902488 T T T
0.3556162014645734 0.2034041549635975 0.6518224856795924 T T T
0.3556382472943013 0.8708626824171168 0.6518446804381628 T T T
0.6054219045723027 0.4960974985410403 0.6782872803927872 T T T
0.6101644063966710 0.1573146140223259 0.6717855436660333 T T T
0.6101435955489074 0.8257157586756552 0.6717484068665116 T T T
0.8688825267344328 0.4443215691415581 0.6888773367016084 T T T
0.8650373599134087 0.1121119139423934 0.6894250999707616 T T T
0.8647181437688384 0.7797894952319931 0.6895531986484725 T T T
0.5395600351682805 0.5481751497398392 0.7501313004754252 T T T
0.4204044709592313 0.5771210472306205 0.7672429640572245 T T T
0.6254828801718310 0.5480004325630966 0.7757301403583156 T T T

CHO/Cu(533) $E_{ads} = -1.50$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F

0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0469947605252026	0.2938506689902048	0.4658269495047345	T	T	T
0.0475666913328802	0.6268709708904655	0.4660033042168268	T	T	T
0.0474627315587113	0.9602977435138459	0.4659427715969904	T	T	T
0.3045608768742632	0.2460050359206633	0.4866561726687982	T	T	T
0.3039457806029212	0.5798085128486907	0.4866292185023259	T	T	T
0.3036731131246488	0.9131398127801559	0.4868794567890031	T	T	T
0.5597635885633425	0.2004561989577338	0.5068998242127178	T	T	T
0.5597027824366486	0.5332690143130987	0.5068702100267510	T	T	T
0.5595481798887523	0.8659105265733021	0.5070340651877048	T	T	T
0.8161182526890687	0.1528738272273430	0.5275929423517277	T	T	T
0.8159533677526146	0.4858835587680986	0.5277118500928110	T	T	T
0.8165623413071792	0.8191727727707300	0.5274207289456563	T	T	T
0.0718891047069320	0.1061422638243546	0.5482473424925214	T	T	T
0.0736276317175249	0.4376902484710266	0.5478629114160810	T	T	T
0.0732773569816516	0.7717377248395161	0.5482631127075653	T	T	T
0.3284476075439607	0.0585752617060906	0.5687460406220248	T	T	T
0.3289061100014586	0.3934548434553006	0.5693717204218824	T	T	T
0.3287767288001012	0.7238576037229520	0.5692485240934189	T	T	T
0.5851966529438586	0.0117081216592072	0.5883068522390587	T	T	T
0.5847106618767007	0.3466066747624752	0.5895914455859304	T	T	T
0.5847113608058100	0.6766259020028176	0.5897537431791210	T	T	T
0.8446178721717708	0.6284106368229184	0.6089822874269528	T	T	T
0.8418978338192706	0.2974107407750652	0.6100476638540834	T	T	T
0.8441448534407753	0.9625940798133631	0.6093146532859361	T	T	T
0.0998002771377031	0.5810092253552549	0.6316014001553655	T	T	T
0.1007621231350968	0.2484278992783399	0.6319767929539092	T	T	T
0.1003941077372573	0.9159334383546727	0.6317152688321429	T	T	T
0.3517289332186282	0.5369045380570902	0.6542946307633860	T	T	T
0.3547532636464524	0.2011399968211054	0.6513428046631642	T	T	T
0.3527352504981958	0.8729912460954445	0.6509875654879489	T	T	T
0.6121003018866183	0.4928103198255704	0.6751884240241005	T	T	T
0.6099469981201378	0.1537478053959278	0.6708619793379477	T	T	T
0.6097581152750421	0.8253200816030875	0.6712828283570622	T	T	T
0.8673415957331015	0.4450117992474955	0.6895345495209273	T	T	T
0.8665511692999984	0.1087051470567452	0.6894426575537497	T	T	T
0.8646575229180392	0.7786200988114924	0.6894284833974368	T	T	T
0.3647544484840821	0.5695526466465999	0.7264432266833465	T	T	T
0.4760882717286659	0.5572437974727392	0.7476040156342042	T	T	T
0.2630964377992258	0.6048007917510891	0.7505203707617715	T	T	T

CHO/Cu(533) $E_{ads} = -1.50$ eV

1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0474661826589866 0.2938460417881409 0.4658797875143154 T T T
0.0475046895359650 0.6272955981544711 0.4658198203045197 T T T
0.0472112678734803 0.9608832671118559 0.4658677832082678 T T T
0.3043700888666567 0.2459022533807334 0.4864695925847868 T T T
0.3036347536643413 0.5811175918799679 0.4866068186027823 T T T
0.3043180578785004 0.9132517898101546 0.4869872881716680 T T T
0.5598695999280989 0.2006641154768521 0.5068346696668679 T T T
0.5594237197141965 0.5335709553088230 0.5070339915697495 T T T
0.5597492659781982 0.8676204521121237 0.5070145579804007 T T T
0.8159850896988472 0.1536584726691939 0.5276291949971894 T T T
0.8165025738614490 0.4863386880723013 0.5274533524466842 T T T
0.8161391792128145 0.8203802414017272 0.5274757457736524 T T T
0.0737246710199751 0.1052294792588792 0.5480435850492161 T T T
0.0734703499059946 0.4385956437108012 0.5477960825602447 T T T
0.0718487904719635 0.7745035654616792 0.5480816113964410 T T T
0.3286774438812095 0.0610355772099882 0.5694883903924045 T T T
0.3288044344361608 0.3931453017090532 0.5680509765528419 T T T
0.3290881126675304 0.7241354696151626 0.5695378714437372 T T T
0.5842837538922840 0.0152725339421819 0.5895597355352825 T T T
0.5838654413683135 0.3454951505098458 0.5898596506969775 T T T
0.5850620103314824 0.6794537599338476 0.5884485844022689 T T T
0.8443639323231172 0.6299561423391624 0.6090357737368902 T T T
0.8449012056464782 0.2962132033832641 0.6091468922586425 T T T
0.8412381103345643 0.9666066825712976 0.6100223479168564 T T T
0.0973177662935108 0.5863180193835689 0.6299649623308146 T T T
0.1005467638994739 0.2488421079816783 0.6321720599349823 T T T

0.1011204967817870 0.9164044732990418 0.6318893483687321 T T T
0.3486229283045481 0.5394487037944203 0.6537493391065990 T T T
0.3498011905506022 0.2106452953428276 0.6530255494398528 T T T
0.3548804087444272 0.8705555951472126 0.6515831483571356 T T T
0.6105409039809655 0.4939002494545230 0.6709419603641117 T T T
0.6164021778858459 0.1543748638526702 0.6753093275183456 T T T
0.6102007033580543 0.8229893610901092 0.6706787807402608 T T T
0.8648873327630997 0.4470942548605276 0.6895491113896544 T T T
0.8691072577030311 0.1120848121883330 0.6896315023204934 T T T
0.8677652916646772 0.7752799357365127 0.6895052928632633 T T T
0.3354161761680333 0.3784602688531585 0.7162947836898670 T T T
0.4622663841657234 0.2807753464291324 0.7422588877997639 T T T
0.2178385355315318 0.4719764806473602 0.7370661025905925 T T T

CHO/Cu(533) $E_{ads} = -1.50$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0476723740516597 0.2935119070426531 0.4658173768024194 T T T
0.0479274519314488 0.6268921556428649 0.4659692841116322 T T T
0.0480600726835427 0.9600828135442151 0.4659052334999901 T T T
0.3053038871205921 0.2457348322259194 0.4867346066459374 T T T
0.3049236017143160 0.5792903568266921 0.4868129073661197 T T T
0.3049828300971922 0.9124604251674691 0.4869312574120528 T T T
0.5605456848877267 0.1999028737489569 0.5069079961628824 T T T
0.5605419295428934 0.5331306548075999 0.5068784822667969 T T T
0.5603901917347313 0.8663726726736342 0.5069236403217243 T T T
0.8175286389112042 0.1520150788684830 0.5275370562320291 T T T

0.8178233650782781 0.4852299663103561 0.5276390983175256 T T T
0.8176939782223621 0.8188372990756382 0.5274665558192302 T T T
0.0752007973373538 0.1041142538251739 0.5479816146829841 T T T
0.0752286552606540 0.4370108257491874 0.5477930339771984 T T T
0.0751786644476419 0.7712736123389188 0.5481850222223612 T T T
0.3302522573451067 0.0583510160139410 0.5692487901945879 T T T
0.3308604855112336 0.3924699136487070 0.5697266358778633 T T T
0.3309158203363888 0.7228480597210961 0.5699051699985982 T T T
0.5874022002977016 0.0112152512032356 0.5887112270451176 T T T
0.5854826669523813 0.3456673527182189 0.5891278992689821 T T T
0.5872044528541839 0.6776619737158612 0.5888062568317021 T T T
0.8470271850646131 0.6281627001308721 0.6093848772832582 T T T
0.8474853034055693 0.2940604953768011 0.6091926692398045 T T T
0.8470438846191306 0.9612256165074660 0.6094752035075319 T T T
0.1022517744638783 0.5798404053744507 0.6306612322328370 T T T
0.1036576285857004 0.2472807056075266 0.6323141443434714 T T T
0.1030476609951539 0.9157581563956151 0.6319091565046486 T T T
0.3524262258454540 0.5394326686826060 0.6578871685841086 T T T
0.3577782039090794 0.2014907550834170 0.6519672054324974 T T T
0.3572639359179519 0.8702135801687482 0.6520478071522562 T T T
0.6133206484698965 0.4916734777213789 0.6708689304561933 T T T
0.6127698087487030 0.1550516944961204 0.6714523986052903 T T T
0.6120580654431387 0.8241870202233422 0.6719850462121838 T T T
0.8666387842482285 0.4454152849118836 0.6895492115220834 T T T
0.8646089803087373 0.1146209815278249 0.6894231777557316 T T T
0.8687740961419180 0.7769550816382306 0.6900506792020608 T T T
0.2944428597529215 0.5816512394374000 0.7303102975484873 T T T
0.1691077159432053 0.6359688792176855 0.7492493093997851 T T T
0.3930896998289713 0.5513533530899024 0.7552088726315956 T T T

CHO/Defected-Cu(533) $E_{ads} = -1.50$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
59 1 1 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F

0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0469259495364511 0.2935646950460153 0.4659528429733797 T T T
0.0468395985732002 0.6266926575754468 0.4660720713033868 T T T
0.0468920807359652 0.9608134727002735 0.4658724960651810 T T T
0.3031505651081119 0.2465819314526101 0.4866991329807675 T T T
0.3035453392113112 0.5796227657257802 0.4866042992930488 T T T
0.3031193457606349 0.9128277787306303 0.4867990287584831 T T T
0.5591952556304065 0.2002149555757526 0.5069043467526981 T T T
0.5591111797723656 0.5335884855262307 0.5065275157115323 T T T
0.5587738417654222 0.8660297622652564 0.5072408736846654 T T T
0.8159986068914336 0.1524301854997390 0.5275152997490267 T T T
0.8153649893256585 0.4860980164251956 0.5275265595800533 T T T
0.8153698935316811 0.8194597545264983 0.5276827850721801 T T T
0.0707964867751443 0.1066898342005089 0.5484911635802021 T T T
0.0708287683797408 0.4393328038225235 0.5484265700276509 T T T
0.0718172736513623 0.7724474116770494 0.5478918265681401 T T T
0.3261015179094429 0.0601035474394394 0.5685945087771955 T T T
0.3274534760818995 0.3930701499359728 0.5690899780012160 T T T
0.3284274450516804 0.7238090507727577 0.5690832894884181 T T T
0.5836896287850379 0.0133100377467557 0.5888168832833145 T T T
0.5849229482280052 0.3455030239905739 0.5884388132768876 T T T
0.5852879403913960 0.6755504049048966 0.5892655417632326 T T T
0.8422588086000573 0.6264227694427120 0.6103575763951739 T T T
0.8419549669567630 0.2998684037465367 0.6110196069081439 T T T
0.8412885477228897 0.9644598084501368 0.6093794191112281 T T T
0.0982752492494541 0.5823636017848060 0.6317532280025446 T T T
0.0938222268954476 0.2534181967761384 0.6331238903604657 T T T
0.1003601799604823 0.9149265638482831 0.6310790179009445 T T T
0.3513038509048272 0.5383177937598305 0.6536746693068309 T T T
0.3496263764227905 0.2039758538526399 0.6508543114867607 T T T
0.3500356877235831 0.8757530043400052 0.6508602993888104 T T T
0.6099439107184494 0.4935082765250343 0.6713911785039670 T T T
0.6032411780241915 0.1616046693005799 0.6737658713020664 T T T
0.6076141679840532 0.8246662713948396 0.6699493802746233 T T T
0.8687360164211029 0.1046317311319029 0.6882912501051024 T T T
0.8597152638186856 0.7817168806045132 0.6881474996002410 T T T
0.4877360660278498 0.4354081465650097 0.7234103061349657 T T T
0.4142987523651911 0.4407366473120859 0.7597319360002359 T T T
0.5654492970602689 0.5073783635041949 0.7336102675530611 T T T

CHO/Cu(533) E_{ads} = −1.49 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F

0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0479400070930162	0.2934790348136527	0.4659187764992857	T	T	T
0.0479988423908150	0.6267409377528370	0.4658377529056034	T	T	T
0.0478650358582716	0.9602756954095161	0.4658937201204223	T	T	T
0.3050590013865405	0.2457942505962603	0.4868199995979449	T	T	T
0.3050212996756142	0.5793077474775240	0.4867658438869871	T	T	T
0.3049961943451682	0.9124420715658715	0.4867486087233482	T	T	T
0.5607628336089964	0.1995681542315846	0.5069628765327161	T	T	T
0.5604673320097475	0.5332922580816248	0.5070229942910405	T	T	T
0.5606269911679744	0.8659452929223728	0.5070702582262810	T	T	T
0.8177037832339172	0.1521829030447894	0.5274673017489012	T	T	T
0.8175958175164801	0.4853369183561653	0.5275382892155164	T	T	T
0.8179165512520837	0.8183501963116958	0.5275658426566951	T	T	T
0.0744400241044143	0.1047680310948340	0.5481798989746184	T	T	T
0.0748651309871327	0.4377810004226030	0.5481544519019973	T	T	T
0.0748886661842814	0.7712399935045767	0.5480911037384499	T	T	T
0.3300139386404631	0.0577979261239167	0.5691834600995191	T	T	T
0.3304907373950023	0.3918789529213793	0.5690574452282552	T	T	T
0.3302321015642741	0.7250642242443370	0.5692852277928042	T	T	T
0.5871428996773339	0.0106901236370291	0.5885871995652003	T	T	T
0.5876415632054712	0.3457157189711201	0.5894447070357933	T	T	T
0.5875381856846000	0.6756672436900124	0.5897181058496037	T	T	T
0.8466276111117168	0.6273352793011138	0.6093103489456438	T	T	T
0.8448479126755485	0.2960655147300354	0.6095199699420021	T	T	T
0.8469783205958521	0.9617686510442190	0.6090954693698198	T	T	T
0.1032791368260877	0.5809071507978495	0.6322258337590118	T	T	T
0.1030047882662363	0.2475553417161186	0.6322742417935666	T	T	T
0.1025328839954716	0.9150705729897755	0.6324923772903209	T	T	T
0.3557894145828719	0.5368199128350580	0.6517367176525387	T	T	T
0.3561785197379291	0.2035059970260825	0.6516520537555448	T	T	T
0.3556313663779585	0.8701665443732995	0.6518834987839290	T	T	T
0.6061815149667090	0.4952078714306152	0.6780810494921702	T	T	T
0.6109762387901243	0.1558675983333517	0.6707432600370176	T	T	T
0.6108515236522233	0.8269149471229360	0.6711630413510083	T	T	T
0.8675573369484486	0.4442013355017985	0.6892035021093808	T	T	T
0.8656371300157535	0.1116160054190763	0.6893161383650185	T	T	T
0.8662814144801887	0.7788210903865694	0.6892495729290036	T	T	T
0.5590653120003646	0.5448045169600768	0.7512560859427596	T	T	T

0.5551485994463343 0.6804117052581520 0.7767750821750991 T T T
0.5336875727034253 0.4339550535568814 0.7686918828237165 T T T

CHO/Cu(533) $E_{ads} = -1.49$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0474587004470008 0.2938686123677135 0.4659453842653855 T T T
0.0476796139432244 0.6270893433976827 0.4659572524345861 T T T
0.0477061640219874 0.9604591701624257 0.4659935489933871 T T T
0.3047193164613683 0.2463716553118201 0.4867360148541682 T T T
0.3044315679591725 0.5799314080176968 0.4868254576895537 T T T
0.3043773046193727 0.9130842873460396 0.4867800378229374 T T T
0.5600384331173346 0.2004008558240978 0.5068201739434199 T T T
0.5600982908082203 0.5334634385743878 0.5068045775307504 T T T
0.5600394614346093 0.8666121068693966 0.5069116353397009 T T T
0.8168639604626201 0.1527221393259502 0.5275588814478890 T T T
0.8173875664064199 0.4855938893816772 0.5276049938472642 T T T
0.8173082372673927 0.8190551734550605 0.5274790387303553 T T T
0.0740191187137411 0.1050712380815600 0.5482371971654968 T T T
0.0746277159464554 0.4384109956399870 0.5480805232776048 T T T
0.0743141003031844 0.7717990001395888 0.5482515824246138 T T T
0.3292831921077226 0.0589706894810155 0.5687929212910512 T T T
0.3295643596927870 0.3938472592473229 0.5696626930098748 T T T
0.3297514723109968 0.7244476231432760 0.5696290867238154 T T T
0.5868898007636184 0.0118264005891274 0.5886102108155649 T T T
0.5847148583943081 0.3464536726040781 0.5890117114144127 T T T
0.5867010824315524 0.6773817971852457 0.5888706173403455 T T T

0.8465673625842414	0.6279573028410909	0.6092367896711751	T	T	T
0.8459609241722462	0.2950342148962813	0.6094608401455635	T	T	T
0.8455732005513099	0.9623213894480026	0.6092837108095690	T	T	T
0.1016121759514932	0.5818425880912236	0.6322195500200062	T	T	T
0.1021935101453006	0.2486689563927187	0.6323712204026307	T	T	T
0.1016271378138404	0.9159136660333342	0.6321323408055061	T	T	T
0.3531145614514545	0.5393739032158689	0.6567423977576566	T	T	T
0.3568987600324591	0.2003158789946628	0.6508110732883576	T	T	T
0.3564994790069494	0.8721965852922582	0.6511812776097938	T	T	T
0.6111598481374272	0.4913965710091102	0.6716143275264086	T	T	T
0.6101543776788705	0.1577804408344688	0.6715778133385688	T	T	T
0.6103979349730494	0.8248612050798972	0.6716972290076290	T	T	T
0.8647407152164831	0.4464795226076742	0.6896413477300173	T	T	T
0.8642521919592023	0.1128401367702036	0.6895746841066926	T	T	T
0.8640491153770340	0.7800866776080360	0.6895326709549906	T	T	T
0.3035576365021989	0.5881406148691650	0.7297631586425126	T	T	T
0.2966917867637015	0.7243717071020912	0.7558784126240907	T	T	T
0.2763842505159537	0.4770328459111567	0.7457963122283386	T	T	T

CHO/Cu(533) $E_{ads} = -1.47$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0475215921740043	0.2934586774128344	0.4658882119672759	T	T	T
0.0476320218151118	0.6272230112764600	0.4658320456208991	T	T	T
0.0475838984545291	0.9603006941234166	0.4658419618872247	T	T	T
0.3046762509957514	0.2457751923271372	0.4865697753359867	T	T	T
0.3046937998010764	0.5794241616004501	0.4867052212011492	T	T	T

0.3039304432899999 0.9131476313615521 0.4868610728604223 T T T
0.5599618199106488 0.2003352789474642 0.5070861134702110 T T T
0.5593694535535523 0.5333656100864433 0.5071735531707059 T T T
0.5599847136704350 0.8662083910876330 0.5072999132764043 T T T
0.8164911992054708 0.1526714556625340 0.5274124088959514 T T T
0.8161282393105289 0.4858165181300754 0.5276653927361258 T T T
0.8166370431911704 0.8187439026939104 0.5272290959733787 T T T
0.0720737791168651 0.1063307751502962 0.5484966432321755 T T T
0.0734499637329230 0.4385380113107211 0.5478478541354026 T T T
0.0738372422006149 0.7721959610075380 0.5479911012657566 T T T
0.3286446151766951 0.0596316027701115 0.5687658820593777 T T T
0.3291911137684236 0.3922244857928010 0.5687703419491315 T T T
0.3268166462584698 0.7276171194903236 0.5693089898729599 T T T
0.5859161153294058 0.0133536591049265 0.5893544684056298 T T T
0.5858123685417598 0.3452357903472807 0.5900503781427138 T T T
0.5847772099326446 0.6772816936973169 0.5895151411647119 T T T
0.8440664135223824 0.6289280822592781 0.6087939155904128 T T T
0.8421407983194108 0.2954487711782917 0.6101120826915272 T T T
0.8449123243750591 0.9614875817232791 0.6085309977524543 T T T
0.1014842324191909 0.5821747941755859 0.6316036785154808 T T T
0.1010789034438721 0.2496555173940933 0.6318046805531412 T T T
0.0965511856977215 0.9200187477906112 0.6337405796897040 T T T
0.3513577810879533 0.5403808572416658 0.6506802157437531 T T T
0.3548675114930214 0.2052128051507781 0.6518268809149048 T T T
0.3506448947261159 0.8765663973181097 0.6514177139367824 T T T
0.6013555380200256 0.5073900906447474 0.6737375109129929 T T T
0.6084582814212232 0.1547693153583982 0.6747610152873689 T T T
0.6090090635224529 0.8262911851763060 0.6710851193541219 T T T
0.8678484077244958 0.4425242234343179 0.6887221041481317 T T T
0.8575935921151920 0.1103356009168974 0.6910562123139440 T T T
0.8695741032441617 0.7695990445333991 0.6885106972650720 T T T
0.6479812765029497 0.2330211465579356 0.7423524408557792 T T T
0.5885453558163997 0.4321542723264348 0.7516815964734292 T T T
0.6688474679232176 0.1282859424045298 0.7756454263275279 T T T

CHO/Cu(533) $E_{ads} = -1.46$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H
60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F

0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0470135314203167	0.2946327755545433	0.4657386263797369	T	T	T
0.0465879152803933	0.6282139239640289	0.4661069886605440	T	T	T
0.0464197731522722	0.9611267854472547	0.4660861286964913	T	T	T
0.3033078638497929	0.2484869746073417	0.4868281763204803	T	T	T
0.3028633802741764	0.5818954176877811	0.4866870245067185	T	T	T
0.3034805464039338	0.9139077594979200	0.4867590345982991	T	T	T
0.5581645519092469	0.2027310445123709	0.5068454680092062	T	T	T
0.5579885036093890	0.5356890812955940	0.5068102908606675	T	T	T
0.5586733133317539	0.8687898829829137	0.5067450814861924	T	T	T
0.8141134647303743	0.1551810736340286	0.5276480996903318	T	T	T
0.8149309304623139	0.4885976925262390	0.5273285365268964	T	T	T
0.8142016345035872	0.8224541571049163	0.5276198998922629	T	T	T
0.0713307795317144	0.1081097265738180	0.5472861102751886	T	T	T
0.0719063614778746	0.4417857627960513	0.5481983522549179	T	T	T
0.0717029811884798	0.7730310965965599	0.5487134218255042	T	T	T
0.3262502964861323	0.0639737853280243	0.5686931210176654	T	T	T
0.3261520896823444	0.3982433769664946	0.5695303228811092	T	T	T
0.3265571816081398	0.7281860050854944	0.5695537914434567	T	T	T
0.5805693052995354	0.0187482973738114	0.5890858093415524	T	T	T
0.5816823922414039	0.3502387699426608	0.5892676101885564	T	T	T
0.5830163172456276	0.6837582007076196	0.5885176333461727	T	T	T
0.8423858075271753	0.6333099996858667	0.6091400228650296	T	T	T
0.8415032514479961	0.3005554557284043	0.6088487132448516	T	T	T
0.8441463146340008	0.9635617978068296	0.6093936442293187	T	T	T
0.0989896507294551	0.5830152227486108	0.6350786386583936	T	T	T
0.0962975470830392	0.2502089357263754	0.6306769357212116	T	T	T
0.0974210442805799	0.9221238249973346	0.6310590561300718	T	T	T
0.3547818272328641	0.5482970799505592	0.6540219294323683	T	T	T
0.3477052339640644	0.2119530026141281	0.6538583597784355	T	T	T
0.3525213439153257	0.8773397360102306	0.6511891162896876	T	T	T
0.6079858237793390	0.4982446295297688	0.6715437181533040	T	T	T
0.6091949247412749	0.1619807471976050	0.6710203751560209	T	T	T
0.6037510777941414	0.8340724008864746	0.6717065551444047	T	T	T
0.8588227453493290	0.4540319179130629	0.6892612185308378	T	T	T
0.8614382559404801	0.1188607149241705	0.6891709800692741	T	T	T
0.8562315926423443	0.7880658685710453	0.6901696229014291	T	T	T
0.2092414970398759	0.4449811998766571	0.7084705734208766	T	T	T
0.2591907419939615	0.5437739486871764	0.7281110211582600	T	T	T
0.1438012014897375	0.4032961204896057	0.7332274397822843	T	T	T

CHO/Cu(533) $E_{ads} = -1.46$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O H

60 1 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0470360684965694 0.2938142604551847 0.4658016173954856 T T T
0.0470878698890864 0.6271205914091308 0.4659697411572086 T T T
0.0470907239395045 0.9606310171622157 0.4658928498531377 T T T
0.3035027247022763 0.2465885365831303 0.4865470069314574 T T T
0.3033379534449616 0.5801156047675248 0.4867467910453661 T T T
0.3031963610781792 0.9132054456044055 0.4868370078367923 T T T
0.5586881269416500 0.2010894223074052 0.5069968729732984 T T T
0.5587448338588894 0.5342715980325400 0.5066692958032997 T T T
0.5590081655136773 0.8664698502269944 0.5071082447448164 T T T
0.8153587178409915 0.1532580521647834 0.5274831997667406 T T T
0.8148801749266040 0.4869440232048924 0.5275685383127866 T T T
0.8153442207280781 0.8202565804584208 0.5275151397377358 T T T
0.0708146226360539 0.1069181887253243 0.5481723029645255 T T T
0.0715488710022362 0.4396458102394805 0.5479141547861404 T T T
0.0712045753711619 0.7734489468026741 0.5480949583215220 T T T
0.3267307460003639 0.0599375595243210 0.5684011290900279 T T T
0.3268267084599786 0.3939072340880593 0.5690811861470965 T T T
0.3275055422916971 0.7250954872445152 0.5691528136530604 T T T
0.5834372084671512 0.0141033113462533 0.5889133658490127 T T T
0.5839112516168919 0.3469601831427845 0.5887539481191678 T T T
0.5834795152977015 0.6779768644786196 0.5894004210368236 T T T
0.8423420023581745 0.6308838316108236 0.6090432924431266 T T T
0.8408519739740123 0.2978119362069277 0.6097545519859829 T T T
0.8405576413112140 0.9658205667262191 0.6095564785481022 T T T
0.0983974847493598 0.5835946896091553 0.6318928360853733 T T T
0.0974593954881218 0.2507432044268149 0.6319062593254993 T T T
0.1002652754221656 0.9144068064163500 0.6314225040356818 T T T
0.3515807849869919 0.5383245851685396 0.6534076962541161 T T T
0.3501995008853367 0.2034676446460159 0.6506112145678343 T T T
0.3504320876628051 0.8753424187403684 0.6510482917387720 T T T
0.6059649429190790 0.4958773990554829 0.6736408069682254 T T T

0.6030409208773729	0.1621394445282515	0.6737740272800399	T	T	T
0.6059029952749646	0.8273287480750340	0.6712463859955990	T	T	T
0.8614999106743849	0.4491455125336974	0.6893400574221189	T	T	T
0.8682550631308005	0.1081270508599752	0.6891490203750403	T	T	T
0.8604284242580484	0.7824671511480377	0.6890661185872728	T	T	T
0.4781652095372569	0.4295941784236362	0.7244785642121642	T	T	T
0.3942393996127057	0.4369725869339956	0.7577640225222039	T	T	T
0.5526374768108003	0.4973276725312376	0.7372402364634725	T	T	T

CHO/Cu(111) $E_{ads} = -1.63$ eV

1.00000000000000

7.6579664403000001	0.0000000000000000	0.0000000000000000
3.8289832201000000	6.6319934786000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.5000000000000000

Cu C O H

45 1 1 1

Selective dynamics

Direct

0.8888888887999968	0.2222222223999992	0.3170124957488483	F	F	F
0.2222222221000010	0.2222222223999992	0.3170124957488483	F	F	F
0.5555555553999980	0.2222222223999992	0.3170124957488483	F	F	F
0.8888888890000004	0.5555555553000033	0.3170124957488483	F	F	F
0.2222222222999974	0.5555555553000033	0.3170124957488483	F	F	F
0.5555555556000016	0.5555555553000033	0.3170124957488483	F	F	F
0.8888888891999969	0.8888888882000003	0.3170124957488483	F	F	F
0.2222222225000010	0.8888888882000003	0.3170124957488483	F	F	F
0.5555555557999980	0.8888888882000003	0.3170124957488483	F	F	F
0.0000000000000000	0.0000000000000000	0.3975777759823913	F	F	F
0.3333333332999970	0.0000000000000000	0.3975777759823913	F	F	F
0.6666666666000012	0.0000000000000000	0.3975777759823913	F	F	F
0.0000000002103135	0.3333333328999970	0.3975777759823913	F	F	F
0.3333333335000006	0.3333333328999970	0.3975777759823913	F	F	F
0.6666666668999994	0.3333333328999970	0.3975777759823913	F	F	F
0.9999999996666986	0.6666666672999995	0.3975777759823913	F	F	F
0.3333333329999988	0.6666666672999995	0.3975777759823913	F	F	F
0.6666666663000029	0.6666666672999995	0.3975777759823913	F	F	F
0.1111111113999996	0.1111111104999978	0.4771948603999974	F	F	F
0.4444444447999985	0.1111111104999978	0.4771948603999974	F	F	F
0.7777777781000026	0.1111111104999978	0.4771948603999974	F	F	F
0.1111111108999978	0.4444444449000002	0.4771948603999974	F	F	F
0.4444444442000020	0.4444444449000002	0.4771948603999974	F	F	F
0.7777777774999990	0.4444444449000002	0.4771948603999974	F	F	F
0.1111111111000014	0.7777777777999972	0.4771948603999974	F	F	F
0.4444444443999984	0.7777777777999972	0.4771948603999974	F	F	F
0.7777777777000026	0.7777777777999972	0.4771948603999974	F	F	F
0.8887777220791762	0.2203607783490611	0.5563783330327539	T	T	T
0.2231581015349633	0.2214573268050088	0.5570099093291105	T	T	T
0.5530899433099634	0.2212345268957776	0.5569619976512854	T	T	T
0.8893035303944856	0.5529160187276716	0.5563554854859163	T	T	T
0.2236196359391016	0.5531262437756510	0.5576534395255166	T	T	T
0.5533055516582266	0.5539048684052332	0.5574572372327395	T	T	T
0.8892204021437564	0.8864149943077706	0.5566454369968952	T	T	T
0.2227174225195228	0.8848926544161912	0.5572887303043217	T	T	T
0.5550496698630667	0.8875708681361303	0.5565937484075221	T	T	T
0.9978260992725367	0.9983255979070762	0.6367326144069594	T	T	T
0.3332411225084186	0.9963961619038386	0.6364717893210070	T	T	T
0.6677247143531702	0.9947770296747223	0.6370698006086783	T	T	T

0.9978493316741606 0.3300080356610451 0.6368911030395807 T T T
0.3329248439142063 0.3251471086379283 0.6405987043205528 T T T
0.6699983663066362 0.3262302941973161 0.6363627877778981 T T T
0.9953646834529195 0.6637998019251654 0.6363432715540256 T T T
0.3324938868990657 0.6710996450860947 0.6399566113283583 T T T
0.6677495213605340 0.6634910920417738 0.6367303506645285 T T T
0.3358274654533417 0.4162586157977728 0.7113237685199678 T T T
0.3341306933862001 0.5764557948859732 0.7206318443235702 T T T
0.3378467915588246 0.3267757107118356 0.7460992150302914 T T T

CHO/Cu(111) $E_{ads} = -1.62$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
3.8289832201000000 6.6319934786000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu C O H
45 1 1 1
Selective dynamics
Direct
0.8888888887999968 0.2222222223999992 0.3170124957488483 F F F
0.2222222221000010 0.2222222223999992 0.3170124957488483 F F F
0.5555555553999980 0.2222222223999992 0.3170124957488483 F F F
0.8888888890000004 0.5555555553000033 0.3170124957488483 F F F
0.2222222222999974 0.5555555553000033 0.3170124957488483 F F F
0.5555555556000016 0.5555555553000033 0.3170124957488483 F F F
0.8888888891999969 0.8888888882000003 0.3170124957488483 F F F
0.2222222225000010 0.8888888882000003 0.3170124957488483 F F F
0.5555555557999980 0.8888888882000003 0.3170124957488483 F F F
0.0000000000000000 0.0000000000000000 0.3975777759823913 F F F
0.3333333332999970 0.0000000000000000 0.3975777759823913 F F F
0.6666666666000012 0.0000000000000000 0.3975777759823913 F F F
0.0000000002103135 0.3333333328999970 0.3975777759823913 F F F
0.3333333335000006 0.3333333328999970 0.3975777759823913 F F F
0.6666666668999994 0.3333333328999970 0.3975777759823913 F F F
0.9999999996666986 0.6666666672999995 0.3975777759823913 F F F
0.3333333329999988 0.6666666672999995 0.3975777759823913 F F F
0.6666666663000029 0.6666666672999995 0.3975777759823913 F F F
0.1111111113999996 0.1111111104999978 0.4771948603999974 F F F
0.4444444447999985 0.1111111104999978 0.4771948603999974 F F F
0.7777777781000026 0.1111111104999978 0.4771948603999974 F F F
0.1111111108999978 0.4444444449000002 0.4771948603999974 F F F
0.4444444442000020 0.4444444449000002 0.4771948603999974 F F F
0.7777777774999990 0.4444444449000002 0.4771948603999974 F F F
0.1111111111000014 0.7777777777999972 0.4771948603999974 F F F
0.4444444443999984 0.7777777777999972 0.4771948603999974 F F F
0.7777777777000026 0.7777777777999972 0.4771948603999974 F F F
0.8857259439675715 0.2242866002793278 0.5571652612971363 T T T
0.2224425015534521 0.2243905113274565 0.5571336034080261 T T T
0.5549056299948631 0.2226805745906120 0.5559142331759972 T T T
0.8887319919292196 0.5551308192822333 0.5563632501590519 T T T
0.2236771367131141 0.5554152033057065 0.5576826503089620 T T T
0.5536373323715509 0.5552135215636298 0.5577202633526994 T T T
0.8889970769303162 0.8894222797753883 0.5564769767546593 T T T
0.2222813955558962 0.8878604346013361 0.5573056171787059 T T T
0.5540600063580001 0.8895515779622087 0.5564786284435215 T T T
0.9960941192893813 0.0038348793009249 0.6369301450031770 T T T
0.3320222884468436 0.0039381251086468 0.6368213673681282 T T T

0.6690279721349341 0.9941972426077115 0.6362548936249226 T T T
0.9986585194732811 0.3345084179043596 0.6371155507521280 T T T
0.3388212065861111 0.3279135919862171 0.6395342300732025 T T T
0.6649764835766234 0.3275427390450787 0.6396228361846639 T T T
0.9970325015173032 0.6673666879462701 0.6363062683808209 T T T
0.3253504129750127 0.6821080540338400 0.6399548960819033 T T T
0.6678851551511116 0.6674103581737469 0.6362787264550533 T T T
0.4723996986954120 0.3797497123375990 0.7033432121953780 T T T
0.3860749748969852 0.5626924091763499 0.7169467483492653 T T T
0.5271503602003520 0.2678719519900810 0.7358480168953747 T T T

CHO/Cu(100) $E_{ads} = -1.74$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu C O H
45 1 1 1
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.3173193249345303 F F F
0.3333333332999970 0.0000000000000000 0.3173193249345303 F F F
0.6666666666000012 0.0000000000000000 0.3173193249345303 F F F
0.0000000000000000 0.3333333332999970 0.3173193249345303 F F F
0.3333333332999970 0.3333333332999970 0.3173193249345303 F F F
0.6666666666000012 0.3333333332999970 0.3173193249345303 F F F
0.0000000000000000 0.6666666666000012 0.3173193249345303 F F F
0.3333333332999970 0.6666666666000012 0.3173193249345303 F F F
0.6666666666000012 0.6666666666000012 0.3173193249345303 F F F
0.1666666667000030 0.1666666667000030 0.3854655552433357 F F F
0.5000000000000000 0.1666666667000030 0.3854655552433357 F F F
0.8333333332999970 0.1666666667000030 0.3854655552433357 F F F
0.1666666667000030 0.5000000000000000 0.3854655552433357 F F F
0.5000000000000000 0.5000000000000000 0.3854655552433357 F F F
0.8333333332999970 0.5000000000000000 0.3854655552433357 F F F
0.1666666667000030 0.8333333332999970 0.3854655552433357 F F F
0.5000000000000000 0.8333333332999970 0.3854655552433357 F F F
0.8333333332999970 0.8333333332999970 0.3854655552433357 F F F
0.0000000000000000 0.0000000000000000 0.4552941175999976 F F F
0.3333333332999970 0.0000000000000000 0.4552941175999976 F F F
0.6666666666000012 0.0000000000000000 0.4552941175999976 F F F
0.0000000000000000 0.3333333332999970 0.4552941175999976 F F F
0.3333333332999970 0.3333333332999970 0.4552941175999976 F F F
0.6666666666000012 0.3333333332999970 0.4552941175999976 F F F
0.0000000000000000 0.6666666666000012 0.4552941175999976 F F F
0.3333333332999970 0.6666666666000012 0.4552941175999976 F F F
0.6666666666000012 0.6666666666000012 0.4552941175999976 F F F
0.1694177123920468 0.1685192826476083 0.5255140592833953 T T T
0.4996143530699939 0.1665487704629953 0.5242056539277229 T T T
0.8335689481839879 0.1679186263755241 0.5251893169873725 T T T
0.1680412339187782 0.4986229113332641 0.5249511328527703 T T T
0.5017740675438489 0.5018529479296916 0.5236599411269651 T T T
0.8309437780959854 0.4999602906597147 0.5257657647353113 T T T
0.1660281373978165 0.8335188495161532 0.5246824241245562 T T T
0.5010180150375163 0.8313186561173964 0.5252916341557778 T T T
0.8321700999043387 0.8317184541880636 0.5255573637513322 T T T
0.0005876770538649 0.0007663105270410 0.5933197752620671 T T T

0.3328178732156601 0.9987393662233046 0.5923299960220589 T T T
0.6669536432706522 0.0014358758218336 0.5926554679403608 T T T
0.0024255436077212 0.3330341812521098 0.5927165927067009 T T T
0.3391115146166328 0.3366606728013579 0.5960631212865195 T T T
0.6650174238856152 0.3254101941674037 0.5948022464939058 T T T
0.0018720563423642 0.6664816003623315 0.5926870923881893 T T T
0.3279087934730640 0.6687708855538972 0.5927834236720315 T T T
0.6714603767020080 0.6750966566146488 0.5967488032530355 T T T
0.4926545594640928 0.4156782556756866 0.6546362046145688 T T T
0.5769044778629606 0.5554937045345838 0.6642901908211982 T T T
0.4583740239451473 0.3387459524971561 0.6904071835103025 T T T

CHO/Cu(100) $E_{ads} = -1.72$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu C O H
45 1 1 1
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.3173193249345303 F F F
0.3333333332999970 0.0000000000000000 0.3173193249345303 F F F
0.6666666666000012 0.0000000000000000 0.3173193249345303 F F F
0.0000000000000000 0.3333333332999970 0.3173193249345303 F F F
0.3333333332999970 0.3333333332999970 0.3173193249345303 F F F
0.6666666666000012 0.3333333332999970 0.3173193249345303 F F F
0.0000000000000000 0.6666666666000012 0.3173193249345303 F F F
0.3333333332999970 0.6666666666000012 0.3173193249345303 F F F
0.6666666666000012 0.6666666666000012 0.3173193249345303 F F F
0.1666666667000030 0.1666666667000030 0.3854655552433357 F F F
0.5000000000000000 0.1666666667000030 0.3854655552433357 F F F
0.8333333332999970 0.1666666667000030 0.3854655552433357 F F F
0.1666666667000030 0.5000000000000000 0.3854655552433357 F F F
0.5000000000000000 0.5000000000000000 0.3854655552433357 F F F
0.8333333332999970 0.5000000000000000 0.3854655552433357 F F F
0.1666666667000030 0.8333333332999970 0.3854655552433357 F F F
0.5000000000000000 0.8333333332999970 0.3854655552433357 F F F
0.8333333332999970 0.8333333332999970 0.3854655552433357 F F F
0.0000000000000000 0.0000000000000000 0.4552941175999976 F F F
0.3333333332999970 0.0000000000000000 0.4552941175999976 F F F
0.6666666666000012 0.0000000000000000 0.4552941175999976 F F F
0.0000000000000000 0.3333333332999970 0.4552941175999976 F F F
0.3333333332999970 0.3333333332999970 0.4552941175999976 F F F
0.6666666666000012 0.3333333332999970 0.4552941175999976 F F F
0.0000000000000000 0.6666666666000012 0.4552941175999976 F F F
0.3333333332999970 0.6666666666000012 0.4552941175999976 F F F
0.6666666666000012 0.6666666666000012 0.4552941175999976 F F F
0.1682402534686998 0.1679853453458016 0.5249498015122205 T T T
0.4984264132313032 0.1679853453458016 0.5249498015122205 T T T
0.8333333332999970 0.1668061393086753 0.5249838505566233 T T T
0.1689917367763764 0.5004175866748169 0.5253559150775220 T T T
0.4976749299236267 0.5004175866748169 0.5253559150775220 T T T
0.8333333332999970 0.4985664545747825 0.5248545960785997 T T T
0.1683741135505344 0.8311110258648554 0.5253286663327550 T T T
0.4982925531494685 0.8311110258648554 0.5253286663327550 T T T
0.8333333332999970 0.8343315177472117 0.5242510580674589 T T T

0.0002043623059010 0.9999353152643828 0.5926879911527674 T T T
0.3333333332999970 0.9990362572863699 0.5926898351388965 T T T
0.6664623042941004 0.9999353152643828 0.5926879911527674 T T T
0.9992734700135669 0.3323995556912049 0.5931524050162862 T T T
0.3333333332999970 0.3253603752906733 0.5971132039455651 T T T
0.6673931965864343 0.3323995556912049 0.5931524050162862 T T T
0.9965719180027339 0.6675725302992156 0.5919750985597086 T T T
0.3333333332999970 0.6744660236393041 0.5974714959053786 T T T
0.6700947485972601 0.6675725302992156 0.5919750985597086 T T T
0.3333333332999970 0.4200580666308052 0.6669735734199529 T T T
0.3333333332999970 0.5797802550373926 0.6757300587200308 T T T
0.3333333332999970 0.3338770865595986 0.7024025157699073 T T T

CHO/Cu(100) $E_{ads} = -1.55$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu C O H
45 1 1 1
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.3173193249345303 F F F
0.3333333332999970 0.0000000000000000 0.3173193249345303 F F F
0.6666666666000012 0.0000000000000000 0.3173193249345303 F F F
0.0000000000000000 0.3333333332999970 0.3173193249345303 F F F
0.3333333332999970 0.3333333332999970 0.3173193249345303 F F F
0.6666666666000012 0.3333333332999970 0.3173193249345303 F F F
0.0000000000000000 0.6666666666000012 0.3173193249345303 F F F
0.3333333332999970 0.6666666666000012 0.3173193249345303 F F F
0.6666666666000012 0.6666666666000012 0.3173193249345303 F F F
0.1666666667000030 0.1666666667000030 0.3854655552433357 F F F
0.5000000000000000 0.1666666667000030 0.3854655552433357 F F F
0.8333333332999970 0.1666666667000030 0.3854655552433357 F F F
0.1666666667000030 0.5000000000000000 0.3854655552433357 F F F
0.5000000000000000 0.5000000000000000 0.3854655552433357 F F F
0.8333333332999970 0.5000000000000000 0.3854655552433357 F F F
0.1666666667000030 0.8333333332999970 0.3854655552433357 F F F
0.5000000000000000 0.8333333332999970 0.3854655552433357 F F F
0.8333333332999970 0.8333333332999970 0.3854655552433357 F F F
0.0000000000000000 0.0000000000000000 0.4552941175999976 F F F
0.3333333332999970 0.0000000000000000 0.4552941175999976 F F F
0.6666666666000012 0.0000000000000000 0.4552941175999976 F F F
0.0000000000000000 0.3333333332999970 0.4552941175999976 F F F
0.3333333332999970 0.3333333332999970 0.4552941175999976 F F F
0.6666666666000012 0.3333333332999970 0.4552941175999976 F F F
0.0000000000000000 0.6666666666000012 0.4552941175999976 F F F
0.3333333332999970 0.6666666666000012 0.4552941175999976 F F F
0.6666666666000012 0.6666666666000012 0.4552941175999976 F F F
0.1679939751956852 0.1678933672674106 0.5252612495705762 T T T
0.4983619882902204 0.1671668784761664 0.5251257827635172 T T T
0.8331116283367876 0.1663648440354635 0.5250648948181507 T T T
0.1674048163107358 0.4983019890044389 0.5251773973790321 T T T
0.4990235151103732 0.4989092486614339 0.5249611688675344 T T T
0.8322732288537864 0.4993595795983339 0.5251683821524509 T T T
0.1663642503620650 0.8329464039101353 0.5250316552839109 T T T
0.4996167826368776 0.8321133217762622 0.5251265172796664 T T T

0.8331796667119065 0.8330865125122102 0.5247494182873211 T T T
0.0001309652970747 0.9999730916435539 0.5930335341185540 T T T
0.3332934518852184 0.9971748146789636 0.5930310958843918 T T T
0.6666834567103379 0.9986518817367340 0.5930139319440713 T T T
0.9977743129682608 0.3332002535325529 0.5931578433685516 T T T
0.3334663842038026 0.3331940937300146 0.5975044507848608 T T T
0.6668740777042501 0.3308025607981051 0.5933233945126659 T T T
0.9988238710553716 0.6665825320817547 0.5930007627713820 T T T
0.3312423940402240 0.6672507040588229 0.5932741545641420 T T T
0.6667891916634119 0.6665653046881417 0.5930134235851909 T T T
0.3600259824669365 0.3589766261941634 0.6733702639700923 T T T
0.4462514510084361 0.4633308303851535 0.6978486982091994 T T T
0.2793624885145363 0.2596514390178797 0.6951137793161664 T T T

CHO/Cu(211) $E_{ads} = -1.88$ eV
1.00000000000000
6.2527034153000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.3164343000000009
Cu C O H
45 1 1 1
Selective dynamics
Direct
0.0061862950247047 0.1666666667000030 0.3120745335338029 F F F
0.0061862950247047 0.5000000000000000 0.3120745335338029 F F F
0.0061862950247047 0.8333333332999970 0.3120745335338029 F F F
0.3355456677560653 0.0000000000000000 0.3354619372229379 F F F
0.3355456677560653 0.3333333332999970 0.3354619372229379 F F F
0.3355456677560653 0.6666666666000012 0.3354619372229379 F F F
0.6630854692850079 0.1666666667000030 0.3607350091654666 F F F
0.6630854692850079 0.5000000000000000 0.3607350091654666 F F F
0.6630854692850079 0.8333333332999970 0.3607350091654666 F F F
0.9944057463905267 0.0000000000000000 0.3915351276171819 F F F
0.9944057463905267 0.3333333332999970 0.3915351276171819 F F F
0.9944057463905267 0.6666666666000012 0.3915351276171819 F F F
0.3330656692422309 0.1666666667000030 0.4179888222780335 F F F
0.3330656692422309 0.5000000000000000 0.4179888222780335 F F F
0.3330656692422309 0.8333333332999970 0.4179888222780335 F F F
0.6656564241704075 0.0000000000000000 0.4448469552356400 F F F
0.6656564241704075 0.3333333332999970 0.4448469552356400 F F F
0.6656564241704075 0.6666666666000012 0.4448469552356400 F F F
0.0003515212697778 0.1666666667000030 0.4732099031121066 F F F
0.0003515212697778 0.5000000000000000 0.4732099031121066 F F F
0.0003515212697778 0.8333333332999970 0.4732099031121066 F F F
0.3333333329999988 0.0000000000000000 0.5000000000000000 F F F
0.3333333329999988 0.3333333332999970 0.5000000000000000 F F F
0.3333333329999988 0.6666666666000012 0.5000000000000000 F F F
0.6663151448302216 0.1666666667000030 0.5267900968878934 F F F
0.6663151448302216 0.5000000000000000 0.5267900968878934 F F F
0.6663151448302216 0.8333333332999970 0.5267900968878934 F F F
0.9989970434845716 0.9999379528500043 0.5550773136246789 T T T
0.9985455687714690 0.3331643129374697 0.5550665085622697 T T T
0.9982058382672392 0.6673281286231685 0.5550049118273108 T T T
0.3322654609721880 0.1667114756887003 0.5817104519774006 T T T
0.3313498731168778 0.5001576613027154 0.5816989280911287 T T T
0.3314458706247549 0.8335810262192282 0.5816805479625344 T T T
0.6676643045115043 0.0023919909198327 0.6087520018609638 T T T

0.6679704757731102 0.3343286578088609 0.6095470733298995 T T T
0.6673091241533626 0.6638877085192973 0.6095661431582826 T T T
0.9970467170847499 0.1667230420748496 0.6388382835882069 T T T
0.9989722386414570 0.5006485940692329 0.6383322093605415 T T T
0.9969360845078441 0.8333831259334659 0.6389319428940610 T T T
0.3243716741579803 0.0002124883777341 0.6636759115274415 T T T
0.3259779513486905 0.3335421244516965 0.6630093850264061 T T T
0.3261345806623197 0.6667147847971080 0.6637318238487211 T T T
0.6566880813464664 0.1600230245223955 0.6910151670363618 T T T
0.6621485038897532 0.5085241232234807 0.6917085932481797 T T T
0.6532942414188909 0.8345352950214817 0.6878916021621890 T T T
0.6674475407866467 0.2548950481508001 0.7583842862773338 T T T
0.6836548229871298 0.4155853490280847 0.7650100704468130 T T T
0.6600625894358600 0.1752585905183182 0.7939977560838898 T T T

CHO/Cu(211) $E_{ads} = -1.70$ eV
1.00000000000000
6.2527034153000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.3164343000000009
Cu C O H
45 1 1 1
Selective dynamics
Direct
0.0061862950247047 0.1666666667000030 0.3120745335338029 F F F
0.0061862950247047 0.5000000000000000 0.3120745335338029 F F F
0.0061862950247047 0.8333333332999970 0.3120745335338029 F F F
0.3355456677560653 0.0000000000000000 0.3354619372229379 F F F
0.3355456677560653 0.3333333332999970 0.3354619372229379 F F F
0.3355456677560653 0.6666666666000012 0.3354619372229379 F F F
0.6630854692850079 0.1666666667000030 0.3607350091654666 F F F
0.6630854692850079 0.5000000000000000 0.3607350091654666 F F F
0.6630854692850079 0.8333333332999970 0.3607350091654666 F F F
0.9944057463905267 0.0000000000000000 0.3915351276171819 F F F
0.9944057463905267 0.3333333332999970 0.3915351276171819 F F F
0.9944057463905267 0.6666666666000012 0.3915351276171819 F F F
0.3330656692422309 0.1666666667000030 0.4179888222780335 F F F
0.3330656692422309 0.5000000000000000 0.4179888222780335 F F F
0.3330656692422309 0.8333333332999970 0.4179888222780335 F F F
0.6656564241704075 0.0000000000000000 0.4448469552356400 F F F
0.6656564241704075 0.3333333332999970 0.4448469552356400 F F F
0.6656564241704075 0.6666666666000012 0.4448469552356400 F F F
0.0003515212697778 0.1666666667000030 0.4732099031121066 F F F
0.0003515212697778 0.5000000000000000 0.4732099031121066 F F F
0.0003515212697778 0.8333333332999970 0.4732099031121066 F F F
0.3333333329999988 0.0000000000000000 0.5000000000000000 F F F
0.3333333329999988 0.3333333332999970 0.5000000000000000 F F F
0.3333333329999988 0.6666666666000012 0.5000000000000000 F F F
0.6663151448302216 0.1666666667000030 0.5267900968878934 F F F
0.6663151448302216 0.5000000000000000 0.5267900968878934 F F F
0.6663151448302216 0.8333333332999970 0.5267900968878934 F F F
0.9988806596548243 0.0003491938222647 0.5550187137093088 T T T
0.9991643718507195 0.3329865817180546 0.5550352026259510 T T T
0.9991649573236170 0.6667406134641488 0.5549771472123740 T T T
0.3315669755307197 0.1664526427682907 0.5817728608559508 T T T
0.3322470034794303 0.4999469787509946 0.5818339580896419 T T T
0.3315439821076094 0.8335719394168563 0.5818155269982387 T T T

0.6687539665248483	0.9994120944444334	0.6091088719915545	T	T	T
0.6685369466914227	0.3351346534742195	0.6090098576333396	T	T	T
0.6684920666542077	0.6655883224412750	0.6084893749459285	T	T	T
0.9983850267090895	0.1663932338140853	0.6389260617612769	T	T	T
0.9991134303807256	0.4995602324025886	0.6382471147113363	T	T	T
0.9985218497227489	0.8338404783882266	0.6386105618144742	T	T	T
0.3268348157888206	0.0000473402801427	0.6643237782322903	T	T	T
0.3266580041261662	0.3330250022562217	0.6637567014819868	T	T	T
0.3250327109248137	0.6668578419443922	0.6635760470315752	T	T	T
0.6555889221803641	0.1663909129246898	0.6885142732283979	T	T	T
0.6559205013160426	0.5014855394239564	0.6907873300249009	T	T	T
0.6548191028086464	0.8314799152526956	0.6889804290502406	T	T	T
0.6856910358742792	0.5553956029842458	0.7626782907096972	T	T	T
0.8559155577013778	0.5830247921365155	0.7830055291449248	T	T	T
0.5356818457833253	0.5469337488643421	0.7859517570304592	T	T	T

11.6 *OH Adsorption

OH/R-Cu_3/Cu(533) E_{ads} = −4.47 eV

1.00000000000000					
10.3878408006999994	0.0000000000000000	0.0000000000000000			
4.5828709415000004	6.0103788927000004	0.0000000000000000			
0.0000000000000000	0.0000000000000000	26.5000000000000000			
Cu O H					
63 1 1					
Selective dynamics					
Direct					
0.0032853599999996	0.9972806999999975	0.3042624500000031	F	F	F
0.0028217400000017	0.3308767700000033	0.3042691500000032	F	F	F
0.0026800899999984	0.6645640400000019	0.3042978000000005	F	F	F
0.2572489900000008	0.6186597399999982	0.3218759499999990	F	F	F
0.2571973700000001	0.2857762699999995	0.3217927099999969	F	F	F
0.2571614599999990	0.9524293899999989	0.3219123699999997	F	F	F
0.5099116399999986	0.5747781399999994	0.3415763200000015	F	F	F
0.5095861200000016	0.2417833900000019	0.3416938299999970	F	F	F
0.5096986000000001	0.9088501900000026	0.3416314700000029	F	F	F
0.7627858999999972	0.5310134699999978	0.3609394899999998	F	F	F
0.7629538699999969	0.1970798500000015	0.3608490599999996	F	F	F
0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F
0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0469612877838644	0.2944834684938215	0.4662008435514574	T	T	T
0.0467952964014302	0.6272115458117237	0.4663449047683694	T	T	T
0.0471133946406247	0.9607418731720138	0.4661110847214745	T	T	T
0.3036448149226213	0.2467900458766102	0.4871891152190972	T	T	T
0.3041824355328846	0.5791652519753803	0.4869058799646176	T	T	T

0.3043567866117367 0.9135245639288256 0.4868854198376543 T T T
0.5596841869676753 0.2003262972139007 0.5070674007159425 T T T
0.5606529247729489 0.5327688405128214 0.5064060628502337 T T T
0.5592441520227432 0.8670728731645481 0.5070184617367198 T T T
0.8173413630982425 0.1518754634824749 0.5275678176083840 T T T
0.8167149568817931 0.4866587098074658 0.5275763085689140 T T T
0.8160618533284947 0.8193465474327498 0.5276225374098737 T T T
0.0736028632136355 0.1064109834206055 0.5480324667951257 T T T
0.0730189004785860 0.4391305574740806 0.5490544194560950 T T T
0.0732482087861885 0.7711042644896933 0.5480901163608151 T T T
0.3288278554615357 0.0607244974659714 0.5699723860035151 T T T
0.3292283782601280 0.3908073671963099 0.5697760681532700 T T T
0.3308727772079127 0.7241972873618794 0.5683758864708449 T T T
0.5852232663316775 0.0119601654584501 0.5894884115134705 T T T
0.5868680179390031 0.3446657008239236 0.5887224654430117 T T T
0.5862024122633397 0.6779787429239653 0.5887992662932033 T T T
0.8443129867738307 0.6300179620126416 0.6103476157746602 T T T
0.8435209745680189 0.2981404633846531 0.6093802185084312 T T T
0.8428320581487114 0.9629957372153882 0.6095090405705775 T T T
0.1013643659325906 0.5812407433363267 0.6332534759420754 T T T
0.1006026316889723 0.2507612701121260 0.6335045487549085 T T T
0.0987892620997135 0.9178000074727282 0.6287581916831676 T T T
0.3531490566861498 0.5376436621551304 0.6504658715276672 T T T
0.3559296361816378 0.2036624975879797 0.6556750440295817 T T T
0.3532191936528017 0.8739259515581987 0.6506569592500158 T T T
0.6143302902253186 0.4865279599463320 0.6723963076684676 T T T
0.6132676101948509 0.1551449589372693 0.6730059551056423 T T T
0.6119070542816342 0.8247818345170375 0.6733387999185463 T T T
0.8663040438524776 0.4443894722285329 0.6913969326305988 T T T
0.8748471304214265 0.1040893818454636 0.6909493788319117 T T T
0.8674967513004894 0.7778822560670657 0.6911052489056722 T T T
0.4601058237576393 0.7903052921300721 0.7352166660334744 T T T
0.4585974044623165 0.4401267070532793 0.7350267036979847 T T T
0.1725115531732616 0.8545337572327973 0.7146523883907504 T T T
0.3251235793887640 0.7277200946613239 0.7746473009494309 T T T
0.2965116631387055 0.7515871649076478 0.8102729342909768 T T T

OH/Cu_3/Cu(533) E_{ads} = −3.92 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu O H
63 1 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F
0.2571614599999990 0.9524293899999989 0.3219123699999997 F F F
0.5099116399999986 0.5747781399999994 0.3415763200000015 F F F
0.5095861200000016 0.2417833900000019 0.3416938299999970 F F F
0.5096986000000001 0.9088501900000026 0.3416314700000029 F F F
0.7627858999999972 0.5310134699999978 0.3609394899999998 F F F
0.7629538699999969 0.1970798500000015 0.3608490599999996 F F F

0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F
0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0466059087464643	0.2943347029577055	0.4664618586298772	T	T	T
0.0460074399265054	0.6287276834785658	0.4668439051663356	T	T	T
0.0466929340388731	0.9611321933957129	0.4664867991448531	T	T	T
0.3026114773046302	0.2476941752484905	0.4871155292307066	T	T	T
0.3027099084452018	0.5811007319629553	0.4870613433539717	T	T	T
0.3031387080163626	0.9141539738917714	0.4869406540910930	T	T	T
0.5578819218540403	0.2015104078667846	0.5068305779182225	T	T	T
0.5587196645507362	0.5344448653222571	0.5063954255331709	T	T	T
0.5582843943680658	0.8684815275586288	0.5067566288271195	T	T	T
0.8155869098258393	0.1531258003334273	0.5274567781844439	T	T	T
0.8155486794969349	0.4872561773609689	0.5275098595733354	T	T	T
0.8144310223445430	0.8216876035875345	0.5279009120922211	T	T	T
0.0720182927526523	0.1060342572483535	0.5490944418608734	T	T	T
0.0706141556959068	0.4412125341546158	0.5489925311026695	T	T	T
0.0714210723794579	0.7748855366147041	0.5496035321905026	T	T	T
0.3259300791826973	0.0618511348112278	0.5691683382537036	T	T	T
0.3248450722883547	0.3959744528057314	0.5694011030301454	T	T	T
0.3266836352686298	0.7279535136559616	0.5689616648993976	T	T	T
0.5825098628325094	0.0149334442364122	0.5890491469530659	T	T	T
0.5839377959929379	0.3466216711194221	0.5880525628389819	T	T	T
0.5841695236897237	0.6801299181398761	0.5881007260217359	T	T	T
0.8409787868638574	0.6333896544422188	0.6101413527855257	T	T	T
0.8430019799785597	0.2968249156471288	0.6096180868497498	T	T	T
0.8420964117107417	0.9651518085846149	0.6104256917393442	T	T	T
0.0930993227767445	0.5884529160304197	0.6344830003268100	T	T	T
0.0951063233582516	0.2546601008838039	0.6332874699657154	T	T	T
0.0977852201234413	0.9191083331975136	0.6358113782140222	T	T	T
0.3480158432766132	0.5397126145800897	0.6506691764720856	T	T	T
0.3483817351175205	0.2097788586620624	0.6517095913729776	T	T	T
0.3486692696822900	0.8801576743561981	0.6508235416889931	T	T	T
0.6035388383465801	0.4968496229761925	0.6693263622216818	T	T	T
0.6023866968508784	0.1616924612225006	0.6715213305430936	T	T	T
0.6022717205170238	0.8348250578787670	0.6715229848829054	T	T	T
0.8593444709835225	0.4524298261429465	0.6910302215567867	T	T	T
0.8593606386767974	0.1157218793793007	0.6917661917052698	T	T	T
0.8528970890845713	0.7894655803151807	0.6929918259830785	T	T	T
0.6278329770925524	0.6489974955538997	0.7483440079994139	T	T	T
0.6273943153693651	0.3044035435748285	0.7485295247313601	T	T	T
0.3542856366592844	0.7045971793118753	0.7266146227167809	T	T	T
0.4917158955983894	0.5901724099248895	0.7898477372079284	T	T	T
0.4598914304241077	0.6167736250999596	0.8252436605491837	T	T	T

OH/Cu_3/Cu(533) E_{ads} = −3.77 eV
1.00000000000000

10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu O H
63 1 1
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F
0.2571614599999990 0.9524293899999989 0.3219123699999997 F F F
0.5099116399999986 0.5747781399999994 0.3415763200000015 F F F
0.5095861200000016 0.2417833900000019 0.3416938299999970 F F F
0.5096986000000001 0.9088501900000026 0.3416314700000029 F F F
0.7627858999999972 0.5310134699999978 0.3609394899999998 F F F
0.7629538699999969 0.1970798500000015 0.3608490599999996 F F F
0.7629705100000024 0.8638077299999978 0.3608832600000014 F F F
0.0188077500000006 0.4844866199999984 0.3845455499999986 F F F
0.0188649600000019 0.1508076399999965 0.3844206699999972 F F F
0.0189457299999987 0.8174492599999965 0.3845321800000008 F F F
0.2777182000000025 0.4350678200000004 0.4051130599999979 F F F
0.2779364200000032 0.1018241299999971 0.4049400600000013 F F F
0.2778532499999997 0.7683188099999967 0.4050370400000034 F F F
0.5346647900000008 0.3873898000000011 0.4243529600000002 F F F
0.5347255300000029 0.0542446099999978 0.4245416400000011 F F F
0.5343893300000033 0.7214487199999979 0.4243017399999971 F F F
0.7896143700000025 0.3418778500000030 0.4451831499999983 F F F
0.7893677400000030 0.0085227100000012 0.4452920299999974 F F F
0.7895473399999986 0.6754118300000016 0.4453449800000016 F F F
0.0469931325947144 0.2934018159196157 0.4663499917105511 T T T
0.0460925918456212 0.6282905593069685 0.4667040356178518 T T T
0.0461425170749692 0.9605519461567198 0.4662866387162126 T T T
0.3028132402141210 0.2469574254204900 0.4868657815661450 T T T
0.3026207930957412 0.5800503436150137 0.4874134919997601 T T T
0.3032540950551237 0.9122869678523600 0.4868029817885926 T T T
0.5580924728468375 0.2000560710715504 0.5068789745235662 T T T
0.5591471572981916 0.5321282383621408 0.5062677740858277 T T T
0.5594280766343616 0.8648729072362258 0.5064248240537950 T T T
0.8158837063585480 0.1505579882655681 0.5280856214586294 T T T
0.8166021474165390 0.4843006818004483 0.5274004301316708 T T T
0.8150955989248914 0.8192409840255266 0.5279543612791571 T T T
0.0722988946712064 0.1032061705242668 0.5484291540883390 T T T
0.0707562627044851 0.4407320915707302 0.5486317712463062 T T T
0.0708650405728122 0.7736114480508292 0.5496744953694730 T T T
0.3278686607545112 0.0587319475809451 0.5679863823242499 T T T
0.3254828244186498 0.3938256438959442 0.5700465734195532 T T T
0.3269430469103867 0.7241749953735805 0.5694186590333672 T T T
0.5833776312849182 0.0096119837933912 0.5881904987846553 T T T
0.5840184510515840 0.3432641466372388 0.5882609524366060 T T T
0.5856094427187699 0.6741349468294757 0.5876927714990430 T T T
0.8410292679370457 0.6289817462800826 0.6109514241838951 T T T
0.8443294584249372 0.2920554370005490 0.6099661586351672 T T T
0.8426019384081798 0.9572086447856734 0.6116279645300011 T T T
0.0944549256248806 0.5854525154157031 0.6345537025752108 T T T
0.0996941125956852 0.2491091186386356 0.6302811083771473 T T T
0.0970001013649124 0.9172572022184156 0.6352658519903329 T T T

0.3485579431997721 0.5383706417941809 0.6535252425449087 T T T
0.3480929115863560 0.2080850541216961 0.6519828927958784 T T T
0.3475300176515930 0.8787326189356435 0.6492263637303566 T T T
0.6088152838699443 0.4893962243065175 0.6689286846646212 T T T
0.6039366036449678 0.1505618817965981 0.6699149620283151 T T T
0.5981974356218700 0.8289709992719239 0.6699117963081775 T T T
0.8795620133626016 0.4201398266231990 0.6900075131213725 T T T
0.8587625632817506 0.1069291516606725 0.6919329259289810 T T T
0.8568563010658252 0.7800026402479432 0.6957725364965910 T T T
0.6485867014793385 0.6111108164925270 0.7506417965666330 T T T
0.6128185991840809 0.3150466233774907 0.7458493662562518 T T T
0.3862476582347654 0.7047927362845527 0.7282550091390405 T T T
0.8430949415537867 0.6076725640566707 0.7542671756143093 T T T
0.9293568597743374 0.5201005170997135 0.7789457118796932 T T T

OH/Cu(533) E_{ads} = −3.69 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu O H
60 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0469647946374039 0.2948932303685083 0.4659873384498070 T T T
0.0464568467273949 0.6284778109930187 0.4658506810491829 T T T
0.0467766751640397 0.9614325154092214 0.4659937551216231 T T T
0.3031493240505299 0.2482519786548565 0.4867281273281847 T T T
0.3030718919232029 0.5813192896683503 0.4866696934715407 T T T
0.3033766018526407 0.9145187166240945 0.4866016943693054 T T T
0.5588300950480871 0.2018859285510928 0.5068102350877908 T T T
0.5588491779357838 0.5350496777129123 0.5067997729727196 T T T
0.5590381188284326 0.8681320400664276 0.5067653249868158 T T T

0.8154519750936657 0.1545932813622670 0.5276384035387167 T T T
0.8156046573933580 0.4878123471189895 0.5276054569418775 T T T
0.8154360349177594 0.8212859758316284 0.5283930380078488 T T T
0.0713964020444422 0.1083588718607160 0.5481471636354485 T T T
0.0710070438011670 0.4426117691842464 0.5482656964073414 T T T
0.0710370172060877 0.7746161492845900 0.5482473989022836 T T T
0.3265175295878180 0.0625002529477854 0.5688572663366642 T T T
0.3258940118998410 0.3964393121467538 0.5690746717257795 T T T
0.3264462823015535 0.7292063436001612 0.5688228554914971 T T T
0.5833619316505860 0.0152805473595663 0.5885489524080540 T T T
0.5836172129388260 0.3482111504434187 0.5885613545683483 T T T
0.5839219808757576 0.6817025431279404 0.5885040741842289 T T T
0.8422830223013875 0.6292251135212084 0.6107110893758332 T T T
0.8425875444402138 0.2992502421216088 0.6102212688310544 T T T
0.8421649745679574 0.9695688590210878 0.6106931765075245 T T T
0.0968597692083293 0.5876818200935858 0.6328736779172388 T T T
0.0977158953287329 0.2536452809599652 0.6318552491040066 T T T
0.0975246024401528 0.9201918530393982 0.6317209516920244 T T T
0.3498657857724297 0.5432206918223201 0.6519051770704252 T T T
0.3501377054794190 0.2098077650254382 0.6517786815276949 T T T
0.3499926642184263 0.8767697201778617 0.6515836422471253 T T T
0.6027319190404086 0.4992815957897676 0.6697546108990835 T T T
0.6030954969614370 0.1656786342671808 0.6711345235817419 T T T
0.6033075656354896 0.8319268312885697 0.6711596922928109 T T T
0.8620821591066132 0.4558959751671168 0.6931627854876510 T T T
0.8619380547897961 0.1099256080839766 0.6930475036596420 T T T
0.8563028815217208 0.7877109379772875 0.6892823290460299 T T T
0.8896022186594621 0.2595859351196736 0.7469921124469039 T T T
0.8006948356470360 0.3334835359606743 0.7710916985148302 T T T

OH/Defected-Cu(533) E_{ads} = −3.69 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu O H
59 1 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F

0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0463976887251505 0.2947309478891995 0.4659954986651229 T T T
0.0468233564963683 0.6271092019132141 0.4659719053865032 T T T
0.0468910113290022 0.9613822421783311 0.4660065250833796 T T T
0.3030189361583098 0.2474075733919960 0.4867769960281692 T T T
0.3038457418043947 0.5799918014085819 0.4864032869231991 T T T
0.3030841143160998 0.9141087179631526 0.4866733078902428 T T T
0.5595320601536713 0.2003085666191069 0.5067868955279806 T T T
0.5595871632794527 0.5335680142725181 0.5068148225563434 T T T
0.5587968198540096 0.8674557200710140 0.5069233745516968 T T T
0.8162608479877704 0.1531681965076146 0.5276483645142491 T T T
0.8158480971706012 0.4868245853610134 0.5284000066026806 T T T
0.8160813723355318 0.8195344115371839 0.5276844186616501 T T T
0.0708503919670775 0.1084874458556655 0.5485861475504805 T T T
0.0707427815401402 0.4401615201612685 0.5486982904606279 T T T
0.0724493963090893 0.7727614784113044 0.5477722786206556 T T T
0.3259609553516185 0.0616175775581098 0.5691482066321001 T T T
0.3276288277214334 0.3936068332560154 0.5687876628416504 T T T
0.3274043875048349 0.7270711223716901 0.5686496363409859 T T T
0.5848304278232064 0.0122060835759541 0.5884436494287755 T T T
0.5853879949265490 0.3457334653107225 0.5884462238257555 T T T
0.5851351248199350 0.6789683363100920 0.5886762676516497 T T T
0.8425147694929009 0.6294266139313578 0.6122106185001002 T T T
0.8429020371066258 0.2989430610484547 0.6121842239083009 T T T
0.8437621826293196 0.9631840429031442 0.6098692648587658 T T T
0.0981453156552519 0.5834882930679939 0.6314757181288542 T T T
0.0945590831962804 0.2543962032381231 0.6336736941674559 T T T
0.0982046000311669 0.9190917078835525 0.6313141391380626 T T T
0.3504047485394963 0.5414001080813620 0.6515599074051721 T T T
0.3500495638390788 0.2078518667231464 0.6519617068533421 T T T
0.3504729104534761 0.8744917387183051 0.6518708819888133 T T T
0.6057500850183573 0.4962556334354957 0.6699211174105244 T T T
0.6035521931090813 0.1635034740136234 0.6697626439259494 T T T
0.6052354357785887 0.8277926661252621 0.6699466807417807 T T T
0.8621716310794696 0.1190106386037328 0.6912290231807390 T T T
0.8617688529163843 0.7764099325071641 0.6913366868609216 T T T
0.8931245865759152 0.9218759779077885 0.7457004243163041 T T T
0.8072534188303067 0.9940356145385607 0.7708453030664089 T T T

OH/Defected-Cu(533) E_{ads} = −3.61 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu O H
59 1 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F

0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0468944941660752	0.2945860382524899	0.4661963801817848	T	T	T
0.0465905532944859	0.6274587072864080	0.4657726110821088	T	T	T
0.0465795189654585	0.9613113698918738	0.4658807924241160	T	T	T
0.3031102628908116	0.2474337329938407	0.4867073608995440	T	T	T
0.3036052742003363	0.5806598408120820	0.4864617428341091	T	T	T
0.3030479026205555	0.9139156457752762	0.4866126409568494	T	T	T
0.5585945876201706	0.2017075659787153	0.5068782719934077	T	T	T
0.5589010049034897	0.5342215958649206	0.5066993363170269	T	T	T
0.5585037165825852	0.8668803228882354	0.5070704561164447	T	T	T
0.8151761929984929	0.1534304604652093	0.5274031839167534	T	T	T
0.8148582872779002	0.4871694805450346	0.5274710592992875	T	T	T
0.8153859317906367	0.8204971711422644	0.5276028813196447	T	T	T
0.0714595303695873	0.1069646945707774	0.5484208568454463	T	T	T
0.0707354516673817	0.4413243841552585	0.5486662911187139	T	T	T
0.0720943755602832	0.7727704801827571	0.5476075331584980	T	T	T
0.3258409937262172	0.0617172185618315	0.5688629902705742	T	T	T
0.3266817237289956	0.3949798425971522	0.5688054040005923	T	T	T
0.3267321820049744	0.7274638510828595	0.5687338892002529	T	T	T
0.5832625722275964	0.0139285356000229	0.5881293617987922	T	T	T
0.5843701692229715	0.3483473796870769	0.5893507271501548	T	T	T
0.5845498668018720	0.6770921647537236	0.5898015099771072	T	T	T
0.8410883661959048	0.6271890009118692	0.6102252533630548	T	T	T
0.8422345656807479	0.2992372877384213	0.6099208570978121	T	T	T
0.8436339026221020	0.9645058724706530	0.6096429327116937	T	T	T
0.0971111031575731	0.5853378410611398	0.6323371035403795	T	T	T
0.0940542167998046	0.2544654267085491	0.6329847348765085	T	T	T
0.0969453635315602	0.9190064965169498	0.6319758894382659	T	T	T
0.3509425090399247	0.5414634605374218	0.6513305883545115	T	T	T
0.3484350836285017	0.2101357011600271	0.6517012864940526	T	T	T
0.3497790534889447	0.8752122513210878	0.6511217481340168	T	T	T
0.6051243404948536	0.5012199191478572	0.6736904247791955	T	T	T
0.6037295891662353	0.1602453775272110	0.6700328295576767	T	T	T
0.6038581591180900	0.8332823311041011	0.6698213542463378	T	T	T
0.8655765102391157	0.1083669955422693	0.6906927963574319	T	T	T
0.8594522131772564	0.7811029285375355	0.6880652146923083	T	T	T
0.7402126835578642	0.3635196014985738	0.7352686791979579	T	T	T
0.6849378612132426	0.3460500892786840	0.7621876261285436	T	T	T

OH/Defected-Cu(533) E_{ads} = −3.54 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu O H
59 1 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0467695334148601 0.2945750812853944 0.4658851010871743 T T T
0.0470084309083774 0.6272026335661067 0.4658019862231413 T T T
0.0468630610389837 0.9615809913863131 0.4657211503168384 T T T
0.3037290663718224 0.2472651892294095 0.4866118344958963 T T T
0.3046163416665166 0.5798691709903068 0.4862824958966314 T T T
0.3034072933444065 0.9141045834341739 0.4865459212981520 T T T
0.5600093910522546 0.2002149820130157 0.5076126487773820 T T T
0.5595379071900410 0.5343564392682225 0.5068804224995560 T T T
0.5590900298616788 0.8674791370541612 0.5069210531678010 T T T
0.8157748716640469 0.1537369701958440 0.5274920299988821 T T T
0.8152506724440087 0.4875539431570459 0.5276397678518592 T T T
0.8155560223872556 0.8207888830803043 0.5274704768957150 T T T
0.0715825126314158 0.1076934313211169 0.5482465093632101 T T T
0.0715892585353473 0.4403425279192348 0.5483070905321412 T T T
0.0729823508630290 0.7730734322030699 0.5473634800839164 T T T
0.3268110290428581 0.0615687954360453 0.5687132079047217 T T T
0.3281800905319301 0.3936951712488224 0.5683164973233445 T T T
0.3281162425774866 0.7268817889125572 0.5684064108395859 T T T
0.5846421412431653 0.0099468299396932 0.5898980914249350 T T T
0.5850873708197213 0.3491790121909304 0.5897945097133146 T T T
0.5853574930598029 0.6792423441681450 0.5898345261031110 T T T
0.8423199422222751 0.6284117117394956 0.6102497391265373 T T T
0.8425221103249712 0.3017529213501575 0.6103654929575626 T T T
0.8432765899683830 0.9642102659956535 0.6085114241338587 T T T
0.0994384222460241 0.5831496415126622 0.6313947645987454 T T T

0.0935299779199354	0.2563495905817064	0.6332551397171429	T	T	T
0.0986814607792681	0.9188378843989398	0.6314172696450768	T	T	T
0.3511799587195554	0.5404112443984488	0.6508650063272796	T	T	T
0.3505104291600816	0.2084338872879314	0.6510276142825191	T	T	T
0.3477171831446171	0.8778341753971048	0.6497550921348179	T	T	T
0.6061996977241435	0.4902075309439979	0.6735431297043348	T	T	T
0.6063190691416267	0.1612720530899878	0.6710030373619986	T	T	T
0.6068627842199490	0.8317628336857368	0.6735688584834421	T	T	T
0.8648962408065941	0.1087222394134741	0.6877603181132628	T	T	T
0.8650784432724166	0.7830552291867292	0.6877401170280422	T	T	T
0.6358539442231503	0.6362949061939958	0.7285385641171018	T	T	T
0.7480188714985232	0.5417114897135207	0.7398844371772739	T	T	T

OH/Defected-Cu(533) E_{ads} = −3.53 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu O H
59 1 1
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0465612232963935	0.2949326204541975	0.4660186752097317	T	T	T
0.0463599813330831	0.6279037709465456	0.4656856881438287	T	T	T
0.0463953572015470	0.9618281596773244	0.4659109464538815	T	T	T
0.3031724439605625	0.2478110678362313	0.4866285794055685	T	T	T
0.3034205237018526	0.5807238557920655	0.4862472326563534	T	T	T
0.3029106875645979	0.9145343381788393	0.4864677998606410	T	T	T
0.5585328313390860	0.2018310435078448	0.5068267224145018	T	T	T
0.5589357355458446	0.5338820461415708	0.5066723556069874	T	T	T
0.5583842236700534	0.8678724598158425	0.5075940216458363	T	T	T
0.8150227799485066	0.1536586100755386	0.5276738183628495	T	T	T
0.8145144902081825	0.4869611346468758	0.5275702780375795	T	T	T

0.8145777995776129	0.8209635016783423	0.5276640918338700	T	T	T
0.0704049007567633	0.1088496794393663	0.5483035555597979	T	T	T
0.0701332125202114	0.4420073681755383	0.5483984198356140	T	T	T
0.0711194399817288	0.7739279538893200	0.5474071517957384	T	T	T
0.3247726490339460	0.0634788914213189	0.5686486156032586	T	T	T
0.3262600200968606	0.3958465480493061	0.5685671461110289	T	T	T
0.3267057467531842	0.7281941451630942	0.5681033946649521	T	T	T
0.5823388854123763	0.0180102174857240	0.5894092483983613	T	T	T
0.5845658952790203	0.3465256764252587	0.5896110633427583	T	T	T
0.5834804581853916	0.6780962061349172	0.5894401089294732	T	T	T
0.8395130004751152	0.6274197197789064	0.6096259879703041	T	T	T
0.8414640358453340	0.2987146883204517	0.6111479417123320	T	T	T
0.8415937563365503	0.9649030128199385	0.6097541999030014	T	T	T
0.0965489512118509	0.5865237454123289	0.6318820802286851	T	T	T
0.0922568333015406	0.2569527252312938	0.6333254201555150	T	T	T
0.0987077623951578	0.9187397875557437	0.6309159665963264	T	T	T
0.3486886272402572	0.5439589836182535	0.6502505671186896	T	T	T
0.3470229406254006	0.2121505568170576	0.6515773139268930	T	T	T
0.3472675781574495	0.8798277618172605	0.6509629608787719	T	T	T
0.6026493450568253	0.5093937431170161	0.6717914186884713	T	T	T
0.6017209545751001	0.1607477353264883	0.6736086316153518	T	T	T
0.6018686946012153	0.8342325242273674	0.6697093210071117	T	T	T
0.8838918605261767	0.0869966513938394	0.6902600410152147	T	T	T
0.8617793217331737	0.7686211622925256	0.6873867824145989	T	T	T
0.6763695275858481	0.2879640993529478	0.7274470674184599	T	T	T
0.6466964484776341	0.3141798926711914	0.7629205490651429	T	T	T

OH/Cu(533) E_{ads} = −3.51 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu O H
60 1 1
Selective dynamics
Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F

0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0473558712275306 0.2939197350188323 0.4659665644544830 T T T
0.0471068998788624 0.6274843074324465 0.4656979759470659 T T T
0.0471506307783400 0.9608998161735371 0.4659653849009047 T T T
0.3038898734499824 0.2469237584320965 0.4866245068776536 T T T
0.3036626741776800 0.5803562108787830 0.4865815575020065 T T T
0.3039721271694162 0.9133223193573912 0.4866304402454560 T T T
0.5592711264478680 0.2012379863990290 0.5070028324667888 T T T
0.5590566557474475 0.5340996513013962 0.5070174106644174 T T T
0.5595149350669146 0.8664486925808816 0.5069888132896310 T T T
0.8155507029710449 0.1540082362451685 0.5276242191344025 T T T
0.8155497131331515 0.4866274673089919 0.5275731673055049 T T T
0.8161996237708919 0.8199340842211313 0.5277923053873934 T T T
0.0717283638215207 0.1070897887215452 0.5482447083181299 T T T
0.0719917399755303 0.4406569363994350 0.5479114735843211 T T T
0.0720875762571183 0.7727518122562742 0.5479758741108682 T T T
0.3267577050664556 0.0609781362446142 0.5687788089196175 T T T
0.3266426986583753 0.3947021590554627 0.5689332344304248 T T T
0.3259663751307684 0.7285217961261239 0.5687555623231404 T T T
0.5842733108921081 0.0132035202520271 0.5882143975146334 T T T
0.5841607261673332 0.3482773981845710 0.5894970018325978 T T T
0.5841630222421159 0.6783135613465561 0.5894711551489351 T T T
0.8431822033345497 0.6280622973425025 0.6095165973260848 T T T
0.8423162193418321 0.2983409098054182 0.6102875545476394 T T T
0.8431686337280553 0.9669131942837552 0.6095661263766132 T T T
0.0983812359833394 0.5851443031434371 0.6326058622610375 T T T
0.0977631945414785 0.2522250869851348 0.6321090621179835 T T T
0.0971738136929474 0.9190385011685223 0.6320294207857913 T T T
0.3503799096398836 0.5417356752903544 0.6516583898702706 T T T
0.3500667685973085 0.2084021894894050 0.6515192110956960 T T T
0.3500855626250257 0.8748260087470427 0.6513831742131657 T T T
0.6018411744921082 0.4986053095986662 0.6737740999550681 T T T
0.6031289430970119 0.1617852881784785 0.6705013114805709 T T T
0.6029914859918790 0.8329450588981970 0.6705441938918142 T T T
0.8660888633750119 0.4578372969974183 0.6915125399656574 T T T
0.8660731068749286 0.0989166677739561 0.6915831913620494 T T T
0.8584744165314504 0.7845800228464626 0.6884121666780985 T T T
0.7742784550813155 0.3550062709882127 0.7375010848663948 T T T
0.7475361747781619 0.3774528527747876 0.7731797222683028 T T T

OH/Cu(533) E_{ads} = −3.33 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu O H
60 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F

0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0467201475345576	0.2944870188845314	0.4658157804903453	T	T	T
0.0466542584157565	0.6278245128448958	0.4657203580808513	T	T	T
0.0468534848176034	0.9610228383389341	0.4656953727113020	T	T	T
0.3034141419772496	0.2472799643278165	0.4865038892256166	T	T	T
0.3034094269541754	0.5806191859896899	0.4865008013816308	T	T	T
0.3034128831078036	0.9137468414873311	0.4864860382599048	T	T	T
0.5583359621769972	0.2018859912014079	0.5069175145796692	T	T	T
0.5582569478059156	0.5344073221957544	0.5069596269679835	T	T	T
0.5588193780396296	0.8676177953051649	0.5075454545903781	T	T	T
0.8146752033979396	0.1542412891732425	0.5274757326929134	T	T	T
0.8144651057913990	0.4874871095108730	0.5275529633985485	T	T	T
0.8146129819306225	0.8216838421476069	0.5275808941103151	T	T	T
0.0707175267550966	0.1075935948514797	0.5478481767215726	T	T	T
0.0712442021107194	0.4408195595361448	0.5478208361607102	T	T	T
0.0708316895040397	0.7744539107290009	0.5477683127081434	T	T	T
0.3259517517461887	0.0616325222731433	0.5684447195279745	T	T	T
0.3261379779205242	0.3950364737059857	0.5685671046797012	T	T	T
0.3252823727887915	0.7291053898781001	0.5687168660080673	T	T	T
0.5828304396497970	0.0168310519111898	0.5896167345583976	T	T	T
0.5834870867513544	0.3472319178708645	0.5897820590533627	T	T	T
0.5825942448553363	0.6788231801931417	0.5896930161488214	T	T	T
0.8410599684601650	0.6324227507998827	0.6084233723416119	T	T	T
0.8407799587367037	0.2975927779429455	0.6098374625473184	T	T	T
0.8409509409533626	0.9678303590597110	0.6098764812720248	T	T	T
0.0975482315686946	0.5856929691554242	0.6316704970053024	T	T	T
0.0974774523684800	0.2517232037317569	0.6316779220061477	T	T	T
0.0964978996647972	0.9200676292038565	0.6323312632586848	T	T	T
0.3478890656116178	0.5435461071828058	0.6502744889480638	T	T	T
0.3487826584785552	0.2084472513865521	0.6511849960430851	T	T	T
0.3487710642262130	0.8769903894536313	0.6513195160936647	T	T	T
0.6000630958712634	0.5071041269591419	0.6733858726307815	T	T	T
0.5997291250988681	0.1598215508927439	0.6733569945541973	T	T	T
0.6041656867508252	0.8300132213620017	0.6713134974966550	T	T	T
0.8636176978359416	0.4514887903000826	0.6883930302771546	T	T	T
0.8770379631254031	0.1027768068093948	0.6916537560218288	T	T	T
0.8638201364514941	0.7758930258665799	0.6883858595827661	T	T	T
0.6637551974199454	0.2800799602115518	0.7292411368802263	T	T	T
0.6296985923676175	0.3085714279684595	0.7643468556589923	T	T	T

OH/Cu(533) E_{ads} = −3.27 eV

1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu O H
60 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0467918757700261 0.2943116860893085 0.4657171548321131 T T T
0.0463766012441482 0.6281387031788412 0.4658448176465697 T T T
0.0465309594610233 0.9612809401711075 0.4657674155415350 T T T
0.3028206173452475 0.2478874217088958 0.4866094097950935 T T T
0.3022500978726654 0.5812852552404308 0.4867364442688498 T T T
0.3031342785950102 0.9140516785270023 0.4872179985671039 T T T
0.5578767633472594 0.2018241673284038 0.5068022605255464 T T T
0.5579169789276435 0.5348348689157945 0.5067647749130799 T T T
0.5578458713090342 0.8686223070203027 0.5068489986999012 T T T
0.8136942499665309 0.1548300093158304 0.5275877908482016 T T T
0.8144316767495354 0.4879724991674124 0.5273051009009038 T T T
0.8135221443804284 0.8223521551330393 0.5275519512166369 T T T
0.0710064103237045 0.1074070683809367 0.5476043793350840 T T T
0.0709031035751124 0.4410300720305784 0.5476136291437683 T T T
0.0692521541037152 0.7759898421184346 0.5479775551056605 T T T
0.3257628165751285 0.0642430163608196 0.5695491094724332 T T T
0.3263756765775980 0.3948658070339093 0.5695415764120710 T T T
0.3262617257802276 0.7258776010826935 0.5694457699550313 T T T
0.5811492773993336 0.0171421322875887 0.5895162893504562 T T T
0.5809954830598159 0.3479569230535873 0.5894844846469667 T T T
0.5824790696070963 0.6813801720053760 0.5882286091827638 T T T
0.8413975929349959 0.6320269448001028 0.6088913786880710 T T T
0.8415838806712159 0.2984498675370659 0.6089047885444430 T T T
0.8380639260046294 0.9687637991643072 0.6100580876260935 T T T
0.0958004394678866 0.5871584456671712 0.6301400929128818 T T T
0.0960626881224087 0.2523125222504419 0.6316337928596027 T T T

0.0966382735710738 0.9206927946525170 0.6312262724605020 T T T
0.3459759952259773 0.5535195457336783 0.6530801369229593 T T T
0.3458400730913169 0.2032745325502034 0.6530627446643109 T T T
0.3520987574854431 0.8732102721008630 0.6511180599166622 T T T
0.6099832242453900 0.4947505232175260 0.6707735441643550 T T T
0.6158924399286434 0.1536082325895407 0.6746699770403097 T T T
0.6097643416484289 0.8221508136963465 0.6707364905270268 T T T
0.8634688427666148 0.4472024773615502 0.6898226336494346 T T T
0.8663929899249538 0.1139057277342062 0.6898428564535735 T T T
0.8666002021349613 0.7754105205111230 0.6895542511072534 T T T
0.3972443434163040 0.3355418005990316 0.7089405854886124 T T T
0.3634473469058435 0.3632645326136128 0.7440499861660683 T T T

OH/Defected-Cu(533) E_{ads} = −3.25 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu O H
59 1 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0467125487144244 0.2945904216096267 0.4658303358311500 T T T
0.0464575445848752 0.6276556705886378 0.4658908367691481 T T T
0.0465362964513361 0.9614741084040617 0.4658339424772180 T T T
0.3029550864706110 0.2481313452184324 0.4869531818167943 T T T
0.3028612635183805 0.5809803022179025 0.4864766449707005 T T T
0.3028019983494161 0.9139652365283766 0.4866795405228785 T T T
0.5584997803794280 0.2019908732914431 0.5068964766032593 T T T
0.5586243094329717 0.5341809760923510 0.5068953002524452 T T T
0.5585626554083518 0.8675644628273957 0.5072242932939091 T T T
0.8144209290265323 0.1545818413612139 0.5277760103601210 T T T
0.8147134950353987 0.4874084428402128 0.5274122799025207 T T T

0.8145898576448758 0.8207032920520660 0.5276319633847137 T T T
0.0701494268561191 0.1088395742758195 0.5481280392729957 T T T
0.0705940932297935 0.4408560343863073 0.5483484212941576 T T T
0.0703768464777852 0.7747975382706116 0.5475993946855056 T T T
0.3255373513269717 0.0620417591281139 0.5684799694185187 T T T
0.3264858654518221 0.3969775445604000 0.5694888818282848 T T T
0.3271470200663984 0.7262247431333364 0.5691486809221047 T T T
0.5827330984476404 0.0166548553963608 0.5888887546833743 T T T
0.5828546140748116 0.3480626932226158 0.5899404614320645 T T T
0.5849908145755052 0.6772877925784897 0.5892925077290130 T T T
0.8416105748602760 0.6271836472151833 0.6100596475783320 T T T
0.8405690059194981 0.3021287638214574 0.6109845452485700 T T T
0.8397128393820523 0.9657310418695175 0.6093484254153054 T T T
0.0967052053269910 0.5849988600703853 0.6313935361404290 T T T
0.0929837543766467 0.2558167313035327 0.6333152312906023 T T T
0.0982940156141652 0.9203516791487729 0.6304352855917870 T T T
0.3431939129410324 0.5474511961643458 0.6534919748485564 T T T
0.3488008601455377 0.2067862135720588 0.6506655320614527 T T T
0.3502659827028154 0.8781633893639622 0.6505435636891619 T T T
0.6153215274229638 0.4977610555097556 0.6726360822547903 T T T
0.6079242567824821 0.1528633195046183 0.6740594388626135 T T T
0.6074156495992327 0.8279404573783822 0.6695922880473475 T T T
0.8715187013249022 0.1002324413823956 0.6879501090964197 T T T
0.8633120949696576 0.7751144906770833 0.6884249793763715 T T T
0.4873857220363931 0.4362764718614685 0.7168616235630267 T T T
0.4534781955052267 0.4633714331814005 0.7519490229088177 T T T

OH/Cu(533) $E_{ads} = -3.23$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu O H
60 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F

0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0468376648321609 0.2943742764521033 0.4656581729418576 T T T
0.0466646456116635 0.6278451654986128 0.4657217231371789 T T T
0.0463545693281091 0.9614599536656456 0.4657887268617529 T T T
0.3035296413007273 0.2475997934167822 0.4866364586935958 T T T
0.3028168895352437 0.5811817943813153 0.4866796051358051 T T T
0.3030958759193538 0.9133893050861062 0.4866613320526696 T T T
0.5583331641702998 0.2018488617131666 0.5069351096439618 T T T
0.5582502174743311 0.5344805044641348 0.5068534647391161 T T T
0.5588647273945995 0.8674412549446870 0.5070382869209098 T T T
0.8139520112503718 0.1548659104497432 0.5277995378188862 T T T
0.8146820754788351 0.4875141884726801 0.5273575734079969 T T T
0.8147386020603022 0.8212061638846109 0.5274217061417232 T T T
0.0704289712361827 0.1080888225109149 0.5478181012657473 T T T
0.0716363765626369 0.4403687292606620 0.5476775976398045 T T T
0.0698810704172459 0.7751935596557828 0.5478247088563180 T T T
0.3268638022971757 0.0607762967370888 0.5681009325366020 T T T
0.3265969502271133 0.3963846757792950 0.5693508268827543 T T T
0.3265677148126258 0.7263090490661810 0.5693314890738606 T T T
0.5833264008035997 0.0155748036663326 0.5890854713919467 T T T
0.5819197961242679 0.3485120340447594 0.5898893747518059 T T T
0.5834859942548363 0.6788723621152926 0.5891198604825334 T T T
0.8427702029029689 0.6308481447935534 0.6087585888088682 T T T
0.8398032309802304 0.3003042162994234 0.6097161219638778 T T T
0.8397167221087543 0.9668276547832804 0.6097137243807822 T T T
0.0975955104976123 0.5844243673469478 0.6313364156758539 T T T
0.0986425878193913 0.2511152379678023 0.6315786902636447 T T T
0.0978341525033031 0.9195237407388461 0.6308636612231311 T T T
0.3432556212528581 0.5472927482401104 0.6533601927958728 T T T
0.3515462521631534 0.2040068461542788 0.6504049942399988 T T T
0.3516396081499025 0.8764640177609095 0.6504741968531320 T T T
0.6102787914078007 0.4986876427548310 0.6739354032460625 T T T
0.6097768184571493 0.1513266182688611 0.6738750568967404 T T T
0.6088799217321466 0.8258914050299140 0.6710512845295256 T T T
0.8660248050704524 0.4468551844838302 0.6896612387946348 T T T
0.8705731132359418 0.1077170780799506 0.6892900839661635 T T T
0.8659897713572491 0.7765424373318055 0.6895698432779938 T T T
0.4826072124438099 0.4312674977448410 0.7170021143176513 T T T
0.4543609352205706 0.4541666347639861 0.7525521453147306 T T T

OH/Cu(533) E_{ads} = −3.21 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu O H
60 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F

0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0473149223972840	0.2949761461330880	0.4659789576694280	T	T	T
0.0472927817221773	0.6276254753242370	0.4661010277509021	T	T	T
0.0472178959576013	0.9602562363254705	0.4660947625435625	T	T	T
0.3037783512421299	0.2473492673666442	0.4866916372735517	T	T	T
0.3039590757935358	0.5801143601230621	0.4867043346059887	T	T	T
0.3041185152171195	0.9135356458903274	0.4866170799705003	T	T	T
0.5591916073096996	0.2011828567680780	0.5069775640011684	T	T	T
0.5597644015459267	0.5337447093598939	0.5068209274963849	T	T	T
0.5598574491804342	0.8673410616102899	0.5067968181754168	T	T	T
0.8165994253576514	0.1527717499130787	0.5277113572208734	T	T	T
0.8168232003764189	0.4871157411527136	0.5277149558901257	T	T	T
0.8168239992849351	0.8197826998299860	0.5276049581219056	T	T	T
0.0729513398065009	0.1070234311303935	0.5475375728478795	T	T	T
0.0733183484056710	0.4408614541714115	0.5492356970939056	T	T	T
0.0732564930511970	0.7713838790510792	0.5492475397644228	T	T	T
0.3287936379960428	0.0598317741694459	0.5687132592614361	T	T	T
0.3279665905273816	0.3940871084737907	0.5694237845061068	T	T	T
0.3280579567580943	0.7269789241719593	0.5688719890738199	T	T	T
0.5866250983583328	0.0119542225218154	0.5885016314986657	T	T	T
0.5848200595476456	0.3466656434977864	0.5888352409124451	T	T	T
0.5856694517352139	0.6795554734160802	0.5886483607566859	T	T	T
0.8446962438003069	0.6319374844464747	0.6099997059749072	T	T	T
0.8440205849122719	0.2977378316261508	0.6091585734644056	T	T	T
0.8443407232216913	0.9629937143277445	0.6099050266309405	T	T	T
0.1039696678539315	0.5810681340029333	0.6346425154812962	T	T	T
0.1007533196475308	0.2481966936871061	0.6318873297711818	T	T	T
0.1000504222275680	0.9212785633996035	0.6312899890072501	T	T	T
0.3563054295872092	0.5386953969623463	0.6519401922109509	T	T	T
0.3577647217438695	0.1994494650140410	0.6506372783659913	T	T	T
0.3542938568003109	0.8726302237278318	0.6516282212115030	T	T	T
0.6058686349603164	0.4965581570840385	0.6719425462858126	T	T	T
0.6088349506739377	0.1586645070345440	0.6716114115249638	T	T	T
0.6087853040519136	0.8280196203327534	0.6718482932963212	T	T	T
0.8596208364099667	0.4484636600590761	0.6894165168090822	T	T	T
0.8593563502967925	0.1221379989756315	0.6894405674149269	T	T	T
0.8577155585699785	0.7854883010400897	0.6940200230413254	T	T	T
0.0855115764945182	0.6154250779551660	0.7123918409808567	T	T	T
0.1293436032511011	0.4718829013145580	0.7278941842362698	T	T	T

OH/Cu(533) E_{ads} = −3.10 eV

1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu O H
60 1 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0467430342657522 0.2950972684929170 0.4659545355794492 T T T
0.0462342744273485 0.6282277824501605 0.4661743016088025 T T T
0.0463450667649354 0.9608674389803227 0.4660838584340112 T T T
0.3027145537288334 0.2482307758014954 0.4868242936356850 T T T
0.3025295656213629 0.5808593176838812 0.4867963758063567 T T T
0.3032927525382689 0.9139791988531059 0.4869203674909883 T T T
0.5574863255054794 0.2022561952937210 0.5068690898432990 T T T
0.5577823537273190 0.5351083465579407 0.5066263613101967 T T T
0.5577910111945954 0.8684968378901488 0.5066780012511884 T T T
0.8136459655465771 0.1552212643556956 0.5275301556489325 T T T
0.8148181221014212 0.4879590780916274 0.5273145666716204 T T T
0.8130003605836222 0.8223518884175931 0.5274955994060377 T T T
0.0709293505118822 0.1076386159159526 0.5474496868324721 T T T
0.0710000897031051 0.4423758494315635 0.5488058095099930 T T T
0.0704224235720901 0.7736571595222017 0.5488148955806764 T T T
0.3255657760150115 0.0636276054967837 0.5692634485505010 T T T
0.3246714616485136 0.3963361798319269 0.5700198288619518 T T T
0.3257971613943695 0.7272197219399743 0.5691941364277753 T T T
0.5799473818096246 0.0167938274489288 0.5889819749945957 T T T
0.5800959184212076 0.3501367078487547 0.5889705890438393 T T T
0.5831370266846321 0.6809040164260978 0.5882277777513352 T T T
0.8410189177646359 0.6327192299337128 0.6092586538543472 T T T
0.8410258191178670 0.2993059228267541 0.6088942925606062 T T T
0.8403118872833204 0.9662818455270354 0.6091822412918617 T T T
0.0911772368136212 0.5911019380226037 0.6338608609371761 T T T
0.0964201692540740 0.2502672641170918 0.6312599258697276 T T T

0.0962111013175644	0.9231071610479091	0.6312802671199265	T	T	T
0.3538950847592943	0.5474660727855678	0.6535328176917687	T	T	T
0.3537513888207400	0.1964883410901805	0.6536897558246295	T	T	T
0.3523634823706274	0.8729662086017029	0.6509865897154299	T	T	T
0.6075966591774105	0.4952815110104254	0.6716243388949366	T	T	T
0.6080107241771628	0.1612111675468313	0.6709479736712964	T	T	T
0.6064945123811540	0.8254027474095835	0.6715318537800741	T	T	T
0.8609394275977493	0.4490829647690759	0.6895138443609454	T	T	T
0.8600737516277732	0.1170709073745400	0.6893866757633020	T	T	T
0.8522450365290410	0.7895310838432081	0.6905839968456320	T	T	T
0.2404036338255153	0.4666145944152404	0.6984048292991645	T	T	T
0.2123489805211634	0.4904728766669137	0.7340267823208748	T	T	T

OH/Cu(111) $E_{ads} = -3.44$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
3.8289832201000000 6.6319934786000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu O H
45 1 1
Selective dynamics
Direct

0.8888888887999968	0.2222222223999992	0.3170124957488483	F	F	F
0.2222222221000010	0.2222222223999992	0.3170124957488483	F	F	F
0.5555555553999980	0.2222222223999992	0.3170124957488483	F	F	F
0.8888888890000004	0.5555555553000033	0.3170124957488483	F	F	F
0.2222222222999974	0.5555555553000033	0.3170124957488483	F	F	F
0.5555555556000016	0.5555555553000033	0.3170124957488483	F	F	F
0.8888888891999969	0.8888888882000003	0.3170124957488483	F	F	F
0.2222222225000010	0.8888888882000003	0.3170124957488483	F	F	F
0.5555555557999980	0.8888888882000003	0.3170124957488483	F	F	F
0.0000000000000000	0.0000000000000000	0.3975777759823913	F	F	F
0.3333333332999970	0.0000000000000000	0.3975777759823913	F	F	F
0.6666666666000012	0.0000000000000000	0.3975777759823913	F	F	F
0.0000000002103135	0.3333333328999970	0.3975777759823913	F	F	F
0.3333333335000006	0.3333333328999970	0.3975777759823913	F	F	F
0.6666666668999994	0.3333333328999970	0.3975777759823913	F	F	F
0.9999999996666986	0.6666666672999995	0.3975777759823913	F	F	F
0.3333333329999988	0.6666666672999995	0.3975777759823913	F	F	F
0.6666666663000029	0.6666666672999995	0.3975777759823913	F	F	F
0.1111111113999996	0.1111111104999978	0.4771948603999974	F	F	F
0.4444444447999985	0.1111111104999978	0.4771948603999974	F	F	F
0.7777777781000026	0.1111111104999978	0.4771948603999974	F	F	F
0.1111111108999978	0.4444444449000002	0.4771948603999974	F	F	F
0.4444444442000020	0.4444444449000002	0.4771948603999974	F	F	F
0.7777777774999990	0.4444444449000002	0.4771948603999974	F	F	F
0.1111111111000014	0.7777777777999972	0.4771948603999974	F	F	F
0.4444444443999984	0.7777777777999972	0.4771948603999974	F	F	F
0.7777777777000026	0.7777777777999972	0.4771948603999974	F	F	F
0.8867836058539436	0.2222885750304104	0.5571099667900797	T	T	T
0.2242611524156433	0.2222885750304104	0.5571099667900797	T	T	T
0.5552403286498639	0.2228526759002671	0.5575312583712991	T	T	T
0.8899388712210974	0.5534555908578088	0.5562494888416596	T	T	T
0.2250426649264002	0.5534087523016119	0.5575609125397025	T	T	T
0.5548819159719839	0.5534087523016119	0.5575609125397025	T	T	T
0.8898410286476208	0.8876416403494938	0.5562637600339979	T	T	T
0.2239681784197447	0.8853969763605063	0.5571550155386263	T	T	T

0.5558506642028803	0.8876416403494938	0.5562637600339979	T	T	T
0.0000782566806131	0.9987853661970392	0.6366377490119725	T	T	T
0.3344697104223449	0.9987853661970392	0.6366377490119725	T	T	T
0.6697355504336927	0.9938622323326177	0.6362525125262217	T	T	T
0.0008107543950250	0.3317118245305669	0.6367052921674639	T	T	T
0.3278789703133345	0.3251988059410654	0.6393746577980866	T	T	T
0.6802555570455970	0.3251988059410654	0.6393746577980866	T	T	T
0.9965549258857809	0.6669355125889515	0.6361334398417982	T	T	T
0.3265261285280473	0.6802810762439095	0.6393535530862832	T	T	T
0.6698428947919681	0.6669355125889515	0.6361334398417982	T	T	T
0.4438305925565914	0.4456721448868191	0.6900002578139632	T	T	T
0.4420546169347806	0.4492240961304403	0.7280967673214698	T	T	T

OH/Cu(111) $E_{ads} = -3.39$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
3.8289832201000000 6.6319934786000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu O H
45 1 1
Selective dynamics
Direct

0.8888888887999968	0.2222222223999992	0.3170124957488483	F	F	F
0.2222222221000010	0.2222222223999992	0.3170124957488483	F	F	F
0.5555555553999980	0.2222222223999992	0.3170124957488483	F	F	F
0.8888888890000004	0.5555555553000033	0.3170124957488483	F	F	F
0.2222222222999974	0.5555555553000033	0.3170124957488483	F	F	F
0.5555555556000016	0.5555555553000033	0.3170124957488483	F	F	F
0.8888888891999969	0.8888888882000003	0.3170124957488483	F	F	F
0.2222222225000010	0.8888888882000003	0.3170124957488483	F	F	F
0.5555555557999980	0.8888888882000003	0.3170124957488483	F	F	F
0.0000000000000000	0.0000000000000000	0.3975777759823913	F	F	F
0.3333333332999970	0.0000000000000000	0.3975777759823913	F	F	F
0.6666666666000012	0.0000000000000000	0.3975777759823913	F	F	F
0.0000000002103135	0.3333333328999970	0.3975777759823913	F	F	F
0.3333333335000006	0.3333333328999970	0.3975777759823913	F	F	F
0.6666666668999994	0.3333333328999970	0.3975777759823913	F	F	F
0.9999999996666986	0.6666666672999995	0.3975777759823913	F	F	F
0.3333333329999988	0.6666666672999995	0.3975777759823913	F	F	F
0.6666666663000029	0.6666666672999995	0.3975777759823913	F	F	F
0.1111111113999996	0.1111111104999978	0.4771948603999974	F	F	F
0.4444444447999985	0.1111111104999978	0.4771948603999974	F	F	F
0.7777777781000026	0.1111111104999978	0.4771948603999974	F	F	F
0.1111111108999978	0.4444444449000002	0.4771948603999974	F	F	F
0.4444444442000020	0.4444444449000002	0.4771948603999974	F	F	F
0.7777777774999990	0.4444444449000002	0.4771948603999974	F	F	F
0.1111111111000014	0.7777777777999972	0.4771948603999974	F	F	F
0.4444444443999984	0.7777777777999972	0.4771948603999974	F	F	F
0.7777777777000026	0.7777777777999972	0.4771948603999974	F	F	F
0.8866422328461404	0.2236470266047137	0.5570322678708760	T	T	T
0.2222222221000010	0.2222222223999992	0.5559885174016669	T	T	T
0.5563774071491401	0.2236470266047137	0.5570322678708760	T	T	T
0.8866422330461440	0.5563774070491454	0.5570322678708760	T	T	T
0.2236470265047119	0.5563774070491454	0.5570322678708760	T	T	T
0.5555555556000016	0.5555555553000033	0.5577505620578841	T	T	T
0.8888888891999969	0.8888888882000003	0.5563889719102202	T	T	T
0.2236470267047155	0.8866422322461439	0.5570322678708760	T	T	T

0.5563774075491401	0.8866422322461439	0.5570322678708760	T	T	T
-0.0002538826869999	-0.0002538826869999	0.6366174954036490	T	T	T
0.3311468683358630	0.0043729299282679	0.6361606558060382	T	T	T
0.6671744319740009	-0.0002538826869999	0.6366174954036490	T	T	T
0.0043729301385814	0.3311468679358630	0.6361606558060382	T	T	T
0.3311468685358666	0.3311468679358630	0.6361606558060382	T	T	T
0.6722147303636590	0.3222372059726775	0.6393600248752667	T	T	T
-0.0002538830203012	0.6671744326739992	0.6366174954036490	T	T	T
0.3222372060726793	0.6722147307636590	0.6393600248752667	T	T	T
0.6722147297636625	0.6722147307636590	0.6393600248752667	T	T	T
0.5555555555555571	0.5555555555555571	0.6913996596834556	T	T	T
0.5555555555555571	0.5555555555555571	0.7295012955233020	T	T	T

OH/Cu(111) $E_{ads} = -2.48$ eV

1.00000000000000

7.6579664403000001	0.0000000000000000	0.0000000000000000
3.8289832201000000	6.6319934786000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.5000000000000000

Cu O H

45 1 1

Selective dynamics

Direct

0.8888888887999968	0.2222222223999992	0.3170124957488483	F	F	F
0.2222222221000010	0.2222222223999992	0.3170124957488483	F	F	F
0.5555555553999980	0.2222222223999992	0.3170124957488483	F	F	F
0.8888888890000004	0.5555555553000033	0.3170124957488483	F	F	F
0.2222222222999974	0.5555555553000033	0.3170124957488483	F	F	F
0.5555555556000016	0.5555555553000033	0.3170124957488483	F	F	F
0.8888888891999969	0.8888888882000003	0.3170124957488483	F	F	F
0.2222222225000010	0.8888888882000003	0.3170124957488483	F	F	F
0.5555555557999980	0.8888888882000003	0.3170124957488483	F	F	F
0.0000000000000000	0.0000000000000000	0.3975777759823913	F	F	F
0.3333333332999970	0.0000000000000000	0.3975777759823913	F	F	F
0.6666666666000012	0.0000000000000000	0.3975777759823913	F	F	F
0.0000000002103135	0.3333333328999970	0.3975777759823913	F	F	F
0.3333333335000006	0.3333333328999970	0.3975777759823913	F	F	F
0.6666666668999994	0.3333333328999970	0.3975777759823913	F	F	F
0.9999999996666986	0.6666666672999995	0.3975777759823913	F	F	F
0.3333333329999988	0.6666666672999995	0.3975777759823913	F	F	F
0.6666666663000029	0.6666666672999995	0.3975777759823913	F	F	F
0.1111111113999996	0.1111111104999978	0.4771948603999974	F	F	F
0.4444444447999985	0.1111111104999978	0.4771948603999974	F	F	F
0.7777777781000026	0.1111111104999978	0.4771948603999974	F	F	F
0.1111111108999978	0.4444444449000002	0.4771948603999974	F	F	F
0.4444444442000020	0.4444444449000002	0.4771948603999974	F	F	F
0.7777777774999990	0.4444444449000002	0.4771948603999974	F	F	F
0.1111111111000014	0.7777777777999972	0.4771948603999974	F	F	F
0.4444444443999984	0.7777777777999972	0.4771948603999974	F	F	F
0.7777777777000026	0.7777777777999972	0.4771948603999974	F	F	F
0.8888483758979362	0.2223032482041205	0.5567330491691109	T	T	T
0.2231443946110261	0.2231443949110243	0.5572956726696887	T	T	T
0.5537112103779549	0.2231443949110243	0.5572956726696887	T	T	T
0.8896640696132252	0.5551679649933945	0.5568155049527022	T	T	T
0.2231443948110226	0.5537112102779602	0.5572956726696887	T	T	T
0.5551679652933927	0.5551679649933945	0.5568155049527022	T	T	T
0.8888483762979362	0.8888483752979397	0.5567330491691109	T	T	T
0.2223032483041223	0.8888483752979397	0.5567330491691109	T	T	T

0.5551679654933892	0.8896640688132251	0.5568155049527022	T	T	T
0.0000000000000000	0.0000000000000000	0.6368140611182938	T	T	T
0.3334035765965950	0.9972899486426670	0.6369327355990251	T	T	T
0.6693064746607362	0.9972899486426670	0.6369327355990251	T	T	T
0.9972899488529805	0.3334035761965950	0.6369327355990251	T	T	T
0.3333333335000006	0.3333333328999970	0.6383628601917621	T	T	T
0.6693064749607345	0.3334035761965950	0.6369327355990251	T	T	T
0.9972899483093656	0.6693064753607345	0.6369327355990251	T	T	T
0.3334035762965968	0.6693064753607345	0.6369327355990251	T	T	T
0.6666666663000029	0.6666666672999995	0.6369850504303685	T	T	T
0.3333333350000061	0.3333333328999970	0.7104286381299403	T	T	T
0.3333333350000061	0.3333333328999970	0.7482693711858772	T	T	T

OH/Cu(100) $E_{ads} = -3.57$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu O H
45 1 1
Selective dynamics
Direct

0.0000000000000000	0.0000000000000000	0.3173193249345303	F	F	F
0.3333333332999970	0.0000000000000000	0.3173193249345303	F	F	F
0.6666666666000012	0.0000000000000000	0.3173193249345303	F	F	F
0.0000000000000000	0.3333333332999970	0.3173193249345303	F	F	F
0.3333333332999970	0.3333333332999970	0.3173193249345303	F	F	F
0.6666666666000012	0.3333333332999970	0.3173193249345303	F	F	F
0.0000000000000000	0.6666666666000012	0.3173193249345303	F	F	F
0.3333333332999970	0.6666666666000012	0.3173193249345303	F	F	F
0.6666666666000012	0.6666666666000012	0.3173193249345303	F	F	F
0.1666666667000030	0.1666666667000030	0.3854655552433357	F	F	F
0.5000000000000000	0.1666666667000030	0.3854655552433357	F	F	F
0.8333333332999970	0.1666666667000030	0.3854655552433357	F	F	F
0.1666666667000030	0.5000000000000000	0.3854655552433357	F	F	F
0.5000000000000000	0.5000000000000000	0.3854655552433357	F	F	F
0.8333333332999970	0.5000000000000000	0.3854655552433357	F	F	F
0.1666666667000030	0.8333333332999970	0.3854655552433357	F	F	F
0.5000000000000000	0.8333333332999970	0.3854655552433357	F	F	F
0.8333333332999970	0.8333333332999970	0.3854655552433357	F	F	F
0.0000000000000000	0.0000000000000000	0.4552941175999976	F	F	F
0.3333333332999970	0.0000000000000000	0.4552941175999976	F	F	F
0.6666666666000012	0.0000000000000000	0.4552941175999976	F	F	F
0.0000000000000000	0.3333333332999970	0.4552941175999976	F	F	F
0.3333333332999970	0.3333333332999970	0.4552941175999976	F	F	F
0.6666666666000012	0.3333333332999970	0.4552941175999976	F	F	F
0.0000000000000000	0.6666666666000012	0.4552941175999976	F	F	F
0.3333333332999970	0.6666666666000012	0.4552941175999976	F	F	F
0.6666666666000012	0.6666666666000012	0.4552941175999976	F	F	F
0.1675614369234821	0.1675614369234821	0.5255247849895783	T	T	T
0.5000000000000000	0.1684184225455872	0.5251627839384573	T	T	T
0.8324385630765176	0.1675614369234821	0.5255247849895783	T	T	T
0.1684184225455872	0.5000000000000000	0.5251627839384573	T	T	T
0.5000000000000000	0.5000000000000000	0.5227388992432409	T	T	T
0.8315815774544121	0.5000000000000000	0.5251627839384573	T	T	T
0.1675614369234821	0.8324385630765176	0.5255247849895783	T	T	T
0.5000000000000000	0.8315815774544121	0.5251627839384573	T	T	T

0.8324385630765176	0.8324385630765176	0.5255247849895783	T	T	T
0.0000000000000000	-0.0000000000000000	0.5938019970247891	T	T	T
0.3336347167826465	-0.0000000000000000	0.5929970207143368	T	T	T
0.6663652831173517	-0.0000000000000000	0.5929970207143368	T	T	T
0.0000000000000000	0.3336347167826465	0.5929970207143368	T	T	T
0.3293965267920760	0.3293965267920760	0.5948304408063135	T	T	T
0.6706034731079220	0.3293965267920760	0.5948304408063135	T	T	T
0.0000000000000000	0.6663652831173517	0.5929970207143368	T	T	T
0.3293965267920760	0.6706034731079220	0.5948304408063135	T	T	T
0.6706034731079220	0.6706034731079220	0.5948304408063135	T	T	T
0.5000000000000000	0.5000000000000000	0.6395444841892041	T	T	T
0.5000000000000000	0.5000000000000000	0.6778049824641966	T	T	T

OH/Cu(100) $E_{ads} = -3.34$ eV

1.00000000000000

7.6579664403000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.6579664403000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.5000000000000000

Cu O H

45 1 1

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.3173193249345303	F	F	F
0.3333333332999970	0.0000000000000000	0.3173193249345303	F	F	F
0.6666666666000012	0.0000000000000000	0.3173193249345303	F	F	F
0.0000000000000000	0.3333333332999970	0.3173193249345303	F	F	F
0.3333333332999970	0.3333333332999970	0.3173193249345303	F	F	F
0.6666666666000012	0.3333333332999970	0.3173193249345303	F	F	F
0.0000000000000000	0.6666666666000012	0.3173193249345303	F	F	F
0.3333333332999970	0.6666666666000012	0.3173193249345303	F	F	F
0.6666666666000012	0.6666666666000012	0.3173193249345303	F	F	F
0.1666666667000030	0.1666666667000030	0.3854655552433357	F	F	F
0.5000000000000000	0.1666666667000030	0.3854655552433357	F	F	F
0.8333333332999970	0.1666666667000030	0.3854655552433357	F	F	F
0.1666666667000030	0.5000000000000000	0.3854655552433357	F	F	F
0.5000000000000000	0.5000000000000000	0.3854655552433357	F	F	F
0.8333333332999970	0.5000000000000000	0.3854655552433357	F	F	F
0.1666666667000030	0.8333333332999970	0.3854655552433357	F	F	F
0.5000000000000000	0.8333333332999970	0.3854655552433357	F	F	F
0.8333333332999970	0.8333333332999970	0.3854655552433357	F	F	F
0.0000000000000000	0.0000000000000000	0.4552941175999976	F	F	F
0.3333333332999970	0.0000000000000000	0.4552941175999976	F	F	F
0.6666666666000012	0.0000000000000000	0.4552941175999976	F	F	F
0.0000000000000000	0.3333333332999970	0.4552941175999976	F	F	F
0.3333333332999970	0.3333333332999970	0.4552941175999976	F	F	F
0.6666666666000012	0.3333333332999970	0.4552941175999976	F	F	F
0.0000000000000000	0.6666666666000012	0.4552941175999976	F	F	F
0.3333333332999970	0.6666666666000012	0.4552941175999976	F	F	F
0.6666666666000012	0.6666666666000012	0.4552941175999976	F	F	F
0.1689107743561634	0.1684953488030024	0.5254901644981929	T	T	T
0.5000000000000000	0.1694399295604257	0.5255345577233553	T	T	T
0.8310892256438370	0.1684953488030024	0.5254901644981929	T	T	T
0.1689107743561634	0.4981713178970006	0.5254901644981929	T	T	T
0.5000000000000000	0.4972267371395772	0.5255345577233553	T	T	T
0.8310892256438370	0.4981713178970006	0.5254901644981929	T	T	T
0.1652419753412003	0.8333333332999970	0.5245163010384049	T	T	T
0.5000000000000000	0.8333333332999970	0.5245441335916355	T	T	T

0.8347580246587998	0.8333333332999970	0.5245163010384049	T	T	T
-0.0000000000000000	0.0004177926348464	0.5931148641075069	T	T	T
0.3321463083205051	-0.0035734131025394	0.5924443146495999	T	T	T
0.6678536915794929	-0.0035734131025394	0.5924443146495999	T	T	T
-0.0000000000000000	0.3333333332999970	0.5929172088910841	T	T	T
0.3201541803005017	0.3333333332999970	0.5981724802348685	T	T	T
0.6798458195994963	0.3333333332999970	0.5981724802348685	T	T	T
-0.0000000000000000	0.6662488739651548	0.5931148641075069	T	T	T
0.3321463083205051	0.6702400797025404	0.5924443146495999	T	T	T
0.6678536915794929	0.6702400797025404	0.5924443146495999	T	T	T
0.5000000000000000	0.3333333332999970	0.6517614644887525	T	T	T
0.5000000000000000	0.3333333332999970	0.6897663718048692	T	T	T

OH/Cu(100) $E_{ads} = -2.59$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu O H
45 1 1
Selective dynamics
Direct

0.0000000000000000	0.0000000000000000	0.3173193249345303	F	F	F
0.3333333332999970	0.0000000000000000	0.3173193249345303	F	F	F
0.6666666666000012	0.0000000000000000	0.3173193249345303	F	F	F
0.0000000000000000	0.3333333332999970	0.3173193249345303	F	F	F
0.3333333332999970	0.3333333332999970	0.3173193249345303	F	F	F
0.6666666666000012	0.3333333332999970	0.3173193249345303	F	F	F
0.0000000000000000	0.6666666666000012	0.3173193249345303	F	F	F
0.3333333332999970	0.6666666666000012	0.3173193249345303	F	F	F
0.6666666666000012	0.6666666666000012	0.3173193249345303	F	F	F
0.1666666667000030	0.1666666667000030	0.3854655552433357	F	F	F
0.5000000000000000	0.1666666667000030	0.3854655552433357	F	F	F
0.8333333332999970	0.1666666667000030	0.3854655552433357	F	F	F
0.1666666667000030	0.5000000000000000	0.3854655552433357	F	F	F
0.5000000000000000	0.5000000000000000	0.3854655552433357	F	F	F
0.8333333332999970	0.5000000000000000	0.3854655552433357	F	F	F
0.1666666667000030	0.8333333332999970	0.3854655552433357	F	F	F
0.5000000000000000	0.8333333332999970	0.3854655552433357	F	F	F
0.8333333332999970	0.8333333332999970	0.3854655552433357	F	F	F
0.0000000000000000	0.0000000000000000	0.4552941175999976	F	F	F
0.3333333332999970	0.0000000000000000	0.4552941175999976	F	F	F
0.6666666666000012	0.0000000000000000	0.4552941175999976	F	F	F
0.0000000000000000	0.3333333332999970	0.4552941175999976	F	F	F
0.3333333332999970	0.3333333332999970	0.4552941175999976	F	F	F
0.6666666666000012	0.3333333332999970	0.4552941175999976	F	F	F
0.0000000000000000	0.6666666666000012	0.4552941175999976	F	F	F
0.3333333332999970	0.6666666666000012	0.4552941175999976	F	F	F
0.6666666666000012	0.6666666666000012	0.4552941175999976	F	F	F
0.1680310308282369	0.1680310308282369	0.5252025890261803	T	T	T
0.4986356358717660	0.1680310308282369	0.5252025890261803	T	T	T
0.8333333332999970	0.1669738027249370	0.5251825854218451	T	T	T
0.1680310308282369	0.4986356358717660	0.5252025890261803	T	T	T
0.4986356358717660	0.4986356358717660	0.5252025890261803	T	T	T
0.8333333332999970	0.4996928639750661	0.5251825854218451	T	T	T
0.1669738027249370	0.8333333332999970	0.5251825854218451	T	T	T
0.4996928639750661	0.8333333332999970	0.5251825854218451	T	T	T

0.8333333332999970 0.8333333332999970 0.5244389780189537 T T T
-0.0009744381699351 -0.0009744381699351 0.5929004715290638 T T T
0.3333333332999970 -0.0025289997939096 0.5934949468078655 T T T
0.6676411047699364 -0.0009744381699351 0.5929004715290638 T T T
-0.0025289997939096 0.3333333332999970 0.5934949468078655 T T T
0.3333333332999970 0.3333333332999970 0.5958693256603037 T T T
0.6691956663939106 0.3333333332999970 0.5934949468078655 T T T
-0.0009744381699351 0.6676411047699364 0.5929004715290638 T T T
0.3333333332999970 0.6691956663939106 0.5934949468078655 T T T
0.6676411047699364 0.6676411047699364 0.5929004715290638 T T T
0.3333333332999970 0.3333333332999970 0.6672750082153597 T T T
0.3333333332999970 0.3333333332999970 0.7051004656440740 T T T

OH/Cu(211) $E_{ads} = -3.73$ eV
1.00000000000000
6.2527034153000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.3164343000000009
Cu O H
45 1 1
Selective dynamics
Direct
0.0061862950247047 0.1666666667000030 0.3120745335338029 F F F
0.0061862950247047 0.5000000000000000 0.3120745335338029 F F F
0.0061862950247047 0.8333333332999970 0.3120745335338029 F F F
0.3355456677560653 0.0000000000000000 0.3354619372229379 F F F
0.3355456677560653 0.3333333332999970 0.3354619372229379 F F F
0.3355456677560653 0.6666666666000012 0.3354619372229379 F F F
0.6630854692850079 0.1666666667000030 0.3607350091654666 F F F
0.6630854692850079 0.5000000000000000 0.3607350091654666 F F F
0.6630854692850079 0.8333333332999970 0.3607350091654666 F F F
0.9944057463905267 0.0000000000000000 0.3915351276171819 F F F
0.9944057463905267 0.3333333332999970 0.3915351276171819 F F F
0.9944057463905267 0.6666666666000012 0.3915351276171819 F F F
0.3330656692422309 0.1666666667000030 0.4179888222780335 F F F
0.3330656692422309 0.5000000000000000 0.4179888222780335 F F F
0.3330656692422309 0.8333333332999970 0.4179888222780335 F F F
0.6656564241704075 0.0000000000000000 0.4448469552356400 F F F
0.6656564241704075 0.3333333332999970 0.4448469552356400 F F F
0.6656564241704075 0.6666666666000012 0.4448469552356400 F F F
0.0003515212697778 0.1666666667000030 0.4732099031121066 F F F
0.0003515212697778 0.5000000000000000 0.4732099031121066 F F F
0.0003515212697778 0.8333333332999970 0.4732099031121066 F F F
0.3333333329999988 0.0000000000000000 0.5000000000000000 F F F
0.3333333329999988 0.3333333332999970 0.5000000000000000 F F F
0.3333333329999988 0.6666666666000012 0.5000000000000000 F F F
0.6663151448302216 0.1666666667000030 0.5267900968878934 F F F
0.6663151448302216 0.5000000000000000 0.5267900968878934 F F F
0.6663151448302216 0.8333333332999970 0.5267900968878934 F F F
0.9988413677702206 0.9991283636572649 0.5549454045927633 T T T
0.9990849625958551 0.3333333332999970 0.5548189635631300 T T T
0.9988413677702206 0.6675383029427363 0.5549454045927633 T T T
0.3333070755782537 0.1664678276416410 0.5815330787621005 T T T
0.3333070755782537 0.5001988390583618 0.5815330787621005 T T T
0.3326534554207899 0.8333333332999970 0.5814810481665975 T T T
0.6694188036123978 0.0033740004698737 0.6095986417420414 T T T
0.6700575386456372 0.3333333332999970 0.6093590948880210 T T T

0.6694188036123978	0.6632926661301275	0.6095986417420414	T	T	T
0.0013581491119469	0.1661550923331538	0.6379370184450875	T	T	T
0.0013581491119469	0.5005115743668491	0.6379370184450875	T	T	T
0.9997756958473720	0.8333333332999970	0.6389699428966732	T	T	T
0.3285369716903703	0.0001695316223694	0.6636580153985132	T	T	T
0.3281258530847670	0.3333333332999970	0.6624056829644568	T	T	T
0.3285369716903703	0.6664971349776317	0.6636580153985132	T	T	T
0.6615925367957555	0.1602846487872361	0.6917893869182772	T	T	T
0.6615925367957555	0.5063820179127597	0.6917893869182772	T	T	T
0.6548067861076426	0.8333333332999970	0.6878984214024783	T	T	T
0.6978759861784607	0.3333333333333357	0.7455456486816515	T	T	T
0.5803254415376518	0.3333333333333357	0.7698106053224408	T	T	T

OH/Cu(211) $E_{ads} = -3.54$ eV
1.00000000000000
6.2527034153000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.3164343000000009
Cu O H
45 1 1
Selective dynamics
Direct

0.0061862950247047	0.1666666667000030	0.3120745335338029	F	F	F
0.0061862950247047	0.5000000000000000	0.3120745335338029	F	F	F
0.0061862950247047	0.8333333332999970	0.3120745335338029	F	F	F
0.3355456677560653	0.0000000000000000	0.3354619372229379	F	F	F
0.3355456677560653	0.3333333332999970	0.3354619372229379	F	F	F
0.3355456677560653	0.6666666666000012	0.3354619372229379	F	F	F
0.6630854692850079	0.1666666667000030	0.3607350091654666	F	F	F
0.6630854692850079	0.5000000000000000	0.3607350091654666	F	F	F
0.6630854692850079	0.8333333332999970	0.3607350091654666	F	F	F
0.9944057463905267	0.0000000000000000	0.3915351276171819	F	F	F
0.9944057463905267	0.3333333332999970	0.3915351276171819	F	F	F
0.9944057463905267	0.6666666666000012	0.3915351276171819	F	F	F
0.3330656692422309	0.1666666667000030	0.4179888222780335	F	F	F
0.3330656692422309	0.5000000000000000	0.4179888222780335	F	F	F
0.3330656692422309	0.8333333332999970	0.4179888222780335	F	F	F
0.6656564241704075	0.0000000000000000	0.4448469552356400	F	F	F
0.6656564241704075	0.3333333332999970	0.4448469552356400	F	F	F
0.6656564241704075	0.6666666666000012	0.4448469552356400	F	F	F
0.0003515212697778	0.1666666667000030	0.4732099031121066	F	F	F
0.0003515212697778	0.5000000000000000	0.4732099031121066	F	F	F
0.0003515212697778	0.8333333332999970	0.4732099031121066	F	F	F
0.3333333329999988	0.0000000000000000	0.5000000000000000	F	F	F
0.3333333329999988	0.3333333332999970	0.5000000000000000	F	F	F
0.3333333329999988	0.6666666666000012	0.5000000000000000	F	F	F
0.6663151448302216	0.1666666667000030	0.5267900968878934	F	F	F
0.6663151448302216	0.5000000000000000	0.5267900968878934	F	F	F
0.6663151448302216	0.8333333332999970	0.5267900968878934	F	F	F
-0.0015230802359130	-0.0004914901244897	0.5549266109932827	T	T	T
-0.0026417191441967	0.3333333332999970	0.5548636571940226	T	T	T
-0.0015230802359130	0.6671581567244907	0.5549266109932827	T	T	T
0.3306730065129213	0.1680841205714876	0.5823356924319611	T	T	T
0.3306730065129213	0.4985825461285153	0.5823356924319611	T	T	T
0.3304088993121366	0.8333333332999970	0.5813515560670947	T	T	T
0.6668489842393905	0.0030041376600401	0.6089056341059170	T	T	T
0.6659385525155256	0.3333333332999970	0.6094501338287679	T	T	T

0.6668489842393905 0.6636625289399614 0.6089056341059170 T T T
-0.0041999694858068 0.1666272351946358 0.6384333806655142 T T T
-0.0041999694858068 0.5000394315053670 0.6384333806655142 T T T
-0.0046023868037221 0.8333333332999970 0.6389589281680330 T T T
0.3224331716173907 -0.0016594445054153 0.6633486336707259 T T T
0.3208180583174229 0.3333333332999970 0.6653004289890013 T T T
0.3224331716173907 0.6683261111054162 0.6633486336707259 T T T
0.6587407051026931 0.1536398295460475 0.6907904023276608 T T T
0.6587407051026931 0.5130268371539553 0.6907904023276608 T T T
0.6513805047723074 0.8333333332999970 0.6874485017442403 T T T
0.5647650980855666 0.3333333333333357 0.7380990878846805 T T T
0.5352227160614142 0.3333333333333357 0.7743129180591767 T T T

OH/Cu(211) $E_{ads} = -3.08$ eV
1.00000000000000
6.2527034153000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.3164343000000009
Cu O H
45 1 1
Selective dynamics
Direct
0.0061862950247047 0.1666666667000030 0.3120745335338029 F F F
0.0061862950247047 0.5000000000000000 0.3120745335338029 F F F
0.0061862950247047 0.8333333332999970 0.3120745335338029 F F F
0.3355456677560653 0.0000000000000000 0.3354619372229379 F F F
0.3355456677560653 0.3333333332999970 0.3354619372229379 F F F
0.3355456677560653 0.6666666666000012 0.3354619372229379 F F F
0.6630854692850079 0.1666666667000030 0.3607350091654666 F F F
0.6630854692850079 0.5000000000000000 0.3607350091654666 F F F
0.6630854692850079 0.8333333332999970 0.3607350091654666 F F F
0.9944057463905267 0.0000000000000000 0.3915351276171819 F F F
0.9944057463905267 0.3333333332999970 0.3915351276171819 F F F
0.9944057463905267 0.6666666666000012 0.3915351276171819 F F F
0.3330656692422309 0.1666666667000030 0.4179888222780335 F F F
0.3330656692422309 0.5000000000000000 0.4179888222780335 F F F
0.3330656692422309 0.8333333332999970 0.4179888222780335 F F F
0.6656564241704075 0.0000000000000000 0.4448469552356400 F F F
0.6656564241704075 0.3333333332999970 0.4448469552356400 F F F
0.6656564241704075 0.6666666666000012 0.4448469552356400 F F F
0.0003515212697778 0.1666666667000030 0.4732099031121066 F F F
0.0003515212697778 0.5000000000000000 0.4732099031121066 F F F
0.0003515212697778 0.8333333332999970 0.4732099031121066 F F F
0.3333333329999988 0.0000000000000000 0.5000000000000000 F F F
0.3333333329999988 0.3333333332999970 0.5000000000000000 F F F
0.3333333329999988 0.6666666666000012 0.5000000000000000 F F F
0.6663151448302216 0.1666666667000030 0.5267900968878934 F F F
0.6663151448302216 0.5000000000000000 0.5267900968878934 F F F
0.6663151448302216 0.8333333332999970 0.5267900968878934 F F F
0.9989603101104587 0.0000000000000000 0.5550203703588971 T T T
0.9990793016611869 0.3327588454759479 0.5550331208916067 T T T
0.9990793016611869 0.6672411544240502 0.5550331208916067 T T T
0.3331175674196165 0.1667112807310795 0.5817390581471077 T T T
0.3328032622402123 0.5000000000000000 0.5818015557025052 T T T
0.3331175674196165 0.8332887192689206 0.5817390581471077 T T T
0.6700548802511747 0.0000000000000000 0.6094771508761940 T T T
0.6694179097271682 0.3356853718638170 0.6094481890238369 T T T

0.6694179097271682	0.6643146280361811	0.6094481890238369	T	T	T
0.0010742217695450	0.1663850686302582	0.6387413774751654	T	T	T
0.0012437429233180	0.5000000000000000	0.6381797533273280	T	T	T
0.0010742217695450	0.8336149313697417	0.6387413774751654	T	T	T
0.3294256492533824	0.0000000000000000	0.6641992523242439	T	T	T
0.3290119580924864	0.3336418277188978	0.6636210492766120	T	T	T
0.3290119580924864	0.6663581721811004	0.6636210492766120	T	T	T
0.6580781390762555	0.1657739281778654	0.6894629209854866	T	T	T
0.6607987113645107	0.5000000000000000	0.6918432752621673	T	T	T
0.6580781390762555	0.8342260718221348	0.6894629209854866	T	T	T
0.7156062361987258	0.5000000000000000	0.7601231334486140	T	T	T
0.5861575505044737	0.5000000000000000	0.7806902922340574	T	T	T

OH/Cu_{13} E_{ads} = −4.13 eV

1.00000000000000

30.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	30.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.0000000000000000

Cu O H

13 1 1

Direct

0.5705989273381248	0.4705282768550885	0.4715855747414887
0.5328048440176064	0.4366825461904391	0.5370267445597295
0.4387659434984427	0.4474807576765399	0.5184601313050118
0.4992998464402892	0.4988921393901645	0.4967383982782480
0.4787841128520886	0.4878452069687509	0.5742643980541584
0.5551071224751979	0.5120256045685103	0.5528560975471251
0.5064203823436872	0.4249768297497862	0.4613230079243963
0.5562300840161067	0.5519188399646424	0.4776869058543584
0.4949820009145779	0.5693747933848066	0.5346083327017036
0.5199586353581830	0.5113538638632569	0.4189493091438399
0.4667536295086003	0.5614851232314585	0.4571408597381773
0.4443407817848193	0.4880099330182798	0.4365478884361563
0.4276043756240507	0.5276546069904774	0.5230346565726945
0.4391061686586733	0.4233061007899956	0.4551546591585334
0.4206216104089307	0.4001021778864847	0.4418983682595152

OH/Cu_{13} E_{ads} = −3.44 eV

1.00000000000000

30.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	30.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.0000000000000000

Cu O H

13 1 1

Direct

0.5718292080022648	0.4717928307231531	0.4781025163292689
0.5279015292371982	0.4379178297771674	0.5414383793677817
0.4461563916638745	0.4451732404000646	0.5247217076084092
0.4991268649285368	0.4995752030549600	0.4988878698180378
0.4830314035301669	0.4990131581749334	0.5775145418464337
0.5597607201594518	0.5137626284437811	0.5491847769786026
0.5019461863725279	0.4278374781548752	0.4630516635547035
0.5538329101203006	0.5535945452370673	0.4751276113559023
0.4990703213090066	0.5703750272198658	0.5366619796282266
0.5166640630044030	0.4997960612384952	0.4214526009784311
0.4712511703526266	0.5608924071812526	0.4576970128456334

0.4381755222001253 0.4833041107453664 0.4481706840476441
0.4279006516802872 0.5276229283519895 0.5217207210205407
0.3908592641694335 0.4588888770701798 0.4201766888310767
0.3972055918425189 0.4287571414221859 0.4100332447311200

OH/Cu_{55} $E_{ads} = -3.59$ eV
1.00000000000000
26.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 26.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.0000000000000000
Cu O H
55 1 1
Direct
0.5006689427853473 0.5000063880440102 0.5004365118734078
0.5010151560803815 0.5000056779139532 0.5933991908214428
0.4974818402705319 0.5000040999947055 0.6857391567700603
0.5712334564750651 0.4464461957334229 0.6373514742701198
0.5677946671495903 0.4514536429927343 0.5421179857542026
0.5677936284232192 0.5485591887838457 0.5421225916866065
0.4750387170697680 0.5785356532617764 0.5417909472342572
0.4174950105941268 0.5000016352597570 0.5418011405414170
0.4750435777242893 0.4214724794347082 0.5417853081721065
0.5261173907276002 0.4213624134231609 0.4588150583767375
0.5834418847066708 0.5000101547555986 0.4585689944785233
0.5261116321188259 0.5786538866814057 0.4588203980652598
0.4331755856741434 0.5484855200318645 0.4592868975263861
0.4331769450541575 0.4515228772764116 0.4592833493002160
0.5005983212843174 0.5000089889462858 0.4077502613694931
0.6344647297593502 0.4032552458314960 0.5797608519177599
0.6344597268905477 0.5967566184940157 0.5797666849033719
0.4504399953172767 0.6557039517805838 0.5823163201656718
0.3369643341946116 0.4999982892273383 0.5828512087784412
0.4504475113586064 0.3443023838298101 0.5823071924542076
0.5503210459740240 0.3443723526022213 0.4176239166733096
0.6642212997414455 0.5000148896557066 0.4168856666275919
0.5503110882700689 0.6556491517533684 0.4176336026745567
0.3677351373817980 0.5959654030577314 0.4186807101427554
0.3677418186678866 0.4040450894719635 0.4186736396488876
0.5006062651435331 0.5000106620536275 0.3170525418338292
0.5712236350131291 0.5535648922406641 0.6373594864860372
0.4729909965429861 0.5795277286486671 0.6366502965167344
0.4168265791945512 0.5000005513972116 0.6379054965628503
0.4729968021769312 0.4204754842912387 0.6366448702516111
0.6401412859176022 0.5000074625869473 0.5799603242466063
0.5431531671251081 0.3706911685152841 0.5841632381685159
0.5953089491705981 0.3703781425368891 0.4989343225114879
0.6532546971189959 0.4492614449327081 0.4979076478489444
0.5431461131301443 0.6293187287059959 0.5841705161834754
0.6532520868119143 0.5507594425340687 0.4979147343767547
0.5953031900403559 0.6296356470648962 0.4989465633697174
0.3902150980011516 0.5798262405997314 0.5853085300380539
0.5005742459057370 0.6606123199159976 0.5002017576871197
0.4057514676711777 0.6290106441072091 0.5008170392783805
0.3902189308124742 0.4201751702329425 0.5853033087579415
0.3470261130829441 0.5497684241683236 0.5008675652992267
0.3470289274209922 0.4502362971795485 0.5008639837992145
0.4057601957371256 0.3709973118140936 0.5008094901510556

0.5005821699686994 0.3394005009707327 0.5001917470560148
0.6104653898063298 0.4199301454229953 0.4143902538307100
0.4580429239553825 0.3700992685964565 0.4163359180890093
0.5273578373108840 0.4202280328084456 0.3633670105721824
0.6104625014347120 0.5800958316133249 0.4143962361609434
0.5847832937420919 0.5000158464385620 0.3626741482681674
0.4580357995106498 0.6299163987210004 0.4163467317925582
0.5273510882976800 0.5797955609819168 0.3633726370951265
0.3626368434171113 0.5000046414181832 0.4170793647972905
0.4323323617249925 0.5502104439291841 0.3645503380642647
0.4323352985318394 0.4498048353735080 0.3645460651462965
0.5760385964935902 0.4999994627814683 0.6943217134567259
0.6015816084156398 0.5000047491987587 0.7217070918218976

OH/Cu_{55} $E_{ads} = -3.54$ eV
1.00000000000000
26.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 26.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.0000000000000000
Cu O H
55 1 1
Direct
0.4995638082546842 0.4996919859204191 0.5014559862390151
0.4989737940200674 0.4992280971269045 0.5945326184142662
0.4988311738821497 0.4995530820886815 0.6864232916218376
0.5701602108499886 0.4466237660626708 0.6404218515017996
0.5656787093767348 0.4510425206036676 0.5448794827611281
0.5662785092152381 0.5483319493335683 0.5430543394128314
0.4739466070287823 0.5785459082429897 0.5423718842782541
0.4162383455456937 0.4998048325261250 0.5417107501237655
0.4731252844321268 0.4209737320759416 0.5421315565280830
0.5252018803143536 0.4210401393254307 0.4601472463955601
0.5826707405059767 0.4995244947381862 0.4607927366892007
0.5256758759070488 0.5785963810270648 0.4601812072747095
0.4330470623067433 0.5485481189615571 0.4593744331621655
0.4325525254456394 0.4513405480735393 0.4591720172148323
0.5004823479820069 0.4997874975058560 0.4087948855030004
0.6316455138377196 0.4025046197251448 0.5826785845795596
0.6317045597059093 0.5962718015340348 0.5837097177641276
0.4488389972774625 0.6554581176433341 0.5829585160111396
0.3352112667805550 0.5000146412645757 0.5818896654854497
0.4469838034997347 0.3435540024763725 0.5816885217947543
0.5498639586200199 0.3438799528114116 0.4192941847680376
0.6640100668724006 0.4997849110784746 0.4206280072233749
0.5511361485204010 0.6556018435170495 0.4196122917909615
0.3682520348463911 0.5962888794173852 0.4178461276353110
0.3672927674663536 0.4040810832185020 0.4175636796957015
0.5017500214227318 0.4996450780709745 0.3180018339268255
0.5655069191962190 0.5524843323720739 0.6367890516142760
0.4718789668029726 0.5789251093484096 0.6381960314997195
0.4150230987772811 0.5006755382155744 0.6378988076052414
0.4681534889843774 0.4193252279473896 0.6358422075436012
0.6354246074967989 0.4997002143611388 0.5863104574357750
0.5400717638516427 0.3694489157795434 0.5850480423682995
0.5933739959250948 0.3700688425528841 0.5014438360715656
0.6516430727732169 0.4497653291653685 0.5021777480983277
0.5411368520430402 0.6306143230862100 0.5851851872409068

0.6523152881204807 0.5501956730244290 0.5015971277225023
0.5941597112848480 0.6297553495307142 0.5017771506191475
0.3890627470964700 0.5797464265079952 0.5852195116604160
0.5002883965702472 0.6609883219870848 0.5015275109445841
0.4059360514233979 0.6297570593806572 0.5001596631166205
0.3868457243626180 0.4195948454589479 0.5835407231858739
0.3468595285668521 0.5492325277905546 0.4994846948435860
0.3459803866936974 0.4502901019378336 0.4998318916530903
0.4043508394030244 0.3703196158169859 0.4996928901851851
0.497755133532095 7 0.3388326431285888 0.4998517918434704
0.6099302036201252 0.4197072221556700 0.4167377653680397
0.4575302760259087 0.3698646768909623 0.4161185396618391
0.5264682190258585 0.4194371261819687 0.3646872309657730
0.6111206409020596 0.5799919162457934 0.4178262035592263
0.5852846548257098 0.4997922923329349 0.3653481420597415
0.4584945033163288 0.6300878937215223 0.4167467708468384
0.5281558219555611 0.5797296837129062 0.3650644817420782
0.3633359357940599 0.5002201778526705 0.4155683933988085
0.4326824903314745 0.5496675199668279 0.3646914474579844
0.4329730605866625 0.4495479723457090 0.3640540713547178
0.5548788429586646 0.4572538658859526 0.7139375752710656
0.5820203582996214 0.4762065966684051 0.7314281772110317

OH/Cu_{55} $E_{ads} = -3.46$ eV
1.00000000000000
26.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 26.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.0000000000000000
Cu O H
55 1 1
Direct
0.5007078966833052 0.4994691665427106 0.4998457114891310
0.5001277619765634 0.4998684395359109 0.5924378944623104
0.4994331241320066 0.5003653503970820 0.6830535101607005
0.5679182684886022 0.4506541398542516 0.6366698923066626
0.5681734752467854 0.4504685369927476 0.5408630168396780
0.5673423942347622 0.5482713923620393 0.5412867249703039
0.4747847109871479 0.5784104619166145 0.5412930385416971
0.4175879737492777 0.4997256840952780 0.5412686881936830
0.4748732044475903 0.4210367431410896 0.5412400294303660
0.5270545812759387 0.4205422769363534 0.4584852654996663
0.5839368407702819 0.4988433580083163 0.4585137344529178
0.5257838221669937 0.5784976947337851 0.4586224778126470
0.4334430414779404 0.5483850470694361 0.4585144020776514
0.4332947455891713 0.4512570219976738 0.4585727631574174
0.5005034854051972 0.4996554013612738 0.4074435381473997
0.6318887823535544 0.4040516996503470 0.5854204275520969
0.6327427669254608 0.5963256864871714 0.5820710974972730
0.4497718168747290 0.6554853740159066 0.5818480756394492
0.3364955581558674 0.4997054021832163 0.5817862880786395
0.4493857104618530 0.3439793984852986 0.5820098236327780
0.5477043464734254 0.3428228410608849 0.4168126752617477
0.6642407683907406 0.5031569705682911 0.4168461113420756
0.5500747458797651 0.6559677410160829 0.4183170413408721
0.3679275210296828 0.5960638903587553 0.4179348503186208
0.3671974467119867 0.4041427558115500 0.4182160748416284
0.5002200303664820 0.4999029623421011 0.3166450974849076

0.5683322019548745 0.5494137706065078 0.6365800741549910
0.4746480890425700 0.5805433310181408 0.6368769965080883
0.4155483927756084 0.4991906064690270 0.6368448286813534
0.4739808102163750 0.4197008011408866 0.6365605737296176
0.6364693511060814 0.5001392357430681 0.5850100252099049
0.5419219818419513 0.3701731955335137 0.5850104580827392
0.5930425177933419 0.3647743080693582 0.5026428777332239
0.6573533164939869 0.4531594399756410 0.5026237606489419
0.5421752055990366 0.6296061378434901 0.5841966552797857
0.6527083918284058 0.5501455202084358 0.4999329011236837
0.5944807631186699 0.6297669525105473 0.4999556744403910
0.3903893958788188 0.5795938741624191 0.5850286585443445
0.5007868753611551 0.6607512804689417 0.5003159333464691
0.4068331478641689 0.6300310412041120 0.4993660677464528
0.3897395736068278 0.4198238720273944 0.5841315316688475
0.3475723310578257 0.5484689328074038 0.4993304229398145
0.3473419634051138 0.4496150413711685 0.5002293649993061
0.4057571984828113 0.3700695437944027 0.4998790573745001
0.4993967850930869 0.3392676817817497 0.4998693182688987
0.6109408475895773 0.4193765908928585 0.4097252641680323
0.4575604060725034 0.3703425620959838 0.4157286890587967
0.5256327874967381 0.4195317460375418 0.3631958443205176
0.6102158389048001 0.5804841817334311 0.4158089962655233
0.5844433380764067 0.5005246570549076 0.3632255390863650
0.4580776552806160 0.6297138297497443 0.4148012443625871
0.5263313389316036 0.5801903611523673 0.3634722822180529
0.3636833806102997 0.4998614239639003 0.4147758890176754
0.4319753581010190 0.5494211598098823 0.3636431766469027
0.4318851061568613 0.4502921981976594 0.3634316602094577
0.6586728093424428 0.3845876294169166 0.4628079053778847
0.6884082107908490 0.3629508156044001 0.4560810914212805

OH/Cu_{55} E_{ads} = −3.06 eV
1.00000000000000
26.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 26.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.0000000000000000
Cu O H
55 1 1
Direct
0.5001028524008427 0.5002607758827861 0.5006699406953273
0.5003044253230454 0.5007646867973833 0.5945567345196786
0.5003597781628051 0.5008999979032330 0.6887511764301650
0.5679607280602710 0.4516711423071873 0.6369359536385572
0.5670229685787572 0.4518141367268109 0.5419622206735308
0.5671317406468170 0.5490030267939882 0.5413591671747521
0.4745452526707413 0.5790682552068953 0.5414158200481114
0.4174978482175413 0.5004234368292567 0.5419910999781792
0.4745896446140425 0.4218467561144499 0.5421352441933768
0.5256562350654537 0.4213690386101301 0.4593841523586426
0.5828695068823364 0.5000243448872219 0.4589512424906669
0.5256468959562868 0.5788368125947936 0.4587765194304445
0.4329902180950350 0.5487543612894658 0.4589925195094176
0.4330080810286439 0.4514588273841408 0.4593974204265660
0.4999711124123775 0.4999314723475528 0.4080161935428954
0.6324298720446991 0.4043401215469694 0.5827648947649193
0.6326944342594885 0.5967692152335236 0.5817878237872584

0.4496330794338651 0.6562220848664437 0.5818591041123983
0.3366778577302891 0.5005358038190901 0.5828311390494245
0.4496492948936606 0.3450480376086944 0.5831983719530948
0.5505263893772290 0.3441569064173900 0.4188505913340614
0.6638382986490867 0.4998942469223839 0.4180167625298584
0.5506127348993118 0.6557109764246691 0.4176628260860546
0.3674453862612149 0.5962621122070464 0.4180793461572007
0.3674721634392496 0.4036169265159477 0.4188813249216368
0.4998507471681440 0.4996058980541194 0.3173394032909686
0.5683268888113794 0.5500578754743963 0.6360994851750331
0.4742756042467646 0.5805679303962562 0.6361931299393975
0.4167165756212179 0.5008515708997255 0.6369588395690083
0.4744061016224426 0.4211555052888042 0.6370382635508801
0.6369734615971845 0.5005180424470769 0.5842925111245603
0.5423726290162492 0.3706210253452305 0.5851003289660136
0.5945925837270172 0.3703385018023260 0.5007575683804373
0.6527671801759926 0.4504460213033278 0.5003687267194757
0.5424425072069980 0.6304905813470387 0.5839895697890731
0.6528962385892396 0.5497779715485364 0.4999927586967851
0.5946364212156231 0.6301607356008718 0.4997392808396821
0.3895963551008226 0.5809423353826987 0.5843483680082910
0.4999914502148706 0.6608447620531906 0.4997622766668768
0.4056090888952523 0.6302237462639552 0.5000506135195196
0.3896921850208582 0.4202838355580775 0.5851527852413247
0.3473185597923480 0.5497039465543344 0.5004243015843587
0.3472989601720131 0.4507672218021471 0.5008036421630507
0.4056789885489941 0.3703366094272033 0.5010981024391691
0.5000567152650734 0.3397199585888962 0.5010779211364527
0.6105561230506845 0.4195386642865676 0.4162917391273274
0.4577513439063514 0.3700253624018554 0.4166644054766503
0.5259886952026235 0.4195298717046708 0.3642242150127106
0.6105462910493586 0.5802339067654427 0.4156900239521246
0.5842900234662383 0.4997272377935053 0.3638362451723167
0.4577560171094754 0.6299185733203233 0.4157361747309737
0.5260154238200377 0.5800045215353170 0.3636161288998332
0.3632220902555043 0.4999321956665120 0.4163313478326178
0.4316037145013649 0.5493350484086365 0.3638751892204958
0.4316280955052518 0.4502417024137786 0.3642649867008830
0.5033403388961833 0.5076102071457542 0.7581205531222243
0.4912843639066494 0.4780422600157049 0.7775524280181781

OH/Cu_{147} $E_{ads} = -3.63$ eV
1.00000000000000
31.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 31.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 31.0000000000000000
Cu O H
147 1 1
Direct
0.4159684964902578 0.3861806328057076 0.4369959848715365
0.6035479886307158 0.4658484277902071 0.4229774448000228
0.4176386271269070 0.5360454177022347 0.3739666687199352
0.4247192253689026 0.5864014374266360 0.7021440165689068
0.3960249094145179 0.6621775888386127 0.4317538388996361
0.5886175674322733 0.3266794347478223 0.4352515215118225
0.6298842313649754 0.4367770126028732 0.3546255422853735
0.5312413162513148 0.4289709627465489 0.5021878920587594

0.7304829152792757	0.4856220232390885	0.4733974237944988
0.6278039017041049	0.5965053700298477	0.6281266322070131
0.6622977378923063	0.4583934481691451	0.6187078101835460
0.5929832370279413	0.2868513403233479	0.5058793819413856
0.6196556607828618	0.4766020822807803	0.5550382621005777
0.4251248910271655	0.3915131908200468	0.5180297449397894
0.4889735261844162	0.3704211394911242	0.4704171351143042
0.4092808706818313	0.4290794927270715	0.6679342432223809
0.4695771323441770	0.5706685205442630	0.4982623200126225
0.6978708445675255	0.4716740831735801	0.5465194561837171
0.3436532509324860	0.3939108265052796	0.5278053443097148
0.4159278066714112	0.4606145320809538	0.4046142098434514
0.5093894994411692	0.4601179445945812	0.2994237013624608
0.3921872612743802	0.3406539848405683	0.5685032518216465
0.3710100753945822	0.5632110368060248	0.6457504214008917
0.3727446178703751	0.4033304632555392	0.3722195067886035
0.3808855563120012	0.5231655588746411	0.4455712616622889
0.6987371560080192	0.5482296888561455	0.5140627182652077
0.6441301323034658	0.5963953508788081	0.3917610176730984
0.4583892169351290	0.4431247359978671	0.4689129655041603
0.4406803604777268	0.3554705169437667	0.3676973795202536
0.6107775942602856	0.5455227921944206	0.4415875240599997
0.4831944277905024	0.4131384703018412	0.4001860489437685
0.5340194741419650	0.6738793939627326	0.3987544861098479
0.4550061049408718	0.3152542103605678	0.5201771020668946
0.4788152943667429	0.3777933812623704	0.6687520749779290
0.6546666456302621	0.4025089183392452	0.5582916580767198
0.4165686711918263	0.5071040684021251	0.6867738148984324
0.6380260855598402	0.3916038233083179	0.4231217847584520
0.3123501461138331	0.4581417726212747	0.5688801913201935
0.6086653825017064	0.6595255269823531	0.4329764721822324
0.5599341214787358	0.6445118514935696	0.6325370330398341
0.6155223955160358	0.3908051456181739	0.6298591221431787
0.5083470006942620	0.3835202732048503	0.3316206802236656
0.6888686253399353	0.5414796488856500	0.4318610205856665
0.5912258012996312	0.5717962483559521	0.3320483142168135
0.5233015613864613	0.6197065357260885	0.3364219937940692
0.5768755684681047	0.4948830848738645	0.4915009486831016
0.3973114337347253	0.5339315028266770	0.5775663207746196
0.3901702524632690	0.4539774374173767	0.5589802880315455
0.4386686794567417	0.6421530351612624	0.4962741508610536
0.5301550607279173	0.3046219460366399	0.5539512194904730
0.4500542335475746	0.5578859969641968	0.6351113552603982
0.6640566176209003	0.6101215935354446	0.5544952611541374
0.4400307697855882	0.4299363298169772	0.3324281855929582
0.3461693212135785	0.5973820902408273	0.4420349328934163
0.5830151863332581	0.3691713117071111	0.3657437577579855
0.6049290916994406	0.3376043238154426	0.5684520426786185
0.4083151172909192	0.7129621162302530	0.4940685103316771
0.3915211089759279	0.5767221550424585	0.5072741180986654
0.5756525916451698	0.6081274241412120	0.4825318855582396
0.5847253166619103	0.6136236355894306	0.5632979392835247
0.4368354206123832	0.3991316545383115	0.5993514947330491
0.4437226137550880	0.6009625655719264	0.5663599375337207
0.4464510685048356	0.3123754384316683	0.4384712158026061
0.3820974055285493	0.3335843372543587	0.4872015100682704
0.3384959422287868	0.5415557422776963	0.3817601864436306
0.5198090564560376	0.2980296473816014	0.4718444012191894

0.5645581777257420	0.5999770268253556	0.4020275094751355
0.3737784119142184	0.4785179738053688	0.3405127637292965
0.3366116423202669	0.3897683355983351	0.4458661050458838
0.3596113834848657	0.6487466367719535	0.5052980269412491
0.3739856661263796	0.3294395224339152	0.4062763670007956
0.6571722799354721	0.6059544949807031	0.4724973216327245
0.5846391254754938	0.5389569622525882	0.5958131212073985
0.6266713265354418	0.6704094639423914	0.5941806655472202
0.4425942723928828	0.5071895391467275	0.3038031308642098
0.4178079256607332	0.6308103543805478	0.6345205249488642
0.5830111365019907	0.4636102961549947	0.6265201076644340
0.5118662524153677	0.6292352278434468	0.5298976692379537
0.4497268804873813	0.5879631373536591	0.3220208065952606
0.6187291188530827	0.6663689114011649	0.5135001144247640
0.6540974174457714	0.4900037887252861	0.4824458226764444
0.4672023432076065	0.3254057202573229	0.5997981832557776
0.3019969223775412	0.4517200285046236	0.4864983965232045
0.5583767601218486	0.4928090780877168	0.6966375941904780
0.6206693384800287	0.5524991755053756	0.5229387243526920
0.4591249860690331	0.5178184978752498	0.4373478228829132
0.3628942190049545	0.6083432039525846	0.5771731761954247
0.5423682779799367	0.5563706488617524	0.5317337114931151
0.5089099814811390	0.4293148054507997	0.6152741674264841
0.4753426495232804	0.5286634753139059	0.5674750140441909
0.4273833234507199	0.5900179920647520	0.4344021295014370
0.5733540729936621	0.4096725664820987	0.5660615597425646
0.3574950211925191	0.4025095796175966	0.6087177092939455
0.3467232802490932	0.5098469030961549	0.5180853574435045
0.3768047284379055	0.5542693019051136	0.3111397886880444
0.2704397315133921	0.5141666162321092	0.5275263621850527
0.5584257282693545	0.5212539721826783	0.3823187526725683
0.5004194341550390	0.4998453404428802	0.5002299547016202
0.5417159512551697	0.3554813842370828	0.6184107327362404
0.4238876519440375	0.5047048115039817	0.5092311530469925
0.5324108007839493	0.5496939802008978	0.4514288496311867
0.4924502547335798	0.6164292165456666	0.6686715157830340
0.5016333121802896	0.6225335477211139	0.4485268627779476
0.5508481720124395	0.4420250314535935	0.3652838864093062
0.4993441965512464	0.3771788381917805	0.5517037513840837
0.5171178745595304	0.5408012827944019	0.3141042563684084
0.6396100226845984	0.5170791873779513	0.3701242619655280
0.3193774387301726	0.5390801097113793	0.5872285244705188
0.5147945664733766	0.3376759423157540	0.3997436791301131
0.6269014037422161	0.5213908967022158	0.6599002438221994
0.5623740963919830	0.3576106354774304	0.5038948335325762
0.5761364144233584	0.4136802671975502	0.2981869702346792
0.3612353215378488	0.4826143049022956	0.6301386102621979
0.6815290663390782	0.4608276598215438	0.4134078256922598
0.3856133445067479	0.6090718694913690	0.3704114128650550
0.4811886695258821	0.7017775523882427	0.5281400022479835
0.3028035792101958	0.5282774486663255	0.4540896441799888
0.6093762261870486	0.4230352291603739	0.4931257199797744
0.6413714117081711	0.3511532511022429	0.4949458022989713
0.3135320307438383	0.5823293051846821	0.5164180590921563
0.3343908413125992	0.4648398573070938	0.4117354611183636
0.5844223995547171	0.4928761396017459	0.3134907987455413
0.5571465325406646	0.3988038890283165	0.4339959708947121
0.5606549032816224	0.5700376841267210	0.6678688839512301

0.6242992782110465 0.4457821213854052 0.6892447944452378
0.5515358348941745 0.4119506246746135 0.6783655071083011
0.4591032777576180 0.6442769101039951 0.3817208889015222
0.4425432840236173 0.4784785348155737 0.6180550012503374
0.5543198477209549 0.6874046632452560 0.5615852875552297
0.4910354639744363 0.5688637904234706 0.3866329063664442
0.3800860483521675 0.4472081162932863 0.4776306220985344
0.4860358367437951 0.6622190298996118 0.6003562155559795
0.5410703378300229 0.4812427343582716 0.5635807702992094
0.6661864594751155 0.5351034997309165 0.5887145610272193
0.4840089786539549 0.4888764679114122 0.3682376429661635
0.5175437432607195 0.5866677829685371 0.6002084635671294
0.4034567167949529 0.3489687059376594 0.6483064559215934
0.4914711348090221 0.5398387851562600 0.7009644641675234
0.6874298911018485 0.4175496278239927 0.4840721485993801
0.4837871230976685 0.4591146466983496 0.6863137577353202
0.5456176288654482 0.6844717950463072 0.4796854977581730
0.5966861811264796 0.6496760982335856 0.3534459896569329
0.4685094850502425 0.4498479005648283 0.5492043949093312
0.4123105341207352 0.6731383549962977 0.5648362021690025
0.4710119646479615 0.6951497631926808 0.4458579850321884
0.5167352630924630 0.5107279627542647 0.6322362217558098
0.5254408327937197 0.4709809525062378 0.4330331197907069
0.4395509040690436 0.3359047495823895 0.6978897722148223
0.4286538505236421 0.3453567552818519 0.7257843593708946

OH/Cu_{147} E_{ads} = −3.63 eV
1.00000000000000
31.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 31.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 31.0000000000000000
Cu O H
147 1 1
Direct
0.4155709113248346 0.3869842557006243 0.4363412309537046
0.6034291316369419 0.4656294809208956 0.4230955261649578
0.4181694713946028 0.5367517462234205 0.3734745599995770
0.4238753521118167 0.5870014980932902 0.7017085706085657
0.3967264452125232 0.6628034461119632 0.4313739964903887
0.5876528138284657 0.3265311912334961 0.4353598110363623
0.6298919602543585 0.4366166436725381 0.3547889857296008
0.5304626959523900 0.4291047183549189 0.5021037408721910
0.7301598975158167 0.4845243617712922 0.4739521205349297
0.6274220597395017 0.5959018021077837 0.6286211258995770
0.6612814596273539 0.4576284833616975 0.6189792720347246
0.5910946830534741 0.2867544465266124 0.5062095578779697
0.6190108587147329 0.4761273458421112 0.5552171893636481
0.4241316289741123 0.3920057770029620 0.5175795664713499
0.4881619104598078 0.3708152913082337 0.4701381175319482
0.4067786202787158 0.4291027303042921 0.6713962025601932
0.4695842518091803 0.5708695502980327 0.4981837178930681
0.6971762365455605 0.4707684377695137 0.5469054627012746
0.3427644749530749 0.3947408995191372 0.5267382877735008
0.4158921680937429 0.4613655231421396 0.4040835021025956
0.5098270469312332 0.4606099218873335 0.2991639896055130
0.3905714688310781 0.3405252326203304 0.5671896771790723
0.3702166631743136 0.5637927809163460 0.6451609586289216

0.3727365471047443	0.4042697790932794	0.3713373443971655
0.3809397411583497	0.5238914373195570	0.4449038241139047
0.6986051665916049	0.5473881594613885	0.5146188565322386
0.6446446845852666	0.5961571162333685	0.3922312274613258
0.4579338869701879	0.4436477561703698	0.4686100279356475
0.4404705609852781	0.3560959256811813	0.3671850031423293
0.6108777022387887	0.5453428761699843	0.4417769542936288
0.4830178841609601	0.4136209477850981	0.3998775033306817
0.5349707641393697	0.6741698262202622	0.3990385337091871
0.4538981103845332	0.3157337927484433	0.5197532675184120
0.4773655717949853	0.3789934545566365	0.6669731742708745
0.6535149884086885	0.4018152639789349	0.5585701277819962
0.4154952786514778	0.5079242082787202	0.6866714804303710
0.6374709656317775	0.3911755963285559	0.4232821533279983
0.3113930367973056	0.4592928647073840	0.5677707283907086
0.6093448105149849	0.6594039190890610	0.4334374905152691
0.5596559151506004	0.6441182780975625	0.6327493348787316
0.6139541704643596	0.3903387950650030	0.6300562233509729
0.5083049857648300	0.3839815544442668	0.3313701074795372
0.6890279959816132	0.5408793110473041	0.4324502093523959
0.5919917932457950	0.5719971296771270	0.3322516709608833
0.5243285580545329	0.6201041964790192	0.3364457729559256
0.5765376770939823	0.4947454391892350	0.4915425108064176
0.3966678463385033	0.5343692210849803	0.5771225008992052
0.3893262933395652	0.4547120487535902	0.5583184662655831
0.4389140555851839	0.6424586141556129	0.4960328804785257
0.5282457442164420	0.3049526603912111	0.5542745995606313
0.4492512494329571	0.5579636242448747	0.6348273518856561
0.6639379828905809	0.6093126425025226	0.5550786052410257
0.4402373251881000	0.4306024252973251	0.3319353924554934
0.3465475354238328	0.5981961635791573	0.4413323286740948
0.5825744452933158	0.3691788297755773	0.3657584818366117
0.6029032804996101	0.3372955367039211	0.5689130994290590
0.4088670405342409	0.7133392704228888	0.4938512843280010
0.3914273420165190	0.5773524426248177	0.5067484194242406
0.5758733649053767	0.6079650734947651	0.4826902395501892
0.5845694305850536	0.6131851906176076	0.5635944756089327
0.4347862512216149	0.3998659423554076	0.5990417619462152
0.4434542957068858	0.6010710853010004	0.5661156850842494
0.4456805531579806	0.3129333732498850	0.4379385427577657
0.3812250931249846	0.3343794511607260	0.4861800476681896
0.3389821625059499	0.5424706891999879	0.3809348241389322
0.5185421413278828	0.2982214883206608	0.4717356328799440
0.5652437149301549	0.6001024469561599	0.4021187211495753
0.3741831142875169	0.4794359611169259	0.3397367794662680
0.3360987671389759	0.3908243294415168	0.4448533525506329
0.3597966784266214	0.6493856624979941	0.5047368953142090
0.3734744794992627	0.3304698290055646	0.4055027166087963
0.6573868534901246	0.6054466616431171	0.4730446116668721
0.5841829576054791	0.5386563233007186	0.5960627863225941
0.6266575470954610	0.6696686260604262	0.5946400891653366
0.4432979058024967	0.5078798895685234	0.3033418019188477
0.4174178423544584	0.6311140219886051	0.6340976096256074
0.5820561460865348	0.4634249363661665	0.6265587354394462
0.5119308398377886	0.6292315510201489	0.5299797360259483
0.4506618243295015	0.5885838281181961	0.3218086236931038
0.6189964725551054	0.6659393473691239	0.5139687492058315
0.6537816930449523	0.4894848799421656	0.4826699714419443

0.4647433334830595	0.3260876189132922	0.6004413739065018
0.3014605478380722	0.4527515642249174	0.4853534813553467
0.5575195982590224	0.4929124344050326	0.6966817416335473
0.6204596020397007	0.5520006895001887	0.5232331992032893
0.4592435900621031	0.5182892833648136	0.4370394939488575
0.3625288610011876	0.6088625050050016	0.5765931120117699
0.5420284612205325	0.5562425119243981	0.5317966614135066
0.5078521142226784	0.4299717868510811	0.6146053220515553
0.4744609965802004	0.5283512476301195	0.5675465292162666
0.4278133362532747	0.5905647808631869	0.4340458688712543
0.5721653016195714	0.4094969772447802	0.5661863533686390
0.3556366795175681	0.4037118676154681	0.6072347876280783
0.3463078806367474	0.5106200740246045	0.5173194484167053
0.3776573037220045	0.5551393964863456	0.3105419014492289
0.2699449359625265	0.5154783413815875	0.5261120485902268
0.5587734303034851	0.5215156677885547	0.3822924050838269
0.5000225179125615	0.5000074922416929	0.5001466449085924
0.5395142043751109	0.3556332688158749	0.6188492171550098
0.4234655248506084	0.5052606142590288	0.5087547266214395
0.5325286281134778	0.5498671906940014	0.4514392866919655
0.4918297628020825	0.6165802054888804	0.6685086140783102
0.5020806650350271	0.6227650443588691	0.4485429167778716
0.5508661921823944	0.4423159949029908	0.3652113475389868
0.4978958001561268	0.3774326805184907	0.5515493990376718
0.5178685028197245	0.5412460864484199	0.3140074512697580
0.6399325211818838	0.5168704138060586	0.3704605343963186
0.3188567387121705	0.5394930490022893	0.5865326780635636
0.5141887795998716	0.3379160302935740	0.3995353101304291
0.6262192275265960	0.5208602936957546	0.6601820917949834
0.5611602576083496	0.3576529076024345	0.5039453494267706
0.5762952480726522	0.4139822588780697	0.2982087011581292
0.3607256504052131	0.4827926935618995	0.6300083740243843
0.6813770316221349	0.4601779556508012	0.4137264661363316
0.3863790213236039	0.6098824737080933	0.3698799233229554
0.4815520837116072	0.7018772590110062	0.5282193138823628
0.3028085566894686	0.5292239680142309	0.4530414701354218
0.6086437372431263	0.4227323916200678	0.4933044436500143
0.6401130276087907	0.3506628743235589	0.4953101478519445
0.3134510319308158	0.5831771098836148	0.5156160354552439
0.3343260850700654	0.4657749647824875	0.4107591246599457
0.5849547763167003	0.4930526687448256	0.3135174310440040
0.5566203498026413	0.3988753966243025	0.4339791955936760
0.5600950832272014	0.5699161189829345	0.6680178654728709
0.6230728373297741	0.4452695428825096	0.6894061126302046
0.5500965762703363	0.4121068229596894	0.6783338012254421
0.4599553442144363	0.6448103146796853	0.3816446493442414
0.4407594689537960	0.4776934181783477	0.6187960206659985
0.5544399259010621	0.6871473431697455	0.5619895989460120
0.4916360548411284	0.5692805579277710	0.3864870588547725
0.3795843232235396	0.4480784199085843	0.4768984134077679
0.4858927012431370	0.6622662727180432	0.6003324975817886
0.5405072827874804	0.4813552522341668	0.5634445744648472
0.6658088307603591	0.5343522596703357	0.5891432237562448
0.4843024999378792	0.4893566377132139	0.3679645988878903
0.5170168900419193	0.5864363304180159	0.6002478138613905
0.3999256093609646	0.3468570232817036	0.6447066729367834
0.4906555428299706	0.5404524609461492	0.7008768170616192
0.6866253244334567	0.4167579171409733	0.4844302555956447

0.4831615235823915 0.4602394012523874 0.6862162684180302
0.5461793054328997 0.6844495261663173 0.4800448643805080
0.5976860146920034 0.6499213486365032 0.3537806570323358
0.4674778946656130 0.4500856638550937 0.5491431254010232
0.4123301932113289 0.6734399558604911 0.5645584011953068
0.4717782323340139 0.6954778544199992 0.4459327359660730
0.5157810581905509 0.5107389918058247 0.6322191677978730
0.5253438194185474 0.4712556974448665 0.4329348379926761
0.4203746666945687 0.3705573726057469 0.7008289879736034
0.4164554342044617 0.3624100968412061 0.7309108785480967

OH/Cu_{147} E_{ads} = −3.61 eV
1.00000000000000
31.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 31.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 31.0000000000000000
Cu O H
147 1 1
Direct
0.4154316115974929 0.3867724359543505 0.4366649990977482
0.6035809878644345 0.4657809676709166 0.4232617011109072
0.4185477008938233 0.5367615012031590 0.3733643181492666
0.4233789127910037 0.5860062129462523 0.7013687562602917
0.3970857616159751 0.6627038903616861 0.4310403880259556
0.5877329891483822 0.3267206670434466 0.4350388382435803
0.6302298538001955 0.4367745334940443 0.3551135636063248
0.5303553643388862 0.4288122604843351 0.5022164612800658
0.7299271221712192 0.4845961622028731 0.4747648763866268
0.6269072535657021 0.5951336163091996 0.6289448215155480
0.6607716784064689 0.4572153532273148 0.6195017221670573
0.5912126481357258 0.2866141014813615 0.5054722275352005
0.6186521581160420 0.4757401491212230 0.5557993064441450
0.4243148458155265 0.3916674067378665 0.5178836507817821
0.4881208821663485 0.3704921601832041 0.4700436340052265
0.4072038349098211 0.4273795771189060 0.6676391428487567
0.4698298190631945 0.5706905535402150 0.4979249031432947
0.6967590907445859 0.4706470305845581 0.5475645301078547
0.3429926581654223 0.3944270635497367 0.5267695615288659
0.4160985755933865 0.4613174255077616 0.4038719843419490
0.5101444899273122 0.4607678097833912 0.2992179650865616
0.3905229256007520 0.3402296102231128 0.5667621032053769
0.3698719418510766 0.5633133176572578 0.6447050277190558
0.3728270588113194 0.4043868694543034 0.3710994384154417
0.3811699686257380 0.5237649726644860 0.4446266728853498
0.6984113318635544 0.5473401355245265 0.5154338520677572
0.6452648028252242 0.5966499325702466 0.3924699907335940
0.4581257767822202 0.4433759614930570 0.4684835881218491
0.4404517257744655 0.3563174095319696 0.3669921428467393
0.6110591445679479 0.5456323950769135 0.4418738321601459
0.4831375049179794 0.4136685625564054 0.3997769233250454
0.5356992391846622 0.6742704921031420 0.3989554279467916
0.4536621398158868 0.3151341351955224 0.5195683076567608
0.4739582228649324 0.3761303600921085 0.6663361236473625
0.6536910733659700 0.4016373255952720 0.5586828569404144
0.4144825907859489 0.5067114437956233 0.6859351066293664
0.6375483461586490 0.3913984683939782 0.4234302560802220
0.3113779087088720 0.4586885419815310 0.5671652440608262

0.6099296337083401	0.6596091596731478	0.4334877341388864
0.5594045232082906	0.6436036689829251	0.6328928749932534
0.6138593148304361	0.3896768984307301	0.6297947873062463
0.5084498714809258	0.3841797192849669	0.3312864428496622
0.6891082992070148	0.5411778556619294	0.4330270741761454
0.5928715943624920	0.5724249573752301	0.3325357643413706
0.5249987790094018	0.6204353968550003	0.3363994291952517
0.5765005735046789	0.4946028364535709	0.4915793642029613
0.3965767592118359	0.5338632734696677	0.5769069881035732
0.3894839480945672	0.4538287910873550	0.5585162678222301
0.4392907388883272	0.6422820930565181	0.4957260335850550
0.5279563057449964	0.3039082636358318	0.5532340386406200
0.4488896894233392	0.5573677472770286	0.6345731967143832
0.6638147412159882	0.6090529662251346	0.5556626576414644
0.4403744752802163	0.4307689194112195	0.3318101072754052
0.3467057756902318	0.5980500085688562	0.4409508771272536
0.5827357451274477	0.3693460255296469	0.3657651984871219
0.6039858644399584	0.3368172543308567	0.5679970499156602
0.4091331230107832	0.7130610907246261	0.4936722020198791
0.3916544010053052	0.5770732369511127	0.5064947759109643
0.5760725284718103	0.6080393813346495	0.4826179011517510
0.5845859628406888	0.6128426943859134	0.5636138996686487
0.4356049494509970	0.3986180465566140	0.5996433380585824
0.4435286722960609	0.6007780958019209	0.5658549046652068
0.4456036948150535	0.3127891670257310	0.4375317616937527
0.3811812568187161	0.3341341128253785	0.4859253673232961
0.3391004759443157	0.5424272582559356	0.3806050352699564
0.5185182110355440	0.2979983985248504	0.4710967853345373
0.5659468999263251	0.6005724561521179	0.4021468797074860
0.3742935965176134	0.4794667554128123	0.3395064343513639
0.3361944360616592	0.3907187421716119	0.4446142191034712
0.3600641454017675	0.6491575035253859	0.5043634183924451
0.3735552801722648	0.3305518897739335	0.4050780676495408
0.6576324314874620	0.6055684422065846	0.4734825013567584
0.5837941880810587	0.5378500853607067	0.5964055529849179
0.6263285315061153	0.6691629296145193	0.5951820038432066
0.4436004187944820	0.5078474302982080	0.3033543938193132
0.4172709270324771	0.6306891179093015	0.6338478138710542
0.5805151610698552	0.4613282299851565	0.6278894181238430
0.5120192398460663	0.6291091446766687	0.5299903434668807
0.4513387888585753	0.5885542055068191	0.3219531333256594
0.6190808602866434	0.6657719522086619	0.5142990197927244
0.6536342557744743	0.4897739458340953	0.4831705253978785
0.4645591168899607	0.3250613018785175	0.6006330830302192
0.3016957936028264	0.4524900729415193	0.4848345206333525
0.5564676260834993	0.4920139682946312	0.6967909091523580
0.6203395889420747	0.5519058781199622	0.5235358518806575
0.4594963437343627	0.5181703559205729	0.4370394769940769
0.3626141975215180	0.6085438500114356	0.5762083955914185
0.5419827161833728	0.5561590168395361	0.5317772772280032
0.5082542170207305	0.4290555099257750	0.6147916184922795
0.4746202706757184	0.5282718026314824	0.5672053691647113
0.4281669838036933	0.5904494016609679	0.4338463195753566
0.5721139502908643	0.4090430353346516	0.5660950182112915
0.3553256650612128	0.4030403785086923	0.6077801853439075
0.3465265410815261	0.5099272940907159	0.5171255347476457
0.3781774573498694	0.5551664364673844	0.3104434501120380
0.2702461845294545	0.5152416126218451	0.5255251715855324

0.5591639589540375	0.5218117861131811	0.3825161342010679
0.5000724322683505	0.4997233381455010	0.5002251424687550
0.5404235124509563	0.3543932278111647	0.6160318221216763
0.4236534620836646	0.5049697335498704	0.5087065163890084
0.5328510541261937	0.5499188969659444	0.4513683338465012
0.4914021054107602	0.6157909731051243	0.6684754187502329
0.5026210180168754	0.6227057264568286	0.4483590192771384
0.5511296091669748	0.4425541328131890	0.3653183598300591
0.4976138888119379	0.3767586613670308	0.5515926598759053
0.5183578743661210	0.5414614088798883	0.3142127614828947
0.6403559281608048	0.5172192643557076	0.3708101504925704
0.3185811570136741	0.5395667581278821	0.5858036168300143
0.5141663773373781	0.3379951275617127	0.3992949638920233
0.6254950261093696	0.5199039509797055	0.6605453870341039
0.5609625628649457	0.3573586410178735	0.5038531994469526
0.5765757507661656	0.4141091333068325	0.2984369120644078
0.3597439641808363	0.4827059308664853	0.6292562102728534
0.6815608027514791	0.4605136651079599	0.4141165092111403
0.3866396865963456	0.6097285160772672	0.3697842197512290
0.4817065194647853	0.7017379732363935	0.5282544697707088
0.3031004944348057	0.5290955548597771	0.4525382296354164
0.6085235397314069	0.4225769949526194	0.4935550500209371
0.6402083096375810	0.3506223078060175	0.4948834477688138
0.3136560105618582	0.5829317525722453	0.5149815321121318
0.3343253402454158	0.4657054283007732	0.4103059426719207
0.5852773793905393	0.4933309487252761	0.3139849987555997
0.5565937739690384	0.3989731931488295	0.4339743969217166
0.5595800552315449	0.5691178033350603	0.6682327975525922
0.6231235941645156	0.4449814411796607	0.6896021368922534
0.5509887393423394	0.4096832624809873	0.6814678149374265
0.4605250140727608	0.6446424289203440	0.3815813552160721
0.4410798320975929	0.4777403579306030	0.6176559132213265
0.5544375776989262	0.6870156810127066	0.5621181988938212
0.4921551699802187	0.5694457423188789	0.3864768011314618
0.3797569023417045	0.4478572888804686	0.4765657543364076
0.4858619991065377	0.6618263875164152	0.6003372633342855
0.5404763195314579	0.4810334297694339	0.5634993431706443
0.6652871375049531	0.5338794018716781	0.5897320077912913
0.4846817067894273	0.4895533721282000	0.3679789806965060
0.5169269927373320	0.5858896423185674	0.6003839620163798
0.4006520976172527	0.3487205553878585	0.6462697434625072
0.4899770754806705	0.5394488949717189	0.7007659817080032
0.6865655752159034	0.4169575232661911	0.4846790499278508
0.4813564099398591	0.4595415141206468	0.6851155208271663
0.5464835645422542	0.6844057751843490	0.4800381459391470
0.5984826639852654	0.6504978889072759	0.3534323943983434
0.4675476395243022	0.4494473912510333	0.5492681125050575
0.4124307838516853	0.6731163399264968	0.5643040583804044
0.4721512495035626	0.6952632996921797	0.4457734333074980
0.5153926883360683	0.5099235921789629	0.6321668743505475
0.5254900302787412	0.4713141669673505	0.4330245222571787
0.5154566622214625	0.3682158345565053	0.7134912659570791
0.5051905517001177	0.3792731947629660	0.7410377969051842

OH/Cu_{147} $E_{ads} = -3.54$ eV

1.00000000000000

31.0000000000000000	0.0000000000000000	0.0000000000000000

0.0000000000000000 31.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 31.0000000000000000
Cu O H
147 1 1
Direct
0.4150913540374904 0.3869530452692184 0.4364553719879319
0.6032318213526006 0.4656929683184961 0.4236979325174879
0.4184909001846151 0.5369889043307365 0.3731986232725658
0.4225846618944291 0.5862224719073416 0.7013226562464503
0.3970388426098982 0.6629690454102398 0.4308972122397539
0.5872116857321206 0.3266893223511827 0.4358492849525012
0.6300683915202289 0.4365118760371213 0.3556986316294949
0.5297085318688010 0.4289591514499507 0.5025408918017629
0.7295459423704468 0.4841491563634074 0.4752577908134708
0.6264631569537099 0.5953472431245452 0.6290802966557699
0.6604958923942283 0.4573818479038311 0.6197342975080909
0.5901818027724907 0.2868057239785392 0.5064943361125793
0.6180562410226731 0.4757533358919105 0.5562409074163840
0.4234839447727237 0.3918808928681617 0.5177849130383371
0.4875217170825984 0.3706015539980072 0.4702512650502824
0.4042843190706908 0.4275691959419719 0.6668030451397081
0.4695238328744745 0.5707171942512836 0.4979821470364939
0.6963318704898218 0.4704951677491414 0.5479661861736682
0.3419628700063375 0.3947830274808974 0.5259217371309007
0.4159636772662924 0.4615082012207280 0.4037268959888465
0.5102748934547198 0.4607979739612810 0.2993732695376062
0.3889998054775633 0.3403213718026395 0.5660184130225131
0.3691338216433262 0.5636079670957045 0.6444467384883095
0.3728736020365668 0.4045914757192035 0.3706735803149830
0.3809234423936019 0.5240066682379706 0.4443196994440469
0.6981116925702084 0.5471422154182392 0.5157015892567095
0.6450978595575929 0.5963823162611023 0.3927378121075144
0.4576237455875258 0.4434895111387485 0.4685920856412580
0.4404513380861223 0.3563990516185975 0.3668982087777786
0.6107754115480521 0.5454622012964396 0.4421889456115515
0.4829172329036113 0.4138117007537089 0.3999113035418775
0.5357329272532226 0.6742861046578611 0.3990287363744726
0.4527483478435871 0.3153987448145406 0.5197793145168070
0.4713577123646720 0.3752051750970000 0.6650933019665349
0.6527572646208925 0.4015885983959711 0.5595063970435906
0.4133896264094807 0.5069235789682039 0.6858343266199054
0.6371626205260130 0.3911209823826503 0.4241366961288293
0.3104103581366789 0.4591573516314383 0.5663259555923297
0.6098156850370896 0.6595008042595770 0.4336283323399075
0.5589288008058717 0.6434923988909781 0.6329528998930889
0.6127050845623888 0.3900315156133540 0.6306817815504643
0.5084922280286218 0.3841342235790232 0.3315787817539016
0.6888171349525307 0.5407903004862248 0.4334234198492197
0.5928150134814787 0.5723243200814163 0.3326624492017381
0.5251206352376567 0.6203720047368544 0.3364313501119658
0.5760651797552695 0.4945624068464003 0.4920006721458021
0.3961138506462165 0.5338072085648241 0.5768228569226980
0.3887310257571082 0.4541997449698097 0.5584061792624623
0.4391792957330977 0.6422987189541232 0.4956378052006443
0.5268434243469579 0.3043596128850847 0.5541412596618023
0.4481550545763303 0.5573995525667569 0.6346362739583106
0.6635207489450355 0.6090104596909375 0.5558242882315786
0.4405011857402052 0.4309314760865601 0.3317796426931369

0.3465093937338727	0.5984286686382874	0.4406160606776149
0.5825998869054060	0.3691606168589577	0.3663939311781836
0.6023509934355502	0.3370218650242854	0.5692286753502994
0.4091659187260557	0.7130986608524532	0.4936228760754504
0.3913128170586258	0.5772111128725921	0.5063309014880385
0.5758426646021446	0.6079522988033467	0.4827695092826976
0.5841983479432225	0.6127783836218865	0.5637671999841793
0.4339067247179503	0.3988287366654149	0.5990872533073259
0.4431539530556390	0.6006845363859759	0.5658811512723874
0.4452037723225910	0.3128815210953855	0.4375362923225587
0.3804435738035876	0.3343403369463470	0.4853518169361886
0.3390388123641292	0.5428278364399552	0.3801780054249058
0.5178255501651079	0.2981048238035232	0.4716103819788857
0.5658354480578335	0.6005205682290762	0.4022641071979929
0.3744247062982001	0.4797379435132914	0.3392091072393669
0.3357635576911666	0.3910555927806996	0.4437641977274340
0.3598787704374868	0.6493517315506653	0.5041173599167980
0.3733732091019248	0.3307296989272794	0.4045800832856102
0.6573534661344246	0.6053476940939376	0.4737301920355621
0.5830688034737024	0.5379479327168470	0.5967742360676050
0.6260206612076124	0.6691398272929591	0.5952740145646975
0.4437844732268331	0.5080896508133768	0.3032155803807662
0.4167874667642902	0.6307803487697211	0.6337477103456615
0.5802282047367047	0.4619892818411262	0.6280193371870808
0.5117691966915997	0.6290802079818127	0.5301332294898244
0.4514628338826678	0.5886199240931669	0.3218539055717225
0.6189264203276950	0.6656602943083119	0.5144360279236729
0.6532126956559451	0.4895423606351016	0.4836183995901345
0.4632316581164038	0.3255023754493566	0.6010724777629678
0.3011011304763294	0.4529541658720891	0.4839485673681983
0.5568692346149712	0.4933579492156089	0.6969915770190623
0.6199546405400755	0.5517919388612478	0.5238622256447710
0.4592505132155891	0.5182976276838909	0.4369753324604361
0.3622202237675793	0.6086764487772663	0.5759000725392487
0.5415649458116880	0.5561625263446741	0.5319470913009552
0.5070746913579237	0.4294950749316918	0.6153917307353431
0.4740621586588321	0.5281317365162242	0.5674997334442050
0.4279935434502209	0.5905940037739702	0.4337284050991223
0.5711176538524100	0.4092365419744897	0.5667078593829552
0.3535319398309186	0.4032381461135301	0.6068127887573781
0.3460265045434807	0.5102395399310031	0.5166752249190888
0.3782331714458628	0.5554185527083563	0.3101374900166175
0.2696661062939926	0.5157900642788464	0.5246889131827261
0.5589674469667119	0.5218279211945041	0.3826799379640853
0.4995893650713400	0.4998055164894458	0.5004334669243425
0.5386875558208668	0.3551108697968479	0.6179299369425240
0.4231461598797971	0.5051443666053745	0.5085546536647617
0.5326025502054272	0.5499269270471208	0.4514748753612642
0.4907130447221065	0.6158606553059401	0.6685210346015704
0.5025485406926974	0.6227589546473880	0.4484185620913703
0.5509723658801080	0.4425367109898063	0.3656775627646138
0.4966566846459577	0.3770606300751302	0.5519827821868327
0.5184009066992316	0.5415732467260421	0.3141460584887735
0.6401093530449131	0.5169516734939771	0.3712579366211981
0.3180080371765537	0.5398764761769661	0.5852137892007313
0.5139341942146213	0.3379838026644393	0.3996276855245114
0.6254542958658784	0.5204428603703294	0.6606115362206982
0.5601099859685050	0.3575062573363441	0.5046177396324083

0.5765962184695014 0.4139496303434118 0.2989522054856106
0.3586861362427540 0.4831457979299024 0.6288042101607234
0.6812322931839745 0.4600935710480573 0.4146905411572661
0.3866428454544580 0.6100329051541490 0.3695766480619077
0.4816614610092650 0.7017674916319158 0.5282883639729605
0.3028050153183132 0.5295218341968294 0.4519154478861653
0.6079422795190893 0.4225343842652695 0.4941039670245909
0.6393816954433006 0.3505262912640060 0.4958797464324686
0.3133122147038060 0.5833164287369136 0.5144764191066624
0.3342195063556526 0.4660672121031260 0.4097633535976503
0.5852380537872672 0.4932019837888624 0.3142985534717834
0.5561682976431070 0.3990115471762579 0.4344132387845192
0.5588494429278538 0.5693346124706219 0.6683567426927329
0.6231504259223101 0.4456633912393517 0.6899566915598073
0.5519223461921180 0.4099335348978690 0.6810342343901598
0.4605463609400012 0.6447426108950727 0.3816786971859474
0.4407948672636047 0.4774576066141130 0.6187116931757194
0.5541898662332500 0.6869674787707646 0.5622700347447815
0.4920787097581322 0.5695202630107715 0.3864800201853139
0.3792538807466197 0.4480784917607308 0.4762949901810888
0.4855382924024281 0.6617567689802232 0.6003522075449405
0.5397464351350110 0.4812218619321246 0.5639873365844825
0.6649179661079575 0.5339865250030676 0.5899189503548320
0.4846002518892023 0.4897304748923302 0.3679871246202397
0.5164106390359627 0.5855961489220820 0.6005732186679777
0.3983664935990346 0.3486278881270502 0.6455167046356819
0.4890386964860683 0.5395308108396172 0.7008741155972619
0.6859895045304764 0.4166303004484768 0.4854666441682677
0.4798978113705321 0.4588604472921069 0.6890186127256113
0.5464369146133334 0.6844548708356520 0.4801930770908044
0.5986444387757364 0.6504014952118202 0.3535867145084224
0.4666792387606334 0.4496694280153012 0.5495331379656736
0.4122686286851867 0.6730779640447691 0.5642012848057438
0.4721956530460622 0.6954000213303174 0.4458073308941113
0.5141436253999184 0.5091083005001875 0.6332232990023506
0.5251594279545917 0.4714001518679435 0.4332161487137107
0.4996564512532747 0.3997165009083303 0.7177031158661812
0.4972522638921043 0.3908311908581416 0.7476831097567437

OH/Cu_{147} E_{ads} = −3.38 eV
1.00000000000000
31.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 31.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 31.0000000000000000
Cu O H
147 1 1
Direct
0.4155489943556289 0.3869462369152631 0.4367067441603182
0.6033158365910084 0.4658688612775167 0.4230014145041486
0.4183260867009709 0.5368514530819285 0.3733869536694517
0.4238156182771282 0.5870538599679674 0.7017458854797122
0.3968933436687527 0.6627351534918193 0.4312825950432290
0.5875989764443551 0.3267943428841495 0.4351798560589757
0.6298080082405565 0.4366717838289927 0.3547926300674786
0.5302457616633655 0.4291549073131058 0.5021425595350247
0.7297853225594629 0.4846028358284363 0.4740533020775668
0.6271937611433234 0.5956480452892643 0.6285884777874845

0.6612639608620139	0.4576250564005759	0.6189462044876645
0.5910305108732008	0.2869913080777485	0.5059429910723925
0.6187172909712666	0.4761539537550226	0.5553437556532447
0.4242282968388507	0.3920670765878781	0.5180658794894781
0.4880333575227599	0.3707611781668785	0.4700313497690069
0.4026885345194743	0.4274114037210109	0.6697367802532418
0.4697806414849533	0.5707821954509450	0.4981232092135771
0.6969110130702521	0.4708309684914361	0.5469137592673184
0.3427903767820804	0.3946620225404595	0.5268250124333105
0.4160384126770808	0.4614785299005495	0.4040387106205595
0.5098373617140030	0.4606791472051603	0.2990556879327272
0.3904449255303892	0.3403795839118898	0.5664458123962519
0.3698846766456035	0.5638571057967092	0.6450048309385413
0.3728763106309716	0.4044116426985137	0.3712883453006018
0.3811231829502550	0.5238374864221153	0.4447986808874600
0.6984535603641882	0.5475288490001573	0.5146306610797844
0.6447141509870553	0.5965168182889569	0.3920377114900189
0.4579364893261639	0.4436396549877645	0.4687320355716413
0.4405104794130293	0.3563101351215246	0.3671326182836495
0.6107795732748628	0.5456757981092248	0.4416083828434154
0.4830395848650838	0.4138039971773295	0.3998366649529471
0.5353089495095399	0.6743696190183180	0.3988180028346055
0.4538199383528723	0.3156985505399379	0.5198025954159421
0.4771657177673260	0.3743119459187695	0.6649426753779984
0.6534034811850419	0.4019775805310228	0.5584829373319674
0.4142252459090149	0.5083978599599560	0.6860777742323767
0.6373846265630490	0.3912865162337129	0.4232014892048684
0.3111609818458005	0.4590470506355400	0.5672456256818345
0.6095057107552025	0.6595743309188046	0.4331418397693502
0.5595090986468849	0.6437644331850257	0.6327407074220764
0.6142102685734281	0.3900139213068340	0.6298234627978166
0.5083315300635799	0.3840652093880136	0.3313279980387644
0.6888464236359502	0.5410138061162790	0.4323742715334972
0.5921141325517846	0.5723529420095644	0.3319666987339084
0.5246162846928064	0.6203501149311629	0.3361162043806006
0.5763759381590728	0.4949044672151680	0.4914975956787055
0.3966774357685167	0.5339699297774261	0.5771910414672974
0.3894386972317238	0.4542946144510999	0.5585884251991660
0.4391880313836122	0.6422563306282619	0.4959274257418479
0.5280938223334857	0.3046447617365033	0.5537523778434631
0.4490556156338388	0.5575488499928004	0.6350037474123974
0.6639206457786664	0.6093186451674355	0.5550569329884252
0.4403551707564948	0.4308161266028971	0.3319993775512991
0.3466671794413104	0.5981662997378731	0.4412681210316480
0.5825912595994135	0.3691564610065458	0.3656419802277228
0.6030110150325648	0.3372182845276464	0.5685796789000521
0.4090746311248569	0.7130151620287819	0.4939223336084895
0.3916271967180369	0.5771396033931934	0.5067011476659367
0.5758819591081843	0.6080118981123146	0.4823580972546380
0.5844508783433947	0.6130367779091485	0.5634642688871236
0.4345600761949910	0.3993753734146276	0.5999723189797510
0.4436008179320656	0.6007610804142872	0.5662414159166138
0.4456907617492896	0.3129026233099887	0.4377552403593662
0.3812072796776151	0.3343810740636453	0.4859749098374214
0.3389236698573560	0.5425087424689015	0.3808505927153480
0.5184464052067673	0.2982372888680012	0.4713453434347815
0.5655190915788642	0.6005235599231655	0.4018134763041407
0.3742147938433171	0.4795235685156091	0.3397045483782496

0.3360390748587680	0.3908401445621657	0.4447090916977193
0.3599836723881830	0.6492391245810071	0.5046640258040221
0.3735923165778975	0.3307045333502070	0.4053386076346197
0.6573425001396785	0.6055139349150700	0.4729697028571561
0.5836185232871378	0.5382915138506332	0.5963650240692419
0.6264446961520743	0.6693719184233289	0.5946702216343405
0.4433198072902706	0.5079449541635089	0.3032366324762774
0.4174655280428765	0.6310215869612590	0.6341187233021683
0.5818138924544231	0.4630917124883484	0.6267200095651965
0.5120453455470350	0.6291430510132512	0.5300984509784115
0.4509118652158927	0.5885252994548580	0.3217955924678333
0.6189228341901477	0.6658314249035374	0.5138597274886830
0.6534787108850408	0.4896815604462129	0.4825803970281764
0.4647620520407614	0.3255009474154623	0.6007936018886578
0.3014813353297280	0.4526928402262892	0.4849184712723175
0.5575386766669127	0.4924032170444586	0.6967117620325308
0.6203445063802120	0.5520729488292391	0.5233763112643799
0.4594274562323370	0.5183620326219809	0.4370115428716932
0.3627105849940870	0.6087865277597149	0.5765475342418214
0.5419910849331858	0.5562015005017114	0.5316984280174023
0.5075021325858622	0.4298113176116919	0.6151741028884415
0.4745694660958356	0.5281493796534352	0.5677528999161610
0.4280647246161869	0.5905652563110469	0.4339270678044493
0.5718584567594618	0.4093672745366506	0.5662419480540150
0.3551889933588550	0.4035184255189566	0.6076974636428132
0.3465175347156562	0.5103536687211869	0.5174096835663273
0.3776987819403252	0.5551932024634274	0.3105287966473076
0.2702001402617289	0.5154885166487735	0.5258647861399415
0.5588580838326311	0.5218308159069912	0.3821536057358353
0.4999199006600530	0.4998475646133158	0.5002955045854783
0.5398851334854403	0.3548508718807229	0.6182702651636769
0.4236032094318117	0.5050579187119066	0.5087928879837327
0.5325951337059589	0.5499940937152848	0.4512083531710626
0.4917864161118427	0.6162411104239660	0.6686961924288943
0.5024128982767214	0.6228136041292729	0.4483437529139506
0.5508730755403800	0.4425163127783242	0.3651259214126405
0.4975404696227596	0.3773519209771303	0.5518388537544594
0.5180530814122273	0.5415322334102717	0.3138148663986624
0.6398511886417543	0.5170913300856441	0.3704539948150952
0.3187811562641966	0.5395176612672711	0.5862846355038143
0.5142393323159232	0.3379242535236195	0.3993258988978398
0.6261091024063906	0.5206982895636223	0.6603232458147253
0.5608646877970105	0.3577385765238499	0.5040376524254656
0.5762879331686073	0.4140504990000652	0.2981914777602896
0.3599373080637424	0.4827814634814934	0.6295687199198423
0.6812424259343590	0.4603040885284694	0.4136436868032421
0.3864368825058391	0.6098467639223658	0.3698855187180888
0.4817382995955851	0.7017797718979316	0.5282193172158453
0.3030587822624481	0.5292657916469194	0.4528907384540035
0.6083800354021760	0.4228420135073867	0.4932478629653480
0.6400140804389604	0.3508263740859904	0.4951357167452468
0.3136720150593114	0.5831320005391460	0.5154815133996891
0.3342909825594934	0.4658505400109662	0.4105604468462462
0.5847809786106608	0.4932759839149405	0.3135278597095796
0.5564849594723584	0.3990312356837120	0.4338675498840762
0.5598226416920172	0.5694099681550834	0.6680742742914513
0.6233259209892453	0.4452189563594355	0.6893504402012662
0.5510976211200074	0.4110597892336802	0.6775859944293193

0.4602058320137911 0.6448349009350971 0.3816067568196983
0.4408892300967118 0.4772166895622488 0.6193263350607937
0.5544448857786939 0.6871275164925920 0.5619669566641518
0.4918846444236776 0.5695026896449864 0.3863220614679636
0.3795738294368856 0.4479501668858122 0.4767886154645435
0.4859872948391075 0.6619491683932530 0.6004133307329615
0.5403256379220469 0.4813753998501150 0.5636733835502751
0.6655410092046387 0.5343345166928434 0.5892060924737632
0.4844999885074489 0.4896644273787031 0.3678626503150221
0.5169199701165741 0.5857133122165209 0.6005320733635379
0.4001410747528168 0.3471176979521394 0.6446430497284773
0.4902495605009849 0.5401760359362358 0.7009600970257106
0.6864031062643696 0.4168760948431837 0.4843297886106419
0.4830835429306896 0.4595735446263536 0.6896934289657872
0.5462942263504899 0.6844472676509692 0.4799355808095619
0.5980539666104999 0.6504366761828694 0.3531561046959234
0.4673691840263107 0.4498263628964508 0.5496988817786185
0.4124921985988358 0.6731906059916637 0.5645800651249038
0.4719718335675255 0.6953664431474184 0.4458345440021348
0.5146301033679982 0.5089867570777585 0.6333276048466038
0.5253284298249012 0.4714555519385107 0.4329175283329565
0.4482035212453421 0.4080686669183404 0.7137168622843346
0.4445683317765702 0.3996861342880587 0.7437588291339248

OH/Cu_{147} $E_{ads} = -3.32$ eV
1.00000000000000
31.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 31.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 31.0000000000000000
Cu O H
147 1 1
Direct
0.4153580722582667 0.3863866667738267 0.4363190685019641
0.6035083561239750 0.4654132637000623 0.4235962617541202
0.4179078212329974 0.5362577795028589 0.3736096410724017
0.4233746830550728 0.5866951331197460 0.7018216668635284
0.3965489238076750 0.6625958740633403 0.4313942548350101
0.5878628604060284 0.3262679397514364 0.4357387313375994
0.6300226549755863 0.4362714931559658 0.3554363647155787
0.5303872334897466 0.4288384616744958 0.5023228172044752
0.7303481550846258 0.4845208914066346 0.4746683101706139
0.6271928664601593 0.5960497380766357 0.6290761233416685
0.6611772879889167 0.4576607205122017 0.6195668430181720
0.5912616680423514 0.2864128957684638 0.5065161653969119
0.6191054990495739 0.4761733037668930 0.5556501826858348
0.4240574360154633 0.3919644554455238 0.5172544631968424
0.4880955912968729 0.3704862887926135 0.4701815547973354
0.4079986751177888 0.4289236970724074 0.6672076483616032
0.4693115966792453 0.5708514520017437 0.4982979834035666
0.6972573613419120 0.4707920325368364 0.5475616672585837
0.3424254948731978 0.3945873667669529 0.5266481863242950
0.4158202770206207 0.4609192977560911 0.4040802531357482
0.5100149124969515 0.4601033381528124 0.2996037274796525
0.3908721308266661 0.3411416589397016 0.5664473130299297
0.3698654471046513 0.5637736947806827 0.6449672882534074
0.3727426468331730 0.4037099651299300 0.3712953872314855
0.3807126894893574 0.5235789581831982 0.4448282178881933

0.6985654827521830	0.5473452603891272	0.5153344700310775
0.6446240930186945	0.5958299424003113	0.3929330658069783
0.4577572899576883	0.4432834921048691	0.4685470643487136
0.4405097905887300	0.3555774538716436	0.3673180111064268
0.6109054546269618	0.5450911112130905	0.4423882897495807
0.4829936857030608	0.4131833622253253	0.4000528765573088
0.5347343639662506	0.6738298672734154	0.3994394374239561
0.4538764191350143	0.3154453854909245	0.5200812376566729
0.4756356158213316	0.3803051682406500	0.6631409334973281
0.6535260507480762	0.4019035065900108	0.5590496781261870
0.4148753684460296	0.5074397711519697	0.6862423933484760
0.6376154428406636	0.3909882417008116	0.4238217989428113
0.3108074546507000	0.4591004745692820	0.5673123639479176
0.6091287959405747	0.6590925825683083	0.4340467436678482
0.5593770236866115	0.6442541157660290	0.6330697267608150
0.6137288033334266	0.3903663078393768	0.6304134949471130
0.5084653188704654	0.3834823877425044	0.3316721791184535
0.6891319199832179	0.5407627744020533	0.4331395844206378
0.5921082345978391	0.5715021366818838	0.3329338513283761
0.5241650870983203	0.6197135839916730	0.3369637661691042
0.5765951906250957	0.4945844497078107	0.4918816857990212
0.3962798832919726	0.5345045474450433	0.5768394972100924
0.3888566462356068	0.4547182222633007	0.5581013863696750
0.4385926929480501	0.6424168341257990	0.4962132753312991
0.5281909594129218	0.3045833830047778	0.5543871960359793
0.4489368161063341	0.5582958338931640	0.6348529213339345
0.6638312072199479	0.6094651988608585	0.5556744514667543
0.4403991595108531	0.4301740423186090	0.3321578958781904
0.3463800755364963	0.5979350979346396	0.4412162520193215
0.5828618411311581	0.3687566306638062	0.3662328077885734
0.6033639421849607	0.3371696111726288	0.5689341110747289
0.4085855140605461	0.7133563787003887	0.4938119530524374
0.3911450371860039	0.5771890017579312	0.5067091796506762
0.5757540981052790	0.6078592786688246	0.4832449898492254
0.5844761814732228	0.6133573479655433	0.5640494288740184
0.4343983971486426	0.3997814898107606	0.5980982163592756
0.4431428278919516	0.6012777326762967	0.5661735090763003
0.4456030728164568	0.3125325645526320	0.4381251327637802
0.3810191905414831	0.3339128700569209	0.4860001167480724
0.3387832474692082	0.5421355613384297	0.3808171841499259
0.5186069849384661	0.2979609244072114	0.4720083877407518
0.5651577096984648	0.5997838619186675	0.4028857990257643
0.3742131097020176	0.4789079485623832	0.3396961844811240
0.3360115404485684	0.3903182834679036	0.4446778103527006
0.3595923311866873	0.6493038723533000	0.5046013255339590
0.3733550951439270	0.3297636062222746	0.4051969873253096
0.6573281634906142	0.6053401261622130	0.4736681523278615
0.5840607150020145	0.5388122454105275	0.5963979330660752
0.6265168936998340	0.6699925629850475	0.5951639917322785
0.4433416538669610	0.5074157256286980	0.3036164126486462
0.4170393782822255	0.6312302615657791	0.6342095278153846
0.5820782593303080	0.4635527675915354	0.6268622676486553
0.5117326573821965	0.6292715433777843	0.5302379127542927
0.4506539554329210	0.5880954907382530	0.3221247569079132
0.6188646623767843	0.6659875397928726	0.5145337588823854
0.6538872277643875	0.4893304153617529	0.4833277163089020
0.4649545756580835	0.3264301416440553	0.6010040146832597
0.3012132889130777	0.4525348473022145	0.4849891970596334

0.5566514534001200	0.4924664518145753	0.6968040325042060
0.6204257928400067	0.5520071488529515	0.5237484307622259
0.4590093566681042	0.5179643864368964	0.4372028569307419
0.3622661765720491	0.6089747096784756	0.5764630696781015
0.5420081435239480	0.5563897119745105	0.5320941165754119
0.5085002456803086	0.4309558053252000	0.6136055348379023
0.4744570429701351	0.5288687178686156	0.5673034554905650
0.4276575526535807	0.5903307893289225	0.4341502270185937
0.5722408145590390	0.4094371647164009	0.5662861789132200
0.3555260594338229	0.4041199911050213	0.6074409128112747
0.3458504051733878	0.5105311230258820	0.5170383464137133
0.3775758445863501	0.5546656098766172	0.3105149474644404
0.2694227106936539	0.5153540651162436	0.5256737755599952
0.5587812093062147	0.5209997146681536	0.3828582184148011
0.5000067356803921	0.5000491468062491	0.5000865846170297
0.5402069327018219	0.3553304606420385	0.6185042252139415
0.4231558684169826	0.5050399755323511	0.5087240470728984
0.5324078303198179	0.5496427712874186	0.4517392734522994
0.4914380458404687	0.6164747036646608	0.6687740784153139
0.5018351499846558	0.6225909088909597	0.4489033017252361
0.5509402204832596	0.4417227222655802	0.3656555428285113
0.4979617821364379	0.3772037253645005	0.5515956703145287
0.5179358541734758	0.5408237281320281	0.3143954689844952
0.6400844099413345	0.5166005252717587	0.3710895130434027
0.3182714045984190	0.5399134682197776	0.5859276106542812
0.5142976122761471	0.3375538164815868	0.3998251049896522
0.6258035836586331	0.5208593394544117	0.6606934717291393
0.5612825225270800	0.3573267476672012	0.5041645606660691
0.5765335398249476	0.4134204981776132	0.2986593552148910
0.3597174661485369	0.4834982921171668	0.6292921773198119
0.6815332552347122	0.4600888399602708	0.4144102558664021
0.3862536358195597	0.6094440786511758	0.3699578839115512
0.4812546305905889	0.7018376088343353	0.5283535524897879
0.3025578136690238	0.5290505582675740	0.4527684924055175
0.6086355449994877	0.4225578726788691	0.4937131054862894
0.6402550255193988	0.3504754707958821	0.4956850814346688
0.3130726024721581	0.5831057267326919	0.5152753356370660
0.3342529320430437	0.4653918653629658	0.4105774597888431
0.5850244310072565	0.4926257432104592	0.3142176169338268
0.5566657612414169	0.3985424983033578	0.4343146905744488
0.5595859877487368	0.5697069028159326	0.6681990784848281
0.6224134320864608	0.4451289687611049	0.6898997712174828
0.5491692421231961	0.4117241389692199	0.6782111197617566
0.4598124100049442	0.6445099186387887	0.3818206987347316
0.4411010968692329	0.4790287832891757	0.6176005720778287
0.5542441860015724	0.6872502536593479	0.5623093095688415
0.4913895457427960	0.5688620706113815	0.3868765859720614
0.3793506176164349	0.4477709675746855	0.4766371894648835
0.4856042873220940	0.6623702314059026	0.6005286309623905
0.5407158264179047	0.4817132916753573	0.5633771255037643
0.6656932824124435	0.5344530510152257	0.5897276423475851
0.4843958297686639	0.4890635351538550	0.3682507592298257
0.5168458549943876	0.5866213316339042	0.6004390096793869
0.4009951702656188	0.3487272590497628	0.6477127080131754
0.4899134436649483	0.5398829876746677	0.7008436613487746
0.6867005903426479	0.4167434754269511	0.4850147938704937
0.4820532022539358	0.4591535034410417	0.6860908448926060
0.5459565106538339	0.6843771072746445	0.4803576008889787

0.5974687142463383 0.6493289861384709 0.3544544596883580
0.4675335674644508 0.4503916522860233 0.5485831075107755
0.4120256688044307 0.6735945439612744 0.5646218684358855
0.4715274217420938 0.6953291561944024 0.4460521742858145
0.5155045885168059 0.5108091872215762 0.6322513494438191
0.5253114004564997 0.4708555359349362 0.4332468724954517
0.3754375402247104 0.3155620219790414 0.6881448184488388
0.3691185585353828 0.2863834434610218 0.6785309595592335

OH/Cu_{309} E_{ads} = −3.64 eV
1.00000000000000
38.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 38.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 38.0000000000000000
Cu O H
309 1 1
Direct
0.4932683051216502 0.4599706726192369 0.4525775271446402
0.5000689844315024 0.5000314964055085 0.5000109452072680
0.4441441604993470 0.4729576612648147 0.4940453044458996
0.5495905413760777 0.4648361955108999 0.4858050846108861
0.4648137968953854 0.5191368199009225 0.4522090455437616
0.4701230245116059 0.4860152001656475 0.5529212947417036
0.5324757814670834 0.4188894125178838 0.5638550967459005
0.5300141801003698 0.5140852296048640 0.4470855143609231
0.4135002499260577 0.5552259847011216 0.4656952442704261
0.5560642698771047 0.5270510936326160 0.5059542845799732
0.5070447454796653 0.5401469219830924 0.5474006705989056
0.5037630519673851 0.5606068847956692 0.4852156910795742
0.4897127695860961 0.3974857962277456 0.4667962676278727
0.4361468631352216 0.4315911063440681 0.4455947430327080
0.4394685307423753 0.4106921034677487 0.5090398155218875
0.5470797112259403 0.4024903824748855 0.5006900315742127
0.5437360175145365 0.4233709599823472 0.4371881761146096
0.4572517445622842 0.4786661034149492 0.4029294560542641
0.4660042023175767 0.4240118175604328 0.5690704257552403
0.4071272973751099 0.4918643186142974 0.4451441144400548
0.4125478860556018 0.4580568078824049 0.5478744758914317
0.5237328878592160 0.4735091325809463 0.3977467710935302
0.5353224803545047 0.4809481627411071 0.5478307521921445
0.3925133888332936 0.5082404693518262 0.5083833798776393
0.5866397753813603 0.4448738604333420 0.5342980084615118
0.5812351843563109 0.4786377921708628 0.4316615885654973
0.5054738030755374 0.4662852982450212 0.6026976555979270
0.4946623328556079 0.5338173731224050 0.3973211325851956
0.4505446340037531 0.5351605963711557 0.5141899989604077
0.4189014575073635 0.5214416157164782 0.5683844418499633
0.6075658014859731 0.4917390392682436 0.4916037132867757
0.4676613798267586 0.5810997337569412 0.4361581254418812
0.4764149667376366 0.5265047003260754 0.6022133344113081
0.5930331648840650 0.5081885892225740 0.5548118393676644
0.5876027646982920 0.5419586071008972 0.4521776581232110
0.5430212171663500 0.5214734747603179 0.5970396263693464
0.5342269081413675 0.5760745934357697 0.4309925329729035
0.4564316592678492 0.5766136363578226 0.5627532316448800
0.4530825950793173 0.5974720481584576 0.4993272629531510
0.5644599545886595 0.5685902056307981 0.5543764122672711

0.5610981898631716	0.5894380238221427	0.4910209511837553
0.5106530883821252	0.6025633428450187	0.5332023740731698
0.4930097111099964	0.3780533869752469	0.5299069509986820
0.4864199827872187	0.4193179601440110	0.4044670112730690
0.3873720759859828	0.4455176698036211	0.4880056905887063
0.5998468793155194	0.4290870375146761	0.4713841441415218
0.4289666906190733	0.5384112860428293	0.4036406598237682
0.4396587491828284	0.4716562623242678	0.6066034458967535
0.5710469014808999	0.4615515945499544	0.5963822789584443
0.5603475381244313	0.5283230608776283	0.3933470710031939
0.4000742156818475	0.5707448778410383	0.5285605668880843
0.6129684451690954	0.5547084899827336	0.5120581094223079
0.5136884137383975	0.5806998055417116	0.5955254423852684
0.5070609080166285	0.6219523663588008	0.4700885506390381
0.4316166989472673	0.3677914975501598	0.4600797335663716
0.5409744282902178	0.3595003687603815	0.4515940981697754
0.3986370565369591	0.4502612076662451	0.3951234276192823
0.4075286862911763	0.3946720848154741	0.5640133973242535
0.5844155947806400	0.3812336555284519	0.5502611337502364
0.5755385467679919	0.4367693389437152	0.3813922716639825
0.4876237700721371	0.4928845194244635	0.3465760102651244
0.5019948146732266	0.4030589815764051	0.6197316242679463
0.3541422142932159	0.5281005847429238	0.4589518033381602
0.3596471099935770	0.4937474385012021	0.5633172190543480
0.6459797891373262	0.4718782024212664	0.5410118804004361
0.6404699182733594	0.5061987562994285	0.4366739281449920
0.5125744808564064	0.5072177331654040	0.6534189541758273
0.4981775886580443	0.5970287049514016	0.3802860928611835
0.4157130147874656	0.6187677593076251	0.4497327826137080
0.4246029178424073	0.5632318106228066	0.6185939894409711
0.6016730169274798	0.5499046127653126	0.6048008626487128
0.5927260533548108	0.6053905098458447	0.4360681964407292
0.4592353248819360	0.6404918604918586	0.5483862142616278
0.5686575007941519	0.6322214140607517	0.5398873167524991
0.4860199186985406	0.3349842463383526	0.4816651868237349
0.4826882509783743	0.3558606444101128	0.4182428108255637
0.4354760346971152	0.3482915784818544	0.5242692560647727
0.4287842001579081	0.3902516722248266	0.3968156499906812
0.5439116050024690	0.3400345466909880	0.5158742328603571
0.5372334910966432	0.3819651561559844	0.3883231752840245
0.3786514990247722	0.4035170171695556	0.4390823190464633
0.3820014017166195	0.3824246840065807	0.5030539726621794
0.3493843386521450	0.4642001429824475	0.4386731225233317
0.4500822557898935	0.4376736265813285	0.3538140450488351
0.3548286398206556	0.4301455520378574	0.5421520154842676
0.4622075093709275	0.3617043701717025	0.5847557382606043
0.5980182659758800	0.3658873399191830	0.4862457998360733
0.5946496919146012	0.3869129017527073	0.4222369897284996
0.5170667010092439	0.4324796654384743	0.3486095069030105
0.5291762781015008	0.3565686019185463	0.5794989482828365
0.3346358574559024	0.4806817088742195	0.5023774393182715
0.4209685836739526	0.4979230660535209	0.3533975507136283
0.4351857569754872	0.4090666592460974	0.6235344315815131
0.3704046119063131	0.5112355904050324	0.3959772139224365
0.3812595017642241	0.4433773191392202	0.6021533425589629
0.6378287145885237	0.4085497867187393	0.5201043559352119
0.6323908158837925	0.4425684338511224	0.4166373151417592
0.5544111432140988	0.4876652509642565	0.3429674153548775

0.5686287882852672	0.3988329431581532	0.6131797884113122
0.6232246912074056	0.4249409956501318	0.5833597290447387
0.6123353067274551	0.4927663667770410	0.3771323779912304
0.4749662360672287	0.4516754438662128	0.6574381210002632
0.4586386720898425	0.5534946287184090	0.3477600132392304
0.6588013592507372	0.4556194958336095	0.4769989387450916
0.3410435401500677	0.5440679877734378	0.5229002168845153
0.3767903717642284	0.5750655037246328	0.4166464508429910
0.5414611513779813	0.4465623422792896	0.6522788957125354
0.3876773344004431	0.5072279501929022	0.6228510471698226
0.5251261088482704	0.5483976178826111	0.3425317354736966
0.3622010057565820	0.5914276404398444	0.4798486151072906
0.3676461297502132	0.5573763255179558	0.5833739081497139
0.4314115528298683	0.6011245674921218	0.3868534224015010
0.4456372865227390	0.5123270338613884	0.6569580747012245
0.6295602285218673	0.4887270955884483	0.6040115529718340
0.6186894910620631	0.5565576914274377	0.3978165887817177
0.6654544799794331	0.5191670301746043	0.4975754020039796
0.5791957340606950	0.5021444054433233	0.6465812917945666
0.5649385802036081	0.5909605657839044	0.3764716209047694
0.6507186084620918	0.5357448195126471	0.5611884806598437
0.4053863503467078	0.6129611319438855	0.5776812905831560
0.6452632774518731	0.5696967249025789	0.4579030492170034
0.4020166140856458	0.6339694075337062	0.5137423542311832
0.4709368389626832	0.6433999222129365	0.4204529961579978
0.4830890647249584	0.5674850336633858	0.6513813628086620
0.5501381678099958	0.5624094871151473	0.6461816971203274
0.5379461936087487	0.6383485335821529	0.4152485740249279
0.4628325588840652	0.6179656769004653	0.6116366176878555
0.4561270006832860	0.6599005847180275	0.4841014480238094
0.6226024436223514	0.5970293630110949	0.5609136980454494
0.6191901165479617	0.6180182050989436	0.4970790172222546
0.5712475878725668	0.6097256379763825	0.6031550918439316
0.5644970510751536	0.6516573986888902	0.4756965386064271
0.5173918746855721	0.6441511702381997	0.5817860871170779
0.4622326525890427	0.7045245541373899	0.5335783168465769
0.4795123853034789	0.3781624826141583	0.3557780458618837
0.4894714243168911	0.3158635183002513	0.5451589344169983
0.3298659004074711	0.4176848308479790	0.4818757176384618
0.6508679719104871	0.3929725846803013	0.4568152507255528
0.3926682797325916	0.5579498953727524	0.3544957927668470
0.4088523479197780	0.4571845112772909	0.6609530510460397
0.6073387440364072	0.4420191613641156	0.6455316083714261
0.5911419501694931	0.5427999664864686	0.3389872385122601
0.3490310217410058	0.6067700292666226	0.5431066985772852
0.6706821442043511	0.5829495718816554	0.5182970824362266
0.5204719502276374	0.6218207063382478	0.6442658170561638
0.5104590767652537	0.6841456856235372	0.4547729292156609
0.4271208170001743	0.3038740787731112	0.4749893080771693
0.4237596130328370	0.3249761394058907	0.4107121286748009
0.5376772233547211	0.2954327021804104	0.4663577808661020
0.5343030484833011	0.3165432606033448	0.4021354122821102
0.3397623624233301	0.4218038785643515	0.3877872639048091
0.3487512729950674	0.3655590506157337	0.5585773437242872
0.5925034888570128	0.3214902984800296	0.4363562276199639
0.3905039569620795	0.4083901908367363	0.3450582331525484
0.4028495770223023	0.3310442979903062	0.5800601423876625
0.3730998797100263	0.3384322958789990	0.4534739653194499

0.5817837457115687	0.3174328081658954	0.5661419480926545
0.5694695993142590	0.3947095256358162	0.3311088030085464
0.3610943623169002	0.4693646147515246	0.3446057466052091
0.3755498053253948	0.3789828220381533	0.6192980637240008
0.6365568036534908	0.3436594206754199	0.5362142049183296
0.4805386051076453	0.4514825139842607	0.2959004640414488
0.4984552432243034	0.3394745060582438	0.6364067468179985
0.6275718218196944	0.3998309170553030	0.3654587297707201
0.2948351700072108	0.5004793274153176	0.4523563066646251
0.3003859814723663	0.4657168914787107	0.5578784352704077
0.6218040711346786	0.3602320738305125	0.6001741751603547
0.6073084267392499	0.4505600677124821	0.3254188582055298
0.4710768040606223	0.3873899530857102	0.6756591044828119
0.4511130352808864	0.5124224219932958	0.2954664991547149
0.5383385729566290	0.3822227899333921	0.6704939749638986
0.5183616100369721	0.5072916931262044	0.2901712625313721
0.3160239288186476	0.5480181056401348	0.4091485996756773
0.3271172132922316	0.4791044568204435	0.6185991966540948
0.3012616782487827	0.5646129794262383	0.4730743223483440
0.3068240886805231	0.5298285790839953	0.5786952310764619
0.6988536969472112	0.4352434902166112	0.5268139026727899
0.6932954137733863	0.4699730026756281	0.4212583603781337
0.6840477786164523	0.4519374839312192	0.5908059649571541
0.6729500214254509	0.5207821679344702	0.3813673462234444
0.4817037830712586	0.4927454718444458	0.7097782132717599
0.4617144234783863	0.6177867227448213	0.3295353688340014
0.5489876547538348	0.4876152759609639	0.7045692044854975
0.3782214007522581	0.6396869720929033	0.3998594627526196
0.5289894697889780	0.6126693862109395	0.3242891244935509
0.3927061309289714	0.5493857447616358	0.6744808656822759
0.7052413739575434	0.4991942131982144	0.5474821303360993
0.6996838633248219	0.5338711514140672	0.4420167401528745
0.3724762314810802	0.6000861772553199	0.6345457845537094
0.3634939362766700	0.6562990431637840	0.4637333119978069
0.5195836192793492	0.5485332687130059	0.7041260484792978
0.5016179230949492	0.6605640900346132	0.3635398321392461
0.6391413158001418	0.5308632540154284	0.6552353092743940
0.6246666296914063	0.6210582221679605	0.3808781849480570
0.4182573490759199	0.6825170898684328	0.4337811270736956
0.4305977942320853	0.6052027582018291	0.6689078266136363
0.6606419329067317	0.5786457811333559	0.6117018112011759
0.4075403877727278	0.6783091183491891	0.5635813050431366
0.6516351181713762	0.6344183248007206	0.4419109901312183
0.6095976471553439	0.5916212844020240	0.6550890330806051
0.5971785747478267	0.6690082752849837	0.4197655185302128
0.4656305343198281	0.6833788495561079	0.5978798634711135
0.5140320718949662	0.6650449656652576	0.5182902887917976
0.6260106927280418	0.6618732824662609	0.5465966482567067
0.5760675545008219	0.6751794857390750	0.5894034600686975
0.5726694100275004	0.6963362590591102	0.5249565958813281
0.4790232303058919	0.2930639930588763	0.4330167636547976
0.3711084256397106	0.3620381550953298	0.3902115291042626
0.3778029641893194	0.3198281638562161	0.5183362224033079
0.5949250802067347	0.3032139769020024	0.5013934401784194
0.5882258415296120	0.3453486247429935	0.3732233758678106
0.3124816779014361	0.4835243994920492	0.3894021387275461
0.3233823442765263	0.4153141756994078	0.5965201205202346
0.4137171292590620	0.4568637559676243	0.3040749267978645

0.4313445163530873	0.3465838185781048	0.6393558804520237
0.5478479399645498	0.4465749462558375	0.2936179689337333
0.5655399378329838	0.3363169792725952	0.6288936636400804
0.2829657716888869	0.5165075591815512	0.5169102466413761
0.6747116161120950	0.3885771102453928	0.5692626121766764
0.6637260839021845	0.4567135152984142	0.3619672073106037
0.5109225594754733	0.4318924390244538	0.7072814454859216
0.4891653812422459	0.5681667749257261	0.2927174204554614
0.3252339110404199	0.6113921985119984	0.4306946148721617
0.3361977887432270	0.5431762368244404	0.6380057135481977
0.7168874147036364	0.4833097606151805	0.4830273659572342
0.4344954578252138	0.6636148738688802	0.3710856239718495
0.4522112682319472	0.5533662991415311	0.7063288494317156
0.6874782914379068	0.5165056996440015	0.6104803693508033
0.6765746794704147	0.5845628250570033	0.4035450914304243
0.5864149275463217	0.5431587532738111	0.6959777281484202
0.5687326742541912	0.6534478394698209	0.3605716085183037
0.4117386278070383	0.6545012433806017	0.6267182342121832
0.4050202020038904	0.6966394259017519	0.4985789181747433
0.6285715051690365	0.6380553956092792	0.6102018767513436
0.6217649659354251	0.6804424912809456	0.4812906368078976
0.5208361117535983	0.7069371671171755	0.5669691976317368
0.5407105467321005	0.2776433417536979	0.5310035275715504
0.5306315896974890	0.3405722847635061	0.3395908651106139
0.3211116944953415	0.3754378688074894	0.4326007512759688
0.3245070374496594	0.3541394357054156	0.4970327052551703
0.4213793102132926	0.3488447344804726	0.3480877003851512
0.5102807912372113	0.3914746716756237	0.2995627426495539
0.5258150296211148	0.2943102799332920	0.5951392532896218
0.4427905677518292	0.3966355209698603	0.3048361149388648
0.4314600406644567	0.2858861249103229	0.5394633519738447
0.4582957056806776	0.2994420962567390	0.6003405402927900
0.2916357580881626	0.4365848339957971	0.4321864090765548
0.2971264722378947	0.4021920283738442	0.5364698004087285
0.4757089339368667	0.3142908121263020	0.3696602684624838
0.2768305018841060	0.4531621024964881	0.4963412768727576
0.6488146760998944	0.3292788988352699	0.4716849134183894
0.4823452172035925	0.2725096874850840	0.4965886812693630
0.6454733359838772	0.3504570910613037	0.4073646470171560
0.3847217211945062	0.5171344760329053	0.3039169919254376
0.4043814911437895	0.3941309960398155	0.6779410866050971
0.3337016786560629	0.5305025723987321	0.3467948182482822
0.6889609905050471	0.3722994263526855	0.5058684463008131
0.6835036327833881	0.4065478664306379	0.4016769884260475
0.3500267955819873	0.4286679418033735	0.6564402095588947
0.5851871322782993	0.5018407483201818	0.2883070997206814
0.6048549057703564	0.3788908818215328	0.6623752521915961
0.7103091568884246	0.4199896873129758	0.4625335280209645
0.4443962161338880	0.4370946950548902	0.7120994551476975
0.4226765144144969	0.5731135199383388	0.2982897330409920
0.6598437482378974	0.4051844804161378	0.6323736827238901
0.6434653074593838	0.5069634910007621	0.3227466001230153
0.3400893183720347	0.5948184400403520	0.3676185641765110
0.3564513538935463	0.4930096699828679	0.6772400352804814
0.5773657311532012	0.4268912665981536	0.7018012683165826
0.5556341461689909	0.5629651865859374	0.2878020939291996
0.2896652088718469	0.5799021113319686	0.5374149797045232
0.3951414250719151	0.6211033147645341	0.3376806378523183

0.4148067419564798 0.4981886132091635 0.7116131791545356
0.3109557561075398 0.6276205213093909 0.4940335587464412
0.3164104493247986 0.5933011329960012 0.5983444070754677
0.6662920352028342 0.4695523078067628 0.6531030457309974
0.6499635007721990 0.5712787215178849 0.3436380130397976
0.6153966867794434 0.4829450973533120 0.6959861129932068
0.5957122895174302 0.6058731576497016 0.3221352329461542
0.7234512117317154 0.5470121843064341 0.5036885597060766
0.3544684530545267 0.6492719299614746 0.5926170278222817
0.3511187969379741 0.6704927806370756 0.5281889131881429
0.7084680282527772 0.5628030897839288 0.5671948077927916
0.7029962696753816 0.5968451058215254 0.4635872308314332
0.4740969322325324 0.7056681098804402 0.4047786351292702
0.4896782747561054 0.6084677428133226 0.7004817859990531
0.5571688228939923 0.6033350657202682 0.6952603789742271
0.5416069498657496 0.7005668943624718 0.3995434688497772
0.4692924075338976 0.6593221711820838 0.6604331904242366
0.4591672330174372 0.7222994152752377 0.4689081060206013
0.6796810917182066 0.6265617113865772 0.5696927257700157
0.6760496035463680 0.6487060872482613 0.5019580073448938
0.5784953197258254 0.6511214228390352 0.6519653163962215
0.5683656725418929 0.7141072495246067 0.4604186007654733
0.5241371672664936 0.6856907410250430 0.6303923566209337
0.5174575195974378 0.7275030807064936 0.5033307396617861
0.4859197414436198 0.2551058125747657 0.5601219096434733
0.4726221943405547 0.3379497309705574 0.3081971409421398
0.2736843051190402 0.3905661335574412 0.4759210239503203
0.7006910712542499 0.3577664954589778 0.4426300206207354
0.3572851151976070 0.5770008942678886 0.3064181482278280
0.3786890132693747 0.4429920926616401 0.7140360089500507
0.6427368871612050 0.4230013619843560 0.6935721155055463
0.6213267731219781 0.5570007332241695 0.2859484230289576
0.2992280357233377 0.6420432731745198 0.5573226793436939
0.7296294244458610 0.6073734131186783 0.5232066856542678
0.5272231080735065 0.6620020181674940 0.6918951627769219
0.5138674097040782 0.7449017474090687 0.4397438235861788
0.4965328761125326 0.4394807002754901 0.5148457159388442
0.7143948525268118 0.6552875274528265 0.5395348682119205
0.7270356133096205 0.6767102405460114 0.5457061159604735

OH/Cu_{309} E_{ads} = −3.62 eV
1.00000000000000
38.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 38.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 38.0000000000000000
Cu O H
309 1 1
Direct
0.4932844445317833 0.4599678197295439 0.4525926901928015
0.5000449506525992 0.5000304775573934 0.5000717888301978
0.4440804296584600 0.4729444399914017 0.4940513683873459
0.5496509882688846 0.4649398653997148 0.4858529892360816
0.4647229556857048 0.5190444726851300 0.4521880266693419
0.4700683570974953 0.4859237051941999 0.5529030226649879
0.5324897695699301 0.4189867096415733 0.5639010322113165
0.5300269966956181 0.5141239055937060 0.4471283633530234
0.4134102498703256 0.5551936605144876 0.4657178618805620

0.5560044697677065	0.5271030461532692	0.5061699144876427
0.5069112307058620	0.5400294487574695	0.5475220601641726
0.5034586198717191	0.5604973782408420	0.4851975394358595
0.4896419762880286	0.3974745164202565	0.4668298890255127
0.4361435276603466	0.4316254663675818	0.4456056255780440
0.4394852417666685	0.4106880275617861	0.5090728064921185
0.5471197151886721	0.4025478296192014	0.5007144003235587
0.5437397728325960	0.4234289874792677	0.4372270952732736
0.4571827484061121	0.4786084352568084	0.4029292783602484
0.4659759458456659	0.4239440229299807	0.5690887188144385
0.4070308960825363	0.4918249646623435	0.4451784062584341
0.4124535807150969	0.4580426917040605	0.5478384287942181
0.5237237919445469	0.4735684209702034	0.3977304071718347
0.5354090136268495	0.4811036456613725	0.5479350886659606
0.3923672234978046	0.5082094779674948	0.5083927049508324
0.5865721581313430	0.4449663538834999	0.5344166871499461
0.5811931696425201	0.4786246872826009	0.4316469388399539
0.5055531575690045	0.4663352817075114	0.6026802725995385
0.4946205177302682	0.5337822866594866	0.3973010621226340
0.4503934194067542	0.5351061853150286	0.5142336818652421
0.4188445302051803	0.5214128361443472	0.5684036701529309
0.6075938354953527	0.4919145797007763	0.4917837930872694
0.4675344435732028	0.5810815929586486	0.4361183434590881
0.4764749780610962	0.5264964606474908	0.6022562580790052
0.5932509598391568	0.5083993580703902	0.5552074876826216
0.5875391033956844	0.5419580440787294	0.4522525482664109
0.5432149439009956	0.5215872315185065	0.5973733272124763
0.5340708819367682	0.5760623291874298	0.4309573680242058
0.4563383414954645	0.5765464466526884	0.5627929683680509
0.4529104501675607	0.5974672699370863	0.4993440926828100
0.5642046574027630	0.5684667593139024	0.5547837572380010
0.5605858564242286	0.5892114244129585	0.4911029404860346
0.5104768169084737	0.6024070574787166	0.5333113826569816
0.4930754949348650	0.3780465026336052	0.5299273774411868
0.4864849066895339	0.4193220529019622	0.4044787814431448
0.3872945502647031	0.4454715381767729	0.4880365553263855
0.6000061697438359	0.4293620377872656	0.4715015482392653
0.4289156522419368	0.5384067088171639	0.4036418689532423
0.4396776958064686	0.4716484106892103	0.6065809097699433
0.5712344832400545	0.4617853906498786	0.5964846614925030
0.5604141186750302	0.5284004564564021	0.3934020946173814
0.3999615671464613	0.5707193731971657	0.5285771055808162
0.6127850637674572	0.5545784660568176	0.5122324661839556
0.5137675896605537	0.5806731163228407	0.5956575967978552
0.5069599420017364	0.6218822688253236	0.4701501087953396
0.4315054342369861	0.3677939654169752	0.4600755808005930
0.5408984218728962	0.3594734253742277	0.4516014035962612
0.3985703711665938	0.4502424553459170	0.3951671001943851
0.4074664274335540	0.3946578355893107	0.5640117438899731
0.5843983483378128	0.3812939829990872	0.5502446244439692
0.5755435873452062	0.4368002687354255	0.3813988699503608
0.4875068566827783	0.4928382753215302	0.3465411579569800
0.5019224424606969	0.4030469301835841	0.6197237147612548
0.3540663741500243	0.5280377571651250	0.4589416504389745
0.3595746521673560	0.4937193905735115	0.5633166195185754
0.6458925954249892	0.4722373964080881	0.5413523001748590
0.6403720643455650	0.5062877495729731	0.4367542333279986
0.5128666428312524	0.5073391334121474	0.6534232839109604

0.4980879885409733	0.5970208135995844	0.3802529223229078
0.4155836928035925	0.6187698972178434	0.4497433918450424
0.4245320843375877	0.5631758028661752	0.6185800892856483
0.6022794678573836	0.5501881829486313	0.6056770318000150
0.5924926051238283	0.6053084652762637	0.4360585489827218
0.4591532026360444	0.6404659729844988	0.5483902057520738
0.5686743772474986	0.6320022955783604	0.5402168279844963
0.4860305580806335	0.3349619416569103	0.4816992911521097
0.4827119888245542	0.3558879709468498	0.4182460879583499
0.4355003182027836	0.3482867901064954	0.5242732752794099
0.4288099006168207	0.3902617005578630	0.3968660583017107
0.5439393885099092	0.3400401027825415	0.5158262591635331
0.5372487347568202	0.3820118718863401	0.3883853453743870
0.3786371696355130	0.4035053940800968	0.4391173363225940
0.3819825362294126	0.3824351402553958	0.5030783564163521
0.3492907140694183	0.4641901735319158	0.4387004631931516
0.4500457532885100	0.4376505713148982	0.3538227151383538
0.3547401363448211	0.4301284917063625	0.5421530552806855
0.4621438707622015	0.3616316518127858	0.5847546860563624
0.5980833912859980	0.3660249927658634	0.4862531575679375
0.5947006966146160	0.3870820465154037	0.4223252337326922
0.5170552072413823	0.4325476088787110	0.3486179185045725
0.5291598895401092	0.3566375739045624	0.5795163773420884
0.3345313445952934	0.4806599537669393	0.5023979159408557
0.4209224133889417	0.4978845969286713	0.3533893082711573
0.4351230521169165	0.4090202664286408	0.6235502987356453
0.3703555491982458	0.5112089252632694	0.3960053559296302
0.3812549059017884	0.4433701452813282	0.6021388609475465
0.6377987108528833	0.4087515304899637	0.5201905597748052
0.6324416353391457	0.4426619917191906	0.4166659548231912
0.5544403734831390	0.4877248706564896	0.3429863696490164
0.5686637022334540	0.3989764703066939	0.6131466085707972
0.6232348043639261	0.4251222587157485	0.5834113564316902
0.6123610473584196	0.4928031267792092	0.3771266095207747
0.4750055320490107	0.4516961532938677	0.6573485402177446
0.4585879086498861	0.5534523810204532	0.3477624112203088
0.6589831746302803	0.4560718453660342	0.4772047101466865
0.3408943658469752	0.5440272898027745	0.5229025766556222
0.3767735263353124	0.5750345731056996	0.4166571097361816
0.5415238313959407	0.4466931199689827	0.6522263480817165
0.3876570277095024	0.5071838890659320	0.6228546039286641
0.5251002824462196	0.5483975650969770	0.3425448795176578
0.3621006090430421	0.5913888217978919	0.4798735392156152
0.3675257854269618	0.5573364934814440	0.5833606643799503
0.4313387468619407	0.6011107050594362	0.3868325826314869
0.4456982379495297	0.5123140274872182	0.6569089436922113
0.6298944562598305	0.4893416018933337	0.6047490138895261
0.6187430210123926	0.5566406288852219	0.3978990462008258
0.6654284486383703	0.5193922995086019	0.4977806124411599
0.5799682583339714	0.5025042217189699	0.6468486843927841
0.5648616018705743	0.5910153935214492	0.3764318205333657
0.6509693816328590	0.5363992402251410	0.5620259566277834
0.4053303478715348	0.6129132640582116	0.5776803716712976
0.6452034616701381	0.5698556079207077	0.4579412447034220
0.4018971723246254	0.6340032826504264	0.5137228445081998
0.4708419833539039	0.6433798425072678	0.4204928368735191
0.4831638764736678	0.5674428309523993	0.6513830015187585
0.5508377183444627	0.5627858023762033	0.6464315370606634

0.5378170386210376	0.6383451440408024	0.4152667814709256
0.4628424659819062	0.6179268815696253	0.6115947958626862
0.4560674991637418	0.6599193749010599	0.4841493215471798
0.6219840154954576	0.5963661376522776	0.5616090502996383
0.6180263677425593	0.6175134007751657	0.4970927405278274
0.5717632750275741	0.6095997156148951	0.6039057601541837
0.5644887335718751	0.6515579209614464	0.4758289958211339
0.5174315903369272	0.6440105489705947	0.5818273654533253
0.4621134452050675	0.7044887317507710	0.5335873273957692
0.4795658062280905	0.3781968073367594	0.3557917979985776
0.4895221589289695	0.3158520817329632	0.5451637361922002
0.3298354803728569	0.4176809293035344	0.4818969765339505
0.6510069092645873	0.3933037748146043	0.4569292309672007
0.3926531929314469	0.5579292848873597	0.3544811160639147
0.4088933044330424	0.4571690040889254	0.6609407056364920
0.6073270936379080	0.4418175462284630	0.6455819813672444
0.5911527557025950	0.5428715016771839	0.3390093663727454
0.3489391388339750	0.6067500489512140	0.5430997125617811
0.6702835324234455	0.5823880834869933	0.5179022392602097
0.5202465674791092	0.6219365276617750	0.6442819444965150
0.5104722470502935	0.6840650638311866	0.4548630130804481
0.4271648557018282	0.3038378868063244	0.4749607037138736
0.4237899151489017	0.3248955719803214	0.4107630335955620
0.5378050358993360	0.2953753175363372	0.4663225245757088
0.5344449092439043	0.3165567152943286	0.4021467642275391
0.3397627008566159	0.4218134241825048	0.3878866952088260
0.3487170855491805	0.3655110519238315	0.5586139400062792
0.5925176642036558	0.3216271285464995	0.4363958790377502
0.3905624802328421	0.4084035177835701	0.3451204026337607
0.4027776946177720	0.3309714205322330	0.5800799188239059
0.3730398482654623	0.3383070857563290	0.4534655011378932
0.5817194839952632	0.3174646510148079	0.5660831702393685
0.5694930643835788	0.3948143321483872	0.3311018068988715
0.3611343567422544	0.4693744533133727	0.3446635435685698
0.3755207433011328	0.3788740246315346	0.6192928604846794
0.6364806677171909	0.3436538337715943	0.5362044994233016
0.4805141768344092	0.4515277050850179	0.2957845148902691
0.4983716530236269	0.3394324721207030	0.6363957746373209
0.6275999150125242	0.3999168973431002	0.3653834619415625
0.2946823122831502	0.5004989191344525	0.4523594615758120
0.3002820467561940	0.4657413912464448	0.5579054722175817
0.6216896328487169	0.3601661051555782	0.6000412056409807
0.6073019565242588	0.4505735379943928	0.3253789429996803
0.4710439928857199	0.3873007034296274	0.6756260235673714
0.4511206344914477	0.5124109774510851	0.2953475102324305
0.5382044523979288	0.3821305711049417	0.6703722805553448
0.5183391430585483	0.5072908687788384	0.2901587107809810
0.3159126078254910	0.5480087876988292	0.4091795734611366
0.3270289430074536	0.4791208992978427	0.6185858498690875
0.3011380025693967	0.5645753625593262	0.4730881915199061
0.3066479583000303	0.5297908035930774	0.5786782866522737
0.6985943419839087	0.4354420246479584	0.5267984621495909
0.6931787109315628	0.4702162051909033	0.4212778109536659
0.6841041903766413	0.4514600976457229	0.5907080611091534
0.6728376971375294	0.5208770297133177	0.3813724945678463
0.4816079101723839	0.4926880017323199	0.7095726800892602
0.4617005608997463	0.6177989038362918	0.3295185149438369
0.5486553806595653	0.4871549118367135	0.7047660772350983

0.3781850209018874	0.6397576780327305	0.3998581614306910
0.5288944011119177	0.6126977139558727	0.3242162278175932
0.3926739510182958	0.5493993088406691	0.6744620039336110
0.7055110823875371	0.4993890811136200	0.5471715403368459
0.6996014519848159	0.5342391294382429	0.4419878866251367
0.3723740309166269	0.6000562185202148	0.6344843731529788
0.3633576164842404	0.6563614069887527	0.4637000041465191
0.5190516611978392	0.5485467518040466	0.7043270255190462
0.5015575091981267	0.6605593401009376	0.3634794928458689
0.6405387720939290	0.5290816816202873	0.6576362814122837
0.6243731247955161	0.6210426965344711	0.3806641063460733
0.4181505115522729	0.6825371635592918	0.4338272511022004
0.4304257493801347	0.6051579608998127	0.6687791459757503
0.6631419760021797	0.5796458958826750	0.6118065858443601
0.4074232200026243	0.6782702208606769	0.5635162985246286
0.6511774807854629	0.6344308959589284	0.4412755285107541
0.6092591654257635	0.5938818500590596	0.6571836015575963
0.5971005510378409	0.6689014007677030	0.4198678349339370
0.4654508051090191	0.6833834978918433	0.5977585916084792
0.5140089835295365	0.6648679636590893	0.5183633906097925
0.6269900450116485	0.6619151508302780	0.5460487044923015
0.5758234878280947	0.6754212679418803	0.5891255480873491
0.5726838060428793	0.6959358683424666	0.5249405946396869
0.4790886566266069	0.2931209409092098	0.4330475744697966
0.3711725067220401	0.3619242350445898	0.3903011810132101
0.3778496141587362	0.3197963586758250	0.5182957784342217
0.5950052804088631	0.3032897806410240	0.5013703319861295
0.5882961591587271	0.3455088306152869	0.3732738841139596
0.3123655627460978	0.4835959488746116	0.3894434204773243
0.3233502802380067	0.4153010842057832	0.5965432255275945
0.4137644660464499	0.4568871468547088	0.3040003125878364
0.4313019771051732	0.3465059787255400	0.6393832737339805
0.5478138119990129	0.4466708593870792	0.2936122129757135
0.5654732359982454	0.3364002340958104	0.6288449336226641
0.2827882299461608	0.5165179099710071	0.5169105255556747
0.6745709337187651	0.3884736768865589	0.5691704469484784
0.6637778854191493	0.4568293319869520	0.3619906646249375
0.5107603472684747	0.4316834373179733	0.7071133698839681
0.4891298123467464	0.5681256155030601	0.2927282518824731
0.3252312918313389	0.6113494594774088	0.4307398025267560
0.3361833843459494	0.5431755834949917	0.6379743246916552
0.7170955788610849	0.4834957034406486	0.4828452582212613
0.4344630684876769	0.6636139310775818	0.3710855887251949
0.4520095696401766	0.5533720462630447	0.7062358639746461
0.6886657343395438	0.5149862706711235	0.6095053271303402
0.6765633245949416	0.5846765130960174	0.4034588932018720
0.5848194554967230	0.5423967615958133	0.6970591014323968
0.5686472971787101	0.6534748857158390	0.3605727124005940
0.4117151493447664	0.6544394762775722	0.6266530661595484
0.4049418273036334	0.6966800836131330	0.4985801540026151
0.6283646840594616	0.6397455861033156	0.6086431525018394
0.6220729917329391	0.6801154328174897	0.4814658429455241
0.5206560199570365	0.7068241270973170	0.5668669200085307
0.5408109599285714	0.2776176034921092	0.5309624656377498
0.5306860799231221	0.3406699979662025	0.3396343275172919
0.3211656631659312	0.3754172094604142	0.4326739855567862
0.3245477249918546	0.3541806021859156	0.4970522560284809
0.4214728949495689	0.3488903501591474	0.3482074959961294

0.5103360491383392	0.3915391564445046	0.2995708100547279
0.5258213279403783	0.2943220174759930	0.5951153193398826
0.4428848183380869	0.3966984878419333	0.3047950833001236
0.4315314281622795	0.2859616201743670	0.5394289902970052
0.4583042446195981	0.2994166621239563	0.6003996959333352
0.2915716202216496	0.4366192366144020	0.4322560127915187
0.2971276328434589	0.4022178109416199	0.5364555306320508
0.4758124681040075	0.3143218893140199	0.3697044261714268
0.2767391429956491	0.4531360402022150	0.4963752312908771
0.6489120933430466	0.3295002643168827	0.4717977405755853
0.4824000876682312	0.2725203665462936	0.4965674114368079
0.6456236005124256	0.3508074337531790	0.4074186001140853
0.3847600663398472	0.5171258884532804	0.3038800594290831
0.4043650354559860	0.3940644118671005	0.6779214973423399
0.3336884346655148	0.5305228688573422	0.3468801887129597
0.6890159250984470	0.3724408271637133	0.5059270280406758
0.6835990267101231	0.4067472783110150	0.4016455188939436
0.3501017217890295	0.4287083181441763	0.6564210949108608
0.5851638176709711	0.5018740857045566	0.2883018510009162
0.6047469731937631	0.3785972474344287	0.6623029330174112
0.7103665605589199	0.4201561620641102	0.4625913147027756
0.4443633616460096	0.4370449790448967	0.7120771321771008
0.4226586599615796	0.5731000688514558	0.2982586103235060
0.6597393640865441	0.4046033569652859	0.6323431259720556
0.6434897274838576	0.5069600198978084	0.3227267746203737
0.3401648200052697	0.5948197499602832	0.3676376871071239
0.3565040876811986	0.4930176754567191	0.6772036856875731
0.5771687818671044	0.4263456429117156	0.7017853989474333
0.5556225522926538	0.5629555773592811	0.2878383041426296
0.2895452088167306	0.5798632731638996	0.5373762722049376
0.3951596820036353	0.6210774769447595	0.3376710357039142
0.4148258425184483	0.4981388939284867	0.7116152238288876
0.3108865363958813	0.6275664490673531	0.4940399130346411
0.3163177289428422	0.5932468601079685	0.5983471259471481
0.6665192535532947	0.4683032623573125	0.6529530510950049
0.6498966372703454	0.5713113514102248	0.3435623289765747
0.6147859669477804	0.4819376110077929	0.6965417929301645
0.5955889039789999	0.6059700686746335	0.3220015718216096
0.7234153150489480	0.5468935255155194	0.5030862120960213
0.3543599723032641	0.6492131545215614	0.5925745778465510
0.3510221291661491	0.6705306694238634	0.5281414916213679
0.7090014758406237	0.5631550092979183	0.5668230130691130
0.7029043998785459	0.5978146711681623	0.4632679134342278
0.4741541961382583	0.7056448049906586	0.4048802899546435
0.4891669366049402	0.6086645514959137	0.7004744705757228
0.5561505519889278	0.6035015558078149	0.6956328500809084
0.5416148569711315	0.7005277915777960	0.3995875509924145
0.4690571725159062	0.6594394645971310	0.6603419531924090
0.4591561270222854	0.7223052834359730	0.4689736210433061
0.6790267354117474	0.6252161801236653	0.5663922981189636
0.6755719182231232	0.6459397504755371	0.5023998465402029
0.5777803384503043	0.6519450130862964	0.6516398476156245
0.5684067123164931	0.7139529710262947	0.4605399472940045
0.5237172473305041	0.6859454508996925	0.6302768759778570
0.5175419982937118	0.7273902347180840	0.5033988547713812
0.4860201505167908	0.2551080729217884	0.5601184205204592
0.4727388170620681	0.3379988259182559	0.3081997403222937
0.2736664342326631	0.3905049748207107	0.4759209920372803

0.7008108987210259 0.3580233405987059 0.4426990880721268
0.3572790872991477 0.5770044473145707 0.3064075537030501
0.3787229122434471 0.4429975051907664 0.7140309830406605
0.6426099769581162 0.4223548152769936 0.6936576017325188
0.6212957563664985 0.5570297030058260 0.2859121384051453
0.2991288559134871 0.6420136495356792 0.5573006910332376
0.7265450015629816 0.6095970419674522 0.5235321402795818
0.5267370251527380 0.6622982358113338 0.6918730569253453
0.5139480781635393 0.7448175635121472 0.4398821320706927
0.4965984638662760 0.4394840827513385 0.5148945339906956
0.6599844258049453 0.5784857749161767 0.6653021839699853
0.6768229069443930 0.5867699236062851 0.6826785623171516

OH/Cu_{309} $E_{ads} = -3.60$ eV
1.00000000000000
38.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 38.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 38.0000000000000000
Cu O H
309 1 1
Direct
0.4933226662740892 0.4600271516072375 0.4526985057536644
0.5001550048718599 0.5000375780861361 0.5001622132970771
0.4441734401596900 0.4729983775370850 0.4940949172790415
0.5497108777061583 0.4649144616910034 0.4859552670705488
0.4648390902363638 0.5191399185236811 0.4522966310032764
0.4701301746420857 0.4859186017099792 0.5529871283770839
0.5325130998248787 0.4188531460116036 0.5639781793581370
0.5300666527193405 0.5141334549822797 0.4472725285929746
0.4135339437795537 0.5552875328006981 0.4657731022804785
0.5561356788091677 0.5270575222541616 0.5062771389373494
0.5070003921133487 0.5400210299701934 0.5476622632731608
0.5036306562975552 0.5605324488916261 0.4853716271843177
0.4896737114974264 0.3975028499009393 0.4668973053666423
0.4361760570785254 0.4316459628574800 0.4456612290526125
0.4395294584681886 0.4107340424175753 0.5091239502478559
0.5471395620257651 0.4024750590611285 0.5007728081516027
0.5437483971786675 0.4234185132924941 0.4372996185621469
0.4572117221288511 0.4787205620070697 0.4030100072968499
0.4659857308032573 0.4239031793958191 0.5691300491220694
0.4071256174230454 0.4919366187980181 0.4451975666723372
0.4124974337746305 0.4580601399710936 0.5478538944803822
0.5237341857316247 0.4736206402305755 0.3978209726241262
0.5354719562672138 0.4809825348169934 0.5480365662384504
0.3924537877919861 0.5082832476470734 0.5083866083225143
0.5866570017306653 0.4447659798408292 0.5344600916431361
0.5812097056146858 0.4786254822196976 0.4317539802878942
0.5055105543123583 0.4661909558432881 0.6027925773430191
0.4946862172963545 0.5338585014751337 0.3974243978065368
0.4505121709073713 0.5351288872707005 0.5142719526134815
0.4189319558876498 0.5214375082606288 0.5684045474402797
0.6077038572903364 0.4918062633871693 0.4918827394378028
0.4676716620387665 0.5811484627897066 0.4362596147497862
0.4765139653684477 0.5264383296998730 0.6023648121797154
0.5932828957272042 0.5082657984608150 0.5552752543424685
0.5876386007168900 0.5419073313831747 0.4524437334203453
0.5432376744113304 0.5214689191375209 0.5974266194322327

0.5341402466586462	0.5760988996934568	0.4311274235642924
0.4565029676835266	0.5765057760544630	0.5628953179292516
0.4530776806063239	0.5974982583270710	0.4994081824317981
0.5643359511546805	0.5684283164701305	0.5549287632161890
0.5607821276130092	0.5892122386695959	0.4912695843748002
0.5106405677093214	0.6024339285127426	0.5334865794196408
0.4931019463811366	0.3780192225365466	0.5299900609897992
0.4864810383621149	0.4193828873950191	0.4045405939930297
0.3873535611260290	0.4455577229948632	0.4880285571275426
0.6000360127422878	0.4292318842537247	0.4715624797128908
0.4290085164571490	0.5385412154722284	0.4037136232679185
0.4396732248680109	0.4715724855439066	0.6066159121612535
0.5712012531431320	0.4614674674707820	0.5965306035002979
0.5604277357482406	0.5284430970066278	0.3935132001574416
0.4000745821743029	0.5707714009852887	0.5285748298384930
0.6129330447267456	0.5545619446018091	0.5125764663487307
0.5140727070525131	0.5806400982508728	0.5958189707610843
0.5071266122948628	0.6219237567347219	0.4703126233228052
0.4315299238159352	0.3678594117374415	0.4601239870173005
0.5408653789158551	0.3594338338523487	0.4516572780488228
0.3986032203553976	0.4504236696531073	0.3951614121191963
0.4074780445503358	0.3946475624523495	0.5640095729505228
0.5844452650966817	0.3811368235433937	0.5503098613054801
0.5754938850970461	0.4367890347724588	0.3814896398878342
0.4875051423701180	0.4928907097573966	0.3466241515706601
0.5019045007840337	0.4029233773110024	0.6198126663188003
0.3541555059471575	0.5281142849463271	0.4589211277741433
0.3596501135279040	0.4937303737473451	0.5632608760431502
0.6460454976938642	0.4719972183800328	0.5413213970129250
0.6404003907277371	0.5061847485168174	0.4368316176411955
0.5127220397067833	0.5072035926950382	0.6535885137366029
0.4981432906446838	0.5970745727774318	0.3803642612819963
0.4156964473241857	0.6188326872605591	0.4497901336366746
0.4245606398292353	0.5631140081790004	0.6185980096256389
0.6023408315351654	0.5502262745891426	0.6057258330374100
0.5925740288031720	0.6052846492051298	0.4362045954591887
0.4593053078275521	0.6404468353713590	0.5484687111271170
0.5688248742571999	0.6320243275994638	0.5403524580664814
0.4860071834081520	0.3349770822963246	0.4817218394737970
0.4826503749783930	0.3559455378783769	0.4182748839077266
0.4354916459475861	0.3483213741518224	0.5242797091259698
0.4287849968279251	0.3903796957829594	0.3968989798441391
0.5439393887013605	0.3399560783579689	0.5158533723178433
0.5372157420907486	0.3819948699396834	0.3884388075420858
0.3786780216034558	0.4036258165753714	0.4390891212672804
0.3819996347906380	0.3825143215404619	0.5030270019054389
0.3493598735830449	0.4643097313272714	0.4386848570579513
0.4500515211516533	0.4377403914333103	0.3538833550214612
0.3547563783979232	0.4301540236828500	0.5421261380119591
0.4621191572822297	0.3615806378372925	0.5847882259516514
0.5980724764911348	0.3659074186213976	0.4863162699924797
0.5946187618963750	0.3869681152856548	0.4223625515232501
0.5170289936001508	0.4325930406163204	0.3486944003560997
0.5291185407930229	0.3564644621566406	0.5795435465467990
0.3346012036065188	0.4807471462871705	0.5023501173098851
0.4209523266641290	0.4980336126867609	0.3534337796411802
0.4351229493591973	0.4089403965651969	0.6235660376471440
0.3704328087215166	0.5113702374750275	0.3959986561378453

0.3812306755908335	0.4433007933373967	0.6020795790821167
0.6378816501138339	0.4085307580676778	0.5202138449097243
0.6323858806141501	0.4425572146412178	0.4167169941411587
0.5543567740743243	0.4877771351521114	0.3430766505675216
0.5686166462918214	0.3986263401693974	0.6131955902488120
0.6233049290710740	0.4247162711336532	0.5834601198641362
0.6122901875511142	0.4927913211877846	0.3772314656613372
0.4749305328238383	0.4515528541138770	0.6574442668036201
0.4586605082164470	0.5535429644974289	0.3478160205211238
0.6590233029253604	0.4558478056080478	0.4772121669477661
0.3409961581062393	0.5440936567233927	0.5227921751306097
0.3768382775092233	0.5751512256099597	0.4166966160163478
0.5414307791847746	0.4463553431584472	0.6523647848969510
0.3876500266968204	0.5071206610425356	0.6227962909448066
0.5250955554797434	0.5484373237684629	0.3426388905518282
0.3621937612081896	0.5914469257209979	0.4798520809174646
0.3676153121585050	0.5573301294709906	0.5832825177826831
0.4314301110895752	0.6012220876438735	0.3869077860980180
0.4456202293374014	0.5121726384065355	0.6569527259753626
0.6297923304881708	0.4884875977051605	0.6042399966704706
0.6187374188335226	0.5566383332854290	0.3980612944377483
0.6655339634004604	0.5191955910578901	0.4979802719571370
0.5792003466001733	0.5018073217202982	0.6468542553973643
0.5648233801321136	0.5910418860597318	0.3765215236074974
0.6511247241816239	0.5361920489789257	0.5622678719384786
0.4054987974758403	0.6129130239819552	0.5776636103730044
0.6452920310487363	0.5697394081426109	0.4581379602558990
0.4020064293629418	0.6340274780135815	0.5136737299924509
0.4709571644765084	0.6434212736332844	0.4206155206961364
0.4832769070143941	0.5672911844678094	0.6515091570948296
0.5509855610215191	0.5626105923112447	0.6466315887081587
0.5379529185564955	0.6383633997005755	0.4154694922988570
0.4629836121086740	0.6178255445805431	0.6117033356125341
0.4562678743097357	0.6599444592244502	0.4843041547227107
0.6220573925328764	0.5966702430179298	0.5622289089178084
0.6182140714990773	0.6174201724170649	0.4972967612957617
0.5724424533720581	0.6097579281291179	0.6039870718953978
0.5647446881249131	0.6515401115299356	0.4760877263825760
0.5175875159166973	0.6439477441619799	0.5820242226402199
0.4623390858387421	0.7044531171895351	0.5336909510048744
0.4795670548951326	0.3782320278815367	0.3558457988058796
0.4894889175363029	0.3158028818225187	0.5451750538974175
0.3298685718245919	0.4177653263087515	0.4818920048293775
0.6509535096109296	0.3930912550918900	0.4568846429797598
0.3927524594272804	0.5581076089533789	0.3545267869055667
0.4087663134980826	0.4570217406427454	0.6608919672002402
0.6072968021965491	0.4415285445884815	0.6456278313734145
0.5911311048660718	0.5429186634510862	0.3391469317264446
0.3490889269290605	0.6068046698204786	0.5430677179643678
0.6704029193755845	0.5821264268373920	0.5181514850153969
0.5203841486501795	0.6217058043195403	0.6444482052211532
0.5106709480439001	0.6840655835544406	0.4550769129241499
0.4271430210363339	0.3039084038906103	0.4749690395644066
0.4237958694666819	0.3249142546227674	0.4108353631942571
0.5377655076950357	0.2953159746389410	0.4663208021839675
0.5343674840905237	0.3164985291464501	0.4021920083867493
0.3398460309993513	0.4219924301029460	0.3878867138866446
0.3487096606654428	0.3654990662608154	0.5585655994094388

0.5924289270329187	0.3215244110760231	0.4364237256203805
0.3905938458036762	0.4085824446594809	0.3451684267853554
0.4027188833101434	0.3309618452197619	0.5800724564795792
0.3730693179969068	0.3383393064802075	0.4535100483833625
0.5817102274948249	0.3172096321030495	0.5660363534096211
0.5693680257233346	0.3947729235820791	0.3311912707698154
0.3611175524308455	0.4695202188208447	0.3446061322170049
0.3754843249189253	0.3788215998870184	0.6192331439328965
0.6364640490658461	0.3433303030109446	0.5362062448338760
0.4804826617475592	0.4516035127921332	0.2958512878155668
0.4982304664851659	0.3392469647268300	0.6364424020354345
0.6274933429073880	0.3997895893354492	0.3654550792812178
0.2947607014233311	0.5006075308972914	0.4522991436439182
0.3003383625716233	0.4657262667708400	0.5577762394221054
0.6217251570967507	0.3598632141872150	0.6000773441999533
0.6071371783528359	0.4505524812079099	0.3254494987055328
0.4709325855757305	0.3870236084218537	0.6756693748180721
0.4511303777512156	0.5125618535842767	0.2953755192331758
0.5381394587145408	0.3819099645150928	0.6704569880370094
0.5182758435426639	0.5073768171386714	0.2902195019238854
0.3159757846174053	0.5481814852351405	0.4091322127247667
0.3270275553573285	0.4790301819422508	0.6184878368092438
0.3012238701923677	0.5646827547789829	0.4729815206400798
0.3067161635631058	0.5297803828127912	0.5784967351754645
0.6986997648488071	0.4350169600893655	0.5267910962972080
0.6931802591838662	0.4700416109490556	0.4213003208032703
0.6841853507970878	0.4510536123964797	0.5907114566090071
0.6727766468863230	0.5208183711017945	0.3814267663665974
0.4814374633565529	0.4923697751375644	0.7097254216778763
0.4617685531480374	0.6178797449232217	0.3295736154454763
0.5485135852791836	0.4868310450287093	0.7049218054777144
0.3782541084229619	0.6398608963817501	0.3999035349313836
0.5289046840407022	0.6127879808409130	0.3242953013178249
0.3926273870289027	0.5492774721771601	0.6744497064736812
0.7056554625597151	0.4988620721570128	0.5473356243995084
0.6995812263296495	0.5340408573730632	0.4420116174445969
0.3724170749836968	0.6000246728190732	0.6344012506083511
0.3634674408864458	0.6564642099002067	0.4636967087482722
0.5190262345076029	0.5481142552802772	0.7045606877781051
0.5016903264130654	0.6605892140868510	0.3636520943910695
0.6388694357983613	0.5287219943528803	0.6558876989976804
0.6243634365484152	0.6210184356266479	0.3807888023117195
0.4183177031216849	0.6825894870765540	0.4339840429820244
0.4303906658214058	0.6049990490128937	0.6687619342863451
0.6640533629693169	0.5763611157646198	0.6126174189288460
0.4075792016377935	0.6782501724942864	0.5634939487439562
0.6512651878268627	0.6343123610359548	0.4414513377847272
0.6089512516000039	0.5909544792951358	0.6589521218120287
0.5971867552409889	0.6688743539305321	0.4200608692009837
0.4655922780644995	0.6832891089031008	0.5978619639513023
0.5142604742769206	0.6648643208043032	0.5186203993841064
0.6272468447707341	0.6615716574642926	0.5467100258106955
0.5763232049040000	0.6750351378794054	0.5895348921992525
0.5729145318871042	0.6959797024742780	0.5251297930731669
0.4791627400642972	0.2931142067504073	0.4330907043224148
0.3712541712042813	0.3619831616716095	0.3904190449533115
0.3778357907896501	0.3198555561873094	0.5184011780757840
0.5949604855913747	0.3031129934853762	0.5013547171308959

0.5881909751813712	0.3453524918584759	0.3733262409910952
0.3124552901596616	0.4837419769474239	0.3894025217708122
0.3233254996311211	0.4151962367307070	0.5964772278622246
0.4137636264375308	0.4570125730482045	0.3040625623525069
0.4311903346613878	0.3463872582139580	0.6393745507999983
0.5477392955154693	0.4466638641038716	0.2936674089108821
0.5653849613955422	0.3361077999662743	0.6288478084376556
0.2828258477693555	0.5165532145378428	0.5168120289509212
0.6746670167990612	0.3880267565647584	0.5691547058997209
0.6636193562713469	0.4567179634975945	0.3619943060974580
0.5105829059386704	0.4313643494654952	0.7072590718795226
0.4891989370282000	0.5681801689177151	0.2927483910495459
0.3252568404546630	0.6114532773338263	0.4307661017906997
0.3361431613845378	0.5430936076788564	0.6378226831295963
0.7171937818840288	0.4831995450566930	0.4828736139158523
0.4345801205668369	0.6637014061591272	0.3712052546889218
0.4519327808136501	0.5531784783941183	0.7063352588436564
0.6883819232396650	0.5147384353696973	0.6103013860841371
0.6765537746625184	0.5846111622595731	0.4034902673478661
0.5854990541721149	0.5419303581326215	0.6969827309014389
0.5686499960090937	0.6535063784303944	0.3606739489760186
0.4117338537224324	0.6544105842410690	0.6266147089677101
0.4050761950372920	0.6967244245884288	0.4985789298304870
0.6298224117085627	0.6418779682904728	0.6097232681590178
0.6222306359116472	0.6799981945780396	0.4818273343605643
0.5210036068938063	0.7066755916783387	0.5670647464198187
0.5407437257807667	0.2775239483527318	0.5309835917735114
0.5305962169985435	0.3405819174305293	0.3397504259453344
0.3212099010771786	0.3754885149664730	0.4327198298545906
0.3245623162066554	0.3542394750318683	0.4970180972025543
0.4215096948110225	0.3489273050937594	0.3482795410480878
0.5102746686874177	0.3915591420678880	0.2996037896327484
0.5257710561775745	0.2941595365337025	0.5951411830281974
0.4428716424894081	0.3967387728918715	0.3048648753248676
0.4314810919127065	0.2859942103520294	0.5394634409643919
0.4582674209577461	0.2993473318578154	0.6003994352564935
0.2916378769273866	0.4367004365488855	0.4322256049129066
0.2971774234296070	0.4021719317918785	0.5363998799106211
0.4757587022378530	0.3143406777025930	0.3697482153378699
0.2767634052291802	0.4532030016050961	0.4962810038073598
0.6488740209274605	0.3293227097107337	0.4718124328679935
0.4823890569198200	0.2725197043519950	0.4965668780310115
0.6455038954476892	0.3506475348569107	0.4073399223726025
0.3848181778146672	0.5172721252883239	0.3039351921769886
0.4042993102986065	0.3939361133206221	0.6779074711065403
0.3337813610814225	0.5306697335359368	0.3468821189953094
0.6889967783891020	0.3721471330878336	0.5058558742115148
0.6835097939109716	0.4065744846166896	0.4016262750911446
0.3499495088239734	0.4286275165559183	0.6563060399556310
0.5850881041321940	0.5018768214972414	0.2884296106014606
0.6047198872192884	0.3783407227311839	0.6623532416860639
0.7103378430038738	0.4199432300669968	0.4624843477168082
0.4441749884381206	0.4368194774367385	0.7120564578243703
0.4227290262481466	0.5732625565530038	0.2983234651261473
0.6597561805779827	0.4044157337440605	0.6323994595420007
0.6433750563052796	0.5069379921538039	0.3228054987723523
0.3402743446918076	0.5949667065158010	0.3676393690831187
0.3564060451677434	0.4928893871061460	0.6770975222455820

0.5771456357013318 0.4261835414382451 0.7018451027662518
0.5555738069614535 0.5629793058147173 0.2879509937340849
0.2896691500765516 0.5798767990009260 0.5373001510894397
0.3952316135084695 0.6212920540533512 0.3376863297980350
0.4146494468940863 0.4980056963995457 0.7115507277769184
0.3110107131623754 0.6276058181771602 0.4939898768180763
0.3164009856321279 0.5932393510672090 0.5982332909187622
0.6665100742581493 0.4682960298135926 0.6531611743945631
0.6498559212670859 0.5712757672594474 0.3436391482604170
0.6149417166008134 0.4818900849253064 0.6965710842283959
0.5955199145559391 0.6059811294954188 0.3220689944645053
0.7235774015159907 0.5465137726325989 0.5030719097702412
0.3544552809021546 0.6492101828773408 0.5925163971213627
0.3511140647075690 0.6705461434285912 0.5280670103350168
0.7094560743059564 0.5624283103428829 0.5667652899411375
0.7029725862805485 0.5975733461033439 0.4632758656320668
0.4742695377550212 0.7056553898040430 0.4049949770701442
0.4890165747689956 0.6083968866178598 0.7006652595239679
0.5558169775879458 0.6030166448612637 0.6961684919690996
0.5416883882120950 0.7005144550655126 0.3996822301726303
0.4689743815650191 0.6592659143130254 0.6604206302610299
0.4592863938800110 0.7223079804091626 0.4690551766185618
0.6796009665240101 0.6246571070083710 0.5658531674541954
0.6757140529211642 0.6457464169608171 0.5026204301717719
0.5770184341740461 0.6517906012018964 0.6521453132420753
0.5686363296111783 0.7139236569710918 0.4606983561767677
0.5238350585129472 0.6857935819369544 0.6304579162626193
0.5177242277108624 0.7273890971098375 0.5036103930227780
0.4859400300319707 0.2550495878027295 0.5601012670039964
0.4726978137354770 0.3380257059073347 0.3082347864598153
0.2736813481402059 0.3905797775334656 0.4758679999189543
0.7007306436743722 0.3577882684769895 0.4426083900899042
0.3573994187910884 0.5772183493956322 0.3064485145184652
0.3785282153313190 0.4428475459484998 0.7139424513960131
0.6425925910288428 0.4221646841686503 0.6937101599373355
0.6212348549566936 0.5570263492625572 0.2860107132922901
0.2992478295087261 0.6420311107591563 0.5572479294037992
0.7269121479860025 0.6090477265387265 0.5233615028773883
0.5263395543574588 0.6619706271832461 0.6922576006561189
0.5141362710063624 0.7447864274373176 0.4400679997914076
0.4966587009763854 0.4394867487552648 0.5149711944869041
0.6558428205315943 0.6144841667980989 0.6490593421159394
0.6726843672805145 0.6223520157108183 0.6666708060501301

OH/Cu_{309} E_{ads} = −3.57 eV
1.00000000000000
38.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 38.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 38.0000000000000000
Cu O H
309 1 1
Direct
0.4932522445886644 0.4599787056640759 0.4525564640923667
0.5000518418330295 0.5000736425178588 0.4999589300524910
0.4441397199486339 0.4729889491636714 0.4939889741787471
0.5496111105227962 0.4649235883695547 0.4857580555005987
0.4647515805528972 0.5191145722627846 0.4521285149677156

0.4701463701154320	0.4860585596080315	0.5528708309607776
0.5325376139458806	0.4189823086140479	0.5638385967309762
0.5299208267870722	0.5140690038595798	0.4470102010596933
0.4134866352544065	0.5552289369976472	0.4656449525492686
0.5560063770542140	0.5271170284937288	0.5058521433739513
0.5070463256726807	0.5402161399223498	0.5473394938568731
0.5035285996637691	0.5606012716564204	0.4850952167934401
0.4897262073694117	0.3975253596513389	0.4668259404074839
0.4361170544194125	0.4316114517967773	0.4455567738645499
0.4395524201629792	0.4107715074108198	0.5090291342689015
0.5471665405044238	0.4025914875139715	0.5006838472006673
0.5437664614335215	0.4234471774454587	0.4371875446951471
0.4572459049597597	0.4786681101548599	0.4028514376754398
0.4660446041792740	0.4240458277575762	0.5690333103070973
0.4070799668251984	0.4918658541113651	0.4451069910483003
0.4125756410475050	0.4581326631515079	0.5478320617056956
0.5237236942236078	0.4735098480948293	0.3977055559304186
0.5353925759543665	0.4810691796773581	0.5477901372751552
0.3924804817210440	0.5082682202769293	0.5083300432174357
0.5866753325162629	0.4449660484988880	0.5342793565345330
0.5812699559995169	0.4787089110285613	0.4316498837975517
0.5055073417183391	0.4663546715796499	0.6026567854300034
0.4946112353245649	0.5337979517474798	0.3972343931310343
0.4504694012118934	0.5351710588138842	0.5141650886890448
0.4189044428249402	0.5215112333182079	0.5683607753562455
0.6076089245955887	0.4918723664632298	0.4915844501721581
0.4675658983390505	0.5811127039548490	0.4360239068826711
0.4764156321366695	0.5265920672540298	0.6021607483382794
0.5930538973591816	0.5083564236991194	0.5547999970172452
0.5875217449450777	0.5419927224155708	0.4520830765854066
0.5429957161914843	0.5215565632119765	0.5970235372372633
0.5341122685713827	0.5760952700893385	0.4308952065071442
0.4563646816153203	0.5766600627838254	0.5627130864851462
0.4529554166883489	0.5975339337075263	0.4992668826857321
0.5645031981428112	0.5687126717456306	0.5542999162062144
0.5605981147695611	0.5893734171599807	0.4909222103628184
0.5104979153345929	0.6026330022007413	0.5331043145995478
0.4931112518086845	0.3781229665811905	0.5299105020511357
0.4864073016111462	0.4193119316560361	0.4044769275463100
0.3873826796720819	0.4455370651378462	0.4879706404566090
0.5999647841547767	0.4292388707492758	0.4714094770723454
0.4289079436532888	0.5383889914945116	0.4035800793060147
0.4397146822057101	0.4717121431715693	0.6065678615262614
0.5711266123040241	0.4616675537094604	0.5963474002474799
0.5602550607168890	0.5283262315754965	0.3932618479551822
0.4000289620271567	0.5707778825150746	0.5285044713138290
0.6128827957721698	0.5547689056902509	0.5120375502112585
0.5136536213737668	0.5807976923896161	0.5954286380583539
0.5068795476875817	0.6219999332064968	0.4699608776268620
0.4316082600681924	0.3678251246181531	0.4600842131692128
0.5409939785129871	0.3595605684219495	0.4516388588809533
0.3986316374141978	0.4502600069934264	0.3951003493698447
0.4075806560721974	0.3947467339994563	0.5639914631095287
0.5845107871242667	0.3813381653961551	0.5502539996496413
0.5755691639924136	0.4368073894382482	0.3814147780703716
0.4876489031663552	0.4928795398839867	0.3465305910656415
0.5020553599631032	0.4031175217636452	0.6197198025117719
0.3541409761165348	0.5281195348046652	0.4589153339709455

0.3596664048154740	0.4937975304586032	0.5632988637488432
0.6460174934525520	0.4721139609835426	0.5410162639395235
0.6405074401278090	0.5063882636212496	0.4366796912536269
0.5125492244948162	0.5072656447328043	0.6534016032580653
0.4980899911713029	0.5970139658936700	0.3801588684741457
0.4156431112506341	0.6188009393174724	0.4496683202353619
0.4245818884851710	0.5633326779309480	0.6185485894047862
0.6015507892123522	0.5500292260221599	0.6048097355774386
0.5925690726627649	0.6053915724710854	0.4359218482672211
0.4591352545089634	0.6406113605945533	0.5483179469688431
0.5685675584971974	0.6323086163852236	0.5398898611975312
0.4860765978573267	0.3350283927877201	0.4817136765173330
0.4827032975774376	0.3558724082856167	0.4182880835455338
0.4355591402221987	0.3483958553664386	0.5242659222605142
0.4287683714041972	0.3902340735076774	0.3968137795679754
0.5440052626572259	0.3401312837270944	0.5158827589368040
0.5372290872802724	0.3820174458921599	0.3883655822265316
0.3786424326647110	0.4035127591996817	0.4390453613151871
0.3820561727326702	0.3824995126828948	0.5030347472313470
0.3493547027410159	0.4642033257663066	0.4386536678776287
0.4500245928787002	0.4376453154035749	0.3538005513878223
0.3548841731682021	0.4302025638069657	0.5421070719109401
0.4622846952365868	0.3617632517369448	0.5847565436663897
0.5981417269859689	0.3660327241639388	0.4862834253234171
0.5946939190012854	0.3870079545625993	0.4223037253385802
0.5170575837179194	0.4324445539316502	0.3486217065764841
0.5292560034202697	0.3566783564617642	0.5795255574071837
0.3346470976638941	0.4807053310673908	0.5023410283424857
0.4209066641077159	0.4978528659723540	0.3533454178508311
0.4352588919037317	0.4091097371762766	0.6235237878886012
0.3703686907679696	0.5111985675429888	0.3959456725601455
0.3813376250707117	0.4434511572588166	0.6021394765745588
0.6379299603809669	0.4087412337967558	0.5201079357144489
0.6324633921167400	0.4427016044864860	0.4166655387971648
0.5544009511070380	0.4876471744353498	0.3429288651589791
0.5687514893899768	0.3989417794353828	0.6131431581153775
0.6233008476553462	0.4250632454753494	0.5833407217706948
0.6123603874610773	0.4928335143563263	0.3771388114340504
0.4750063438504309	0.4517322747740009	0.6574117498455800
0.4585768116007990	0.5534506598143520	0.3476697427091365
0.6589662601296393	0.4559446321207844	0.4770538040329334
0.3410070991853821	0.5440836196607562	0.5228826810035841
0.3768047960112034	0.5750545046853048	0.4165927644360447
0.5415100090960723	0.4466253357325745	0.6522449234991036
0.3877314311495371	0.5073014443503245	0.6228257002076700
0.5250819856031289	0.5483936403624918	0.3424436195173644
0.3621868779615015	0.5914305495073361	0.4798210667724539
0.3676227692681535	0.5574212224573304	0.5833376387059739
0.4313435885217025	0.6011094385865797	0.3867439067567487
0.4456609441204352	0.5123799473316795	0.6569327757705610
0.6295973109412609	0.4888760946017686	0.6039800379458263
0.6185861634465482	0.5565844596274727	0.3976775326375824
0.6654526581045789	0.5195831154428451	0.4975591736781944
0.5791646678059232	0.5022258984470773	0.6465872505091388
0.5648654913726749	0.5909671964502211	0.3763830446840541
0.6506312714102767	0.5360388694747400	0.5612553563377752
0.4053396433397001	0.6130410087600109	0.5776220597740607
0.6452840771057159	0.5698929696819910	0.4578405420454901

0.4019559074824976	0.6340408224838213	0.5136811433746684
0.4708062232630031	0.6434228217566991	0.4203113730251469
0.4830056295979580	0.5675850771726084	0.6512978793666961
0.5500493228062162	0.5625010736875485	0.6461447019865857
0.5377763965964399	0.6383581092881084	0.4151114605683836
0.4627985130595170	0.6180888478385055	0.6115328739471774
0.4560435355465607	0.6599959000567677	0.4840327739273098
0.6229517390899547	0.5973595454948530	0.5610235636133806
0.6179583595044560	0.6176000890817278	0.4968942345323055
0.5711822192778878	0.6098355056221960	0.6030974939428146
0.5643471982274025	0.6516978640984149	0.4755751762333317
0.5173456694867921	0.6442595395702120	0.5816783021370291
0.4621510571164956	0.7046523700143457	0.5334976176185189
0.4794911445617931	0.3781381184093252	0.3558114136423686
0.4895650032618208	0.3159485746690798	0.5452011968675152
0.3298955943428658	0.4176968178392413	0.4818275632459610
0.6509981670666155	0.3931935180358044	0.4568564656501110
0.3926248931815068	0.5578908437338064	0.3544177450757268
0.4089253083432041	0.4572383469201609	0.6609424224157562
0.6074028098436638	0.4421239067786708	0.6455150435382092
0.5910189544820357	0.5427545440261458	0.3388481384101322
0.3489947228457950	0.6067957972105834	0.5430824726573784
0.6705610826375329	0.5832290978844572	0.5186440168295947
0.5204017741077384	0.6219334387563094	0.6441716168133705
0.5103801338788432	0.6841768604904136	0.4546331048617345
0.4272045394692517	0.3039075696886424	0.4750197341408081
0.4237859864094596	0.3249822299899112	0.4107614216631821
0.5377630685870688	0.2955111504414913	0.4664300297420181
0.5343671073475641	0.3166244695424977	0.4022078787344452
0.3397333044129934	0.4217877408179886	0.3877685718265547
0.3488477785193733	0.3656410018055661	0.5585538705216528
0.5925939067413493	0.3216271364280503	0.4364389732519979
0.3904596682656593	0.4083377081799591	0.3450584570274325
0.4029624138541255	0.3311541814178385	0.5800679468288439
0.3730832012270097	0.3384183571085443	0.4534700115233829
0.5818473488248250	0.3175689660019996	0.5661455162651885
0.5695006742411357	0.3947487121623772	0.3311600558376903
0.3610376854210650	0.4692992780628811	0.3445558551859534
0.3756439436579597	0.3790303937874939	0.6192882301699054
0.6366738985650024	0.3438040254313594	0.5362328563676358
0.4804850698577420	0.4514361030108464	0.2959245433611707
0.4985231525948450	0.3395497737624337	0.6364434596839157
0.6276263193371661	0.3998993207131964	0.3655061977134933
0.2948630491650113	0.5004836700491767	0.4523486758872124
0.3004434628995625	0.4657672123810860	0.5578629005589782
0.6219255486271155	0.3603711651995934	0.6001627860827691
0.6073309394652469	0.4506033982868672	0.3254786061032621
0.4711632169728601	0.3874568986699171	0.6756745619930850
0.4510438173694125	0.5123085713507484	0.2954449466224392
0.5384344298296266	0.3823126082490966	0.6704759323400455
0.5183559040017808	0.5072224497858565	0.2900811176230412
0.3160605105884805	0.5479839037040889	0.4091374762616490
0.3271784244076692	0.4791785623424232	0.6185936959685056
0.3012428245580593	0.5646048533494484	0.4730885651659349
0.3068178490535083	0.5298751957497101	0.5786914460280366
0.6989245496984685	0.4355776578834736	0.5268149489235747
0.6933242115007932	0.4702396090913773	0.4212800018767495
0.6840877275082858	0.4521011523942514	0.5907703415670279

0.6729607956116168	0.5209461727315746	0.3813257052996969
0.4817169454067772	0.4928349244540094	0.7097900139068309
0.4616404389825468	0.6176997790233189	0.3294010895740956
0.5489714386309993	0.4876754423826892	0.7045682148976543
0.3781901655882554	0.6397029980021128	0.3997521086390854
0.5289182896277012	0.6126034008388208	0.3241800207868415
0.3927480971239953	0.5494939028174565	0.6744537511843384
0.7053282688351409	0.4996454481509742	0.5473467568986012
0.6996850609238037	0.5342863731772989	0.4419457235009534
0.3724496568596473	0.6001424246771193	0.6345017702162756
0.3634353271582131	0.6563340390549233	0.4636937321003226
0.5195317518365223	0.5486150009176274	0.7040830569618950
0.5015131169190973	0.6605527832830689	0.3633594886672490
0.6389796344453765	0.5307905735780276	0.6554106154519166
0.6244660793822265	0.6210223430023492	0.3804698428457973
0.4181872383630629	0.6825446269611225	0.4337170658428641
0.4305541350736735	0.6053353699635315	0.6688313489980109
0.6602892831141811	0.5782648328487469	0.6122264735683628
0.4074530265301729	0.6784287089671854	0.5635230322521655
0.6513246472265776	0.6342795510274992	0.4408968239631579
0.6094864805887196	0.5917911052167046	0.6551084651999540
0.5970903375408722	0.6689744301453068	0.4196525224189707
0.4655792141376755	0.6835242036492460	0.5977735757619832
0.5139334613733210	0.6651031141377775	0.5181728499306389
0.6267741608725266	0.6616778805887108	0.5462549031056272
0.5760910273019937	0.6752470668993595	0.5892382880788501
0.5727533911177679	0.6962299158388753	0.5248455180046738
0.4790835516335953	0.2931147757082250	0.4330864272002549
0.3711010740636606	0.3619851825109958	0.3902124511658449
0.3778996138738207	0.3199207116194726	0.5183137920670505
0.5950693282526763	0.3033602434424155	0.5014239794163018
0.5882541045535049	0.3454515567632224	0.3733019250132000
0.3124526094338046	0.4834992380216931	0.3893714927679324
0.3234987806055502	0.4153750005536875	0.5964992786962326
0.4136482293273615	0.4567818416200377	0.3040147664384393
0.4314207761536607	0.3466271760776595	0.6393980474174649
0.5477983526730553	0.4465154095751122	0.2936373460825031
0.5656209164776479	0.3364490936215173	0.6289131029442779
0.2829513356283225	0.5165254339444351	0.5169005950044540
0.6748175842223328	0.3887623841131360	0.5692507975873380
0.6637882270050272	0.4568242250968620	0.3619966402161393
0.5109563513529732	0.4319831849200795	0.7072648848644004
0.4890819860453934	0.5680563953347522	0.2926156970556095
0.3252725437460436	0.6113762263919088	0.4306860859212090
0.3362162838047362	0.5432372478604650	0.6379815167445326
0.7169954725590687	0.4838360045403214	0.4830509944809232
0.4344292315446892	0.6636122044306885	0.3709421339877129
0.4522123219262521	0.5534462293785805	0.7062880606799117
0.6875125063849966	0.5164972016614936	0.6105926020365513
0.6765651226643017	0.5846277066514439	0.4036080294272110
0.5863386366977099	0.5432532713653268	0.6959618542864481
0.5685879423114004	0.6534276473884980	0.3604123486619593
0.4116914895894614	0.6545896088218492	0.6266364578615969
0.4049596399729314	0.6967320605948598	0.4985168094649235
0.6283950832455351	0.6382143701920541	0.6101032309485342
0.6218428899338593	0.6802849112298271	0.4813040533920710
0.5208480223916445	0.7070088323962628	0.5668257992112353
0.5408294470935929	0.2777455196232512	0.5310490435207575

0.5306284250777117	0.3405770295650229	0.3396427880655729
0.3211056964963952	0.3754036966069277	0.4325662539648424
0.3245893062198718	0.3541762060738138	0.4969878232046397
0.4213499125493188	0.3488097048869445	0.3480895659499909
0.5102905665643058	0.3914127180791009	0.2996169202392458
0.5259136987748091	0.2944289709497313	0.5951794341672666
0.4427795229176660	0.3965745587942363	0.3048417921634787
0.4315743356813704	0.2860267993609303	0.5395311146271748
0.4583891521722078	0.2995055316287419	0.6004216276422155
0.2916074128959383	0.4365695078040514	0.4321434021641100
0.2972316970790138	0.4022402813739095	0.5364086661676432
0.4756961510699730	0.3142816158976132	0.3697243912831121
0.2768612001823406	0.4531625107626315	0.4963016280921582
0.6489508388953766	0.3294314417786882	0.4717753183106489
0.4824430421828527	0.2725643110723613	0.4966473033404045
0.6455878366508703	0.3506677454962943	0.4074372609078202
0.3846617709724262	0.5170533767570963	0.3038513445130684
0.4044686947524017	0.3941829488265050	0.6779358182024005
0.3336527268073781	0.5304635886888013	0.3467633219362020
0.6890905247013986	0.3725272490206128	0.5059135585205586
0.6836282791620678	0.4067181131599843	0.4017061922078348
0.3501330581056910	0.4287440032100747	0.6564132972302071
0.5850960227965157	0.5017923013736012	0.2881905780139538
0.6049257790931254	0.3789470562931777	0.6623783267908432
0.7103945157841643	0.4202686879133749	0.4625675440809618
0.4444658726044082	0.4371581587777389	0.7121035447458492
0.4226234454334662	0.5729892568744436	0.2981740037791247
0.6599440698092759	0.4052751578634490	0.6323569773390049
0.6434185793396549	0.5069769621069584	0.3227008549784904
0.3401048742250550	0.5947657102702885	0.3675584947189441
0.3565646365821971	0.4930948694997526	0.6772325174574999
0.5774292548383368	0.4269888333881239	0.7017662867689287
0.5555414345089453	0.5628340092578065	0.2876232962254914
0.2896065194633903	0.5798992469220524	0.5374010369373549
0.3950985508273879	0.6210391563812822	0.3375546987516133
0.4148634371513760	0.4982738920439023	0.7116118938368936
0.3109563361183075	0.6276142706908200	0.4940213602829432
0.3163713316697954	0.5933270271758270	0.5983432032846880
0.6663164201674546	0.4695920526504588	0.6531034476118697
0.6498861504729663	0.5712435709495631	0.3435577997764096
0.6153274564904647	0.4829656593194339	0.6960686164906021
0.5955341158070003	0.6058034320939947	0.3219026960917042
0.7231782433392293	0.5480029132619380	0.5034338579773074
0.3544056960580064	0.6492929917175561	0.5926021222859728
0.3510723331594635	0.6705277365311370	0.5281642900309212
0.7081636465916337	0.5624902850956247	0.5675986333586073
0.7033980792676046	0.5975990980981072	0.4644345387679693
0.4740373114581064	0.7056840586308639	0.4046471946088895
0.4896064591792897	0.6085948882783361	0.7003620595184865
0.5570488894895576	0.6034443897827790	0.6951954993799896
0.5415519011781926	0.7005601549916138	0.3993945175674447
0.4692355266823955	0.6594511347960613	0.6603510333895940
0.4591327950760517	0.7223886486613140	0.4688013741574477
0.6800772336905014	0.6275666878862325	0.5701817615981774
0.6746201161098941	0.6459792816198379	0.5013299470128276
0.5784484697225772	0.6512666398160569	0.6519160343025276
0.5683346675069696	0.7140478475311639	0.4602753666889755
0.5241036163573357	0.6858069880281951	0.6302576692264082

0.5174934324022616 0.7275090162472688 0.5032164842980631
0.4860538825484911 0.2552147398084080 0.5602047269782426
0.4725968841587993 0.3378920874708817 0.3082515235335487
0.2737176929972311 0.3905488539069275 0.4759216210799285
0.7008373444006606 0.3579805827539449 0.4426870400689329
0.3572174774583645 0.5769328228924527 0.3063619371657186
0.3787845165285035 0.4430645020490561 0.7140304475097420
0.6427952760382605 0.4230599886453836 0.6935652277513511
0.6212339647963530 0.5569318841898606 0.2858157272628404
0.2991810065405024 0.6420441950476888 0.5572888873058371
0.7279396282709798 0.6102980865618505 0.5243672435704397
0.5271401953611382 0.6621371292749006 0.6917763570906837
0.5138717337881131 0.7449070516040596 0.4396079584960513
0.4966238648580949 0.4395506760725678 0.5148400184714579
0.7286966364974491 0.6445096625635179 0.5629545176228183
0.7447362139745676 0.6396632216514161 0.5823349227452370

OH/Cu_{309} E_{ads} = −3.54 eV
1.00000000000000
38.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 38.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 38.0000000000000000
Cu O H
309 1 1
Direct
0.4933975130641834 0.4599959094332662 0.4527199542326617
0.5000642201321485 0.5000342558595846 0.5002063883563674
0.4441026048128238 0.4729761310603079 0.4940824613858465
0.5497063164492675 0.4649387519456061 0.4861019113554243
0.4648218020903843 0.5191204624923670 0.4523104248253336
0.4699954188820576 0.4859026685685586 0.5530205227343200
0.5323967191714479 0.4188395598185669 0.5640083361791702
0.5301384143966317 0.5141450814299927 0.4474113246288180
0.4135333919341148 0.5552832817585169 0.4657440541261900
0.5560606883037837 0.5270946221978292 0.5064842304434601
0.5067385088770512 0.5400236560248688 0.5477241095439895
0.5035224646424812 0.5605297944209576 0.4854295453972350
0.4897520421782794 0.3975339523221806 0.4668702648873536
0.4362733938076864 0.4316724965034918 0.4456076336714995
0.4395173482325971 0.4107158764928620 0.5090180740118118
0.5471555327907394 0.4025300070527565 0.5008101875363121
0.5438930475611323 0.4234881656626910 0.4373922428963323
0.4573783528202758 0.4787024078163809 0.4029910560707429
0.4658527510699679 0.4238914060715852 0.5690777152581536
0.4071369772167049 0.4919421294131572 0.4451745639502034
0.4124117970821108 0.4580613376302844 0.5478155494309829
0.5239237941769945 0.4736460285578617 0.3979579428918646
0.5352848316747411 0.4809528840968520 0.5481406789631341
0.3923848755543709 0.5082792323005713 0.5083314473103401
0.5865324090280545 0.4448118423230513 0.5346350000141943
0.5813835750975164 0.4787135631445038 0.4320131046886262
0.5052862904051804 0.4662113440403408 0.6028419002958787
0.4948297097154555 0.5338455814080916 0.3975251310554902
0.4503779735127916 0.5351294691562145 0.5142890999301207
0.4187158075235547 0.5213947665102208 0.5683894325817092
0.6076858791808731 0.4918534499336897 0.4922354409412244
0.4677095979270715 0.5811586578052289 0.4362704212087044

0.4762113130818337	0.5263867453943264	0.6024131488797806
0.5932016615221362	0.5083030332201888	0.5554913003971060
0.5877100944079301	0.5419905204149705	0.4527905446404640
0.5430155397922798	0.5214825503677678	0.5973885276857789
0.5343009760192409	0.5761029394266228	0.4313134325004957
0.4561821444385594	0.5765798052222008	0.5628944709838020
0.4529443093875831	0.5975199495375930	0.4994201068526660
0.5641249145521821	0.5684530770048681	0.5550518581503937
0.5606337320412601	0.5892533067058804	0.4915330159678272
0.5103567747272858	0.6024680460708487	0.5335076313853003
0.4930836245168475	0.3780214199406563	0.5299462838374860
0.4866491904366472	0.4194232973316092	0.4045661863810981
0.3873993539480458	0.4455754314415861	0.4879828133771086
0.6001053039900758	0.4293341374211703	0.4717204572926573
0.4291073307449573	0.5384890783128883	0.4037155984648383
0.4394270819258773	0.4715646085537705	0.6066442846358215
0.5708896455014867	0.4614415305102345	0.5966924964924584
0.5605893832349909	0.5284327272157400	0.3937403538066933
0.3999442370795318	0.5707939947323161	0.5285863379210467
0.6129381972667790	0.5546070839437820	0.5130062357189604
0.5133120206150091	0.5806227011021079	0.5958358061881798
0.5070467055704789	0.6219473128862512	0.4703567455237310
0.4315794774046233	0.3678819641112037	0.4600248654625408
0.5409913220165157	0.3595100393884306	0.4516318460609817
0.3987919065641864	0.4503889856268498	0.3951256526932735
0.4073794117628231	0.3946469159915802	0.5639229092047714
0.5843255409402427	0.3811379353558312	0.5504060458269824
0.5757557845188105	0.4368958049512133	0.3816670776077588
0.4878406522974354	0.4929721787319220	0.3466726397732275
0.5016569180811580	0.4028018109123226	0.6197422612510433
0.3541591378889489	0.5281295510064136	0.4588852111577089
0.3594796896629740	0.4937405593488185	0.5632311518525418
0.6458942200167933	0.4719673475429298	0.5417184593123913
0.6405992805719963	0.5064158039679432	0.4373688658329193
0.5120331025890708	0.5069484776978168	0.6536106605488275
0.4983443564799835	0.5970753855914914	0.3805049126314780
0.4156989913986188	0.6188503109428674	0.4497516034911964
0.4241762483563770	0.5631666759810684	0.6185855412769599
0.6019994672424605	0.5500192826966437	0.6057395056533469
0.5927832949278661	0.6053202335007872	0.4366335892314110
0.4590180679488903	0.6405333111310783	0.5485325924818443
0.5684995481909187	0.6321352601244949	0.5405607473017574
0.4860815358746019	0.3350269136472976	0.4816763489871561
0.4828691075739140	0.3559765346034084	0.4182411280352205
0.4354725203810714	0.3483330306518754	0.5241965486350977
0.4290140912915818	0.3903878319412730	0.3968039487389975
0.5439467047998188	0.3400280484193542	0.5158569237208038
0.5374615167002680	0.3820727019960157	0.3884742723555963
0.3787795434520435	0.4036310643248016	0.4390272031924630
0.3820213573228516	0.3824773633121655	0.5029438544944151
0.3494344094921198	0.4643344041348926	0.4386160598181489
0.4503172963960494	0.4377781415009362	0.3538421616973901
0.3546862871468069	0.4301566929230935	0.5420531830304997
0.4620204890890692	0.3615600957258914	0.5847050302597476
0.5981059224264162	0.3660209317099185	0.4863490591126498
0.5948570263869396	0.3871142093220057	0.4224821173985647
0.5173147905330042	0.4326601586225577	0.3487570732198291
0.5290186426013009	0.3564167544142732	0.5795565648398456

0.3345473418974914	0.4807631340048373	0.5022762779223937
0.4211936921539634	0.4980247853338182	0.3534052907702135
0.4349325588265369	0.4089139615947268	0.6235072137235794
0.3705658315134981	0.5113758935008371	0.3959387218317680
0.3810673396267475	0.4433286871495138	0.6020651661962324
0.6377919271313336	0.4085591261999145	0.5204819185791040
0.6326692872418374	0.4428162298874352	0.4170469913847474
0.5546922596141630	0.4878453201285583	0.3432550491260852
0.5683647331413462	0.3985762140176826	0.6133464572007785
0.6229900717298369	0.4246841858577256	0.5837343833458688
0.6126160690124806	0.4928779294398721	0.3775771866474153
0.4745294868746245	0.4514312209800609	0.6574891290239578
0.4588756312845413	0.5535608440244515	0.3478893712608889
0.6590965595205339	0.4560602952234849	0.4776921643090168
0.3408858881840139	0.5440732936956084	0.5228222769162345
0.3769561900131851	0.5751673059358564	0.4166334534773681
0.5409329601520305	0.4461218851079130	0.6524583754849663
0.3874238884171121	0.5071711377595581	0.6228017199804801
0.5253929048308251	0.5484308369078272	0.3428178792714947
0.3621898760279836	0.5914573766081320	0.4798426028923852
0.3673799434250651	0.5573601455041213	0.5833044557851488
0.4315650924348905	0.6012467763234405	0.3868928968096287
0.4451678219032577	0.5121582181810571	0.6570491978778783
0.6292681355154384	0.4884394555156125	0.6046464052864158
0.6189055770482169	0.5566489322556251	0.3985033179737075
0.6653823886356965	0.5194588899270749	0.4985947911809602
0.5785183806845356	0.5017324616250469	0.6470928378666665
0.5651257938584271	0.5910618400230061	0.3768552484537840
0.6513882517023167	0.5363448300761910	0.5626591495106636
0.4050908141550542	0.6129923789690942	0.5777044372542187
0.6453986529206160	0.5698992561821936	0.4589745591207330
0.4019150583714164	0.6340574214969832	0.5137337059383347
0.4710141300249471	0.6434704336817318	0.4206159620523127
0.4823509152095608	0.5673733632580795	0.6515812495598501
0.5493444084852532	0.5621506035357500	0.6466667673280123
0.5381223442160071	0.6383667036391845	0.4156135127378062
0.4623790070682798	0.6179736600863850	0.6117704933857867
0.4561262979390938	0.6599443167590722	0.4842145920109799
0.6222408199934668	0.5966496092755748	0.5622186817012597
0.6180808456632315	0.6173596286398980	0.4978683852624331
0.5707470881593378	0.6096227393744279	0.6037745578936393
0.5646145247148702	0.6515901318730252	0.4762686633999584
0.5169845253470652	0.6441071087576926	0.5821318372050974
0.4620727022368472	0.7045611755616561	0.5337028540606308
0.4798531279775066	0.3782963322037797	0.3558094153546189
0.4894732827813992	0.3158157575811882	0.5451132671189229
0.3298511604565315	0.4177604253150901	0.4818131630354939
0.6511429973472876	0.3933715699621972	0.4571736207080617
0.3929356544938351	0.5581165719871682	0.3544804002321693
0.4084949447517853	0.4570192307762592	0.6609164613592053
0.6068133733856620	0.4415232590585359	0.6459666637194604
0.5915126448777934	0.5429651326940002	0.3395148697949614
0.3488852676898429	0.6068091472171111	0.5430522607731622
0.6707397418041472	0.5825736150602406	0.5202308412393255
0.5197462416141130	0.6217374236947822	0.6446254938738919
0.5106768947177341	0.6841007662468829	0.4550711145309964
0.4271905099502541	0.3039615720024291	0.4748857938539066
0.4239610940036380	0.3250307437977613	0.4106794002879770

0.5378443175828224	0.2954281883971401	0.4662997870667340
0.5346349130973042	0.3166150454088364	0.4021219055393505
0.3400162013671824	0.4220148933936126	0.3877932870016979
0.3486414835615523	0.3655103378166767	0.5583962926608662
0.5926763899130918	0.3216917896343235	0.4364709025754618
0.3907097156627584	0.4085220488458499	0.3450449882125744
0.4027001992166265	0.3309487993360019	0.5799649847035255
0.3731359022588029	0.3384330543243125	0.4533541405537013
0.5816212865611216	0.3172348631626818	0.5661389796405047
0.5697399346240741	0.3949423246460178	0.3313261129883415
0.3612761734849631	0.4694941224041218	0.3445902657976292
0.3753914890239486	0.3788496862999416	0.6191732985904296
0.6364662277406028	0.3435417765686342	0.5363533832865712
0.4807805076492550	0.4516276664127808	0.2958923182214188
0.4981303443850954	0.3391705973920286	0.6363590108198335
0.6279112258810797	0.4000638612718921	0.3657417446303717
0.2948009220232738	0.5006097303874293	0.4522671564737757
0.3001986635577246	0.4657667369424570	0.5577187054555574
0.6214362589539316	0.3598766079353926	0.6003278390630938
0.6076557327252520	0.4508058600069489	0.3258075396264793
0.4706778963915440	0.3870581441123004	0.6756288198774274
0.4514039011600420	0.5125488285790688	0.2954575869395996
0.5378684735521341	0.3817924001349478	0.6705191178404738
0.5186726755853719	0.5074145680277550	0.2903149028453390
0.3161063443234902	0.5481720295550968	0.4090975542724055
0.3268882649564450	0.4791192639961870	0.6184691338068831
0.3012276557147995	0.5646310154997191	0.4730180618261833
0.3065574464046231	0.5298510549383442	0.5785682716958100
0.6986967007706362	0.4352867027680433	0.5273858818541329
0.6934058018659738	0.4703086425039333	0.4218794696538227
0.6838241316751112	0.4511547521964011	0.5913585713059594
0.6730866060684192	0.5209782317529775	0.3820617119947721
0.4810698638126326	0.4924329606982743	0.7099050008209798
0.4620078912168833	0.6178778094781613	0.3296925552597390
0.5482171732399188	0.4870837388663038	0.7049057832797008
0.3783977756357336	0.6399132520436512	0.3997978372474905
0.5293373935207040	0.6127467884270621	0.3246204655346780
0.3922278324655312	0.5493311169371610	0.6744539182476280
0.7053194407245306	0.4993582549150219	0.5483500683299936
0.6997358228591057	0.5343075623627734	0.4429980345701018
0.3720234542368259	0.6001107294302286	0.6344503623038545
0.3634639299281004	0.6564208798649135	0.4636611155316338
0.5187351486148128	0.5482521188141037	0.7044595925606502
0.5019393947273445	0.6606537186831131	0.3637973412503878
0.6381034158429476	0.5297076937678353	0.6566040591442460
0.6246745774759512	0.6210509316923429	0.3813170233849308
0.4183575200608597	0.6826418390116678	0.4338622383132596
0.4299419539439543	0.6051463272194060	0.6689167483326921
0.6595835195525583	0.5778503250646555	0.6163602737319090
0.4072128984397195	0.6783871400487623	0.5635474443259737
0.6513752453904246	0.6343842825424073	0.4422622918374264
0.6083209214560752	0.5915084727474306	0.6561665867436635
0.5973895644745566	0.6689353445621155	0.4203936795811410
0.4651064086159131	0.6834069684633789	0.5980268643251211
0.5139104283553705	0.6649821830217973	0.5186246381981083
0.6268649882091530	0.6617351980235886	0.5471771322973605
0.5754886216829881	0.6753793919098846	0.5897460013964279
0.5726905053941185	0.6960693006861355	0.5254640623801687

0.4791803461104936	0.2932377918728152	0.4329797868422020
0.3713460462434007	0.3620846725993330	0.3902760890712029
0.3777922401083687	0.3198628229016769	0.5182133830955786
0.5950017876516057	0.3032418666986290	0.5013457808027053
0.5885709598737391	0.3456079874792594	0.3733581179811461
0.3125599973259869	0.4837671321354457	0.3894193791576457
0.3232330056449985	0.4152825968421724	0.5963778367480247
0.4138979564435567	0.4569662934100570	0.3040644745573915
0.4310392158863981	0.3463182499145001	0.6392892004658817
0.5481504806724851	0.4468094513079314	0.2938366747606905
0.5652030093393320	0.3359658781605482	0.6289535505886816
0.2827662551639130	0.5165400284111069	0.5168453962785833
0.6744502273658854	0.3882242821005696	0.5696231384702535
0.6641512104576999	0.4569236798159958	0.3623896083166315
0.5102728893201641	0.4314294501689570	0.7074246013639962
0.4895178421481118	0.5682642696487800	0.2929433889292146
0.3253971558645627	0.6114416920273814	0.4306577649449519
0.3358394044157967	0.5431985233655009	0.6378846096551098
0.7171249165071732	0.4833976458084618	0.4836649051677628
0.4347779044451278	0.6637663675560221	0.3711196570389526
0.4515207340760590	0.5531858636848845	0.7065227112218274
0.6871687970780007	0.5143381179427668	0.6113853366512253
0.6766715880510299	0.5846476081532500	0.4043999387178996
0.5853813894288685	0.5426624330964818	0.6966017045722660
0.5690369604549963	0.6535908635106720	0.3609580547854217
0.4112247661294128	0.6545500976744127	0.6267401336335332
0.4049597925091908	0.6967484038156746	0.4985158478728569
0.6270024845430110	0.6389433189256986	0.6104498098380414
0.6220850924526611	0.6801196639676267	0.4821759812897681
0.5204343309660704	0.7069015437481067	0.5672806771569511
0.5407342507715033	0.2775749049618093	0.5308867481718970
0.5309448247753382	0.3406523987698141	0.3397095111117958
0.3212257444749026	0.3755287740516428	0.4326038480566925
0.3245298544490882	0.3542023001729146	0.4969296319950738
0.4217026843823437	0.3490852124913681	0.3481166101266217
0.5106050016620105	0.3916865010741586	0.2996705750158061
0.5256602455372265	0.2941140903567838	0.5950878506868155
0.4431090677421984	0.3968055718602990	0.3048399363164097
0.4314936831484785	0.2859807394531561	0.5392698067890697
0.4581264116730079	0.2993094341509340	0.6002851189390628
0.2916385004505642	0.4367319728303856	0.4321815323502123
0.2970798663499264	0.4022521420948633	0.5363537591651520
0.4758935137932636	0.3144064803536453	0.3696879422750828
0.2766994025531886	0.4532213472265579	0.4962756899090398
0.6489824827154959	0.3295271881650611	0.4719194185988207
0.4823996603662832	0.2725685026733005	0.4964523951645252
0.6457906798711393	0.3508931859782811	0.4075949456760065
0.3850032469323074	0.5172727273850172	0.3039149264830939
0.4040438440223545	0.3939252925386820	0.6778552850683645
0.3339578369876599	0.5306605635750552	0.3467713033193940
0.6890021203202765	0.3723640405973156	0.5062484173427781
0.6838504299254202	0.4068838177469656	0.4020112382170072
0.3497919227818448	0.4286186140591199	0.6562712823468738
0.5855183196685203	0.5020798767174361	0.2886845872041659
0.6043602063074192	0.3782528968664592	0.6625975173690279
0.7104988235007379	0.4201928751107537	0.4630664899738898
0.4438700246670664	0.4367879299379037	0.7121186389673307
0.4229917028839972	0.5732094365531475	0.2983274910981171

0.6593450663734929 0.4045666824734934 0.6328154919430292
0.6438587691322972 0.5071946848317624 0.3232943258949203
0.3403104488659089 0.5948919324250022 0.3675946571312357
0.3561660106879918 0.4929332066869681 0.6771185118962536
0.5766636743192272 0.4262662685151571 0.7020985847692435
0.5560670432042442 0.5630171538950677 0.2882255794455103
0.2895113954079884 0.5799237727003573 0.5372303670799413
0.3953480350124151 0.6212984332017920 0.3377045327373086
0.4143201305157183 0.4979874793290515 0.7116601057673648
0.3109437852767268 0.6276283889490772 0.4939156665633602
0.3161139442604864 0.5932841677221202 0.5982301847386537
0.6657128087992560 0.4685657492077039 0.6540307382449013
0.6503003790054056 0.5714086081991744 0.3443290649743188
0.6144525486639848 0.4820938735123854 0.6967797842338789
0.5960399283325847 0.6059890486260059 0.3225412461174901
0.7231016294834370 0.5467281182626793 0.5046380642573278
0.3541135517239472 0.6492893398707563 0.5925358665351400
0.3509796548715530 0.6705726279520540 0.5280618759958694
0.7119308234153177 0.5613765266343301 0.5685217987563999
0.7028318350173944 0.5977126463411661 0.4644040848253689
0.4744173313798234 0.7056947852176519 0.4049970303469335
0.4888154313376535 0.6083226902874139 0.7007463448239307
0.5560973387129995 0.6031436163572657 0.6958556250089341
0.5419568946225608 0.7005736431356747 0.3998889466289597
0.4685475352224152 0.6593674349149073 0.6606047902062601
0.4593146790608105 0.7223431827052538 0.4690581070137014
0.6794484891863428 0.6286052277785625 0.5679917437659446
0.6752755625473487 0.6457165468386969 0.5039504443693784
0.5775321850492245 0.6511282552589038 0.6526609490791313
0.5685808418818179 0.7139715351418092 0.4609616022283922
0.5235139960167465 0.6856955209957809 0.6307275037772213
0.5175513351450626 0.7274264433615913 0.5036612443242678
0.4859136658041799 0.2550493924166447 0.5599622073083298
0.4730303013409528 0.3381247369506626 0.3081965568808753
0.2736985663727632 0.3905982282153458 0.4757878230201279
0.7009609549824509 0.3581086123153540 0.4430024573385684
0.3575844451979979 0.5771866593118339 0.3063742975931010
0.3782226567207100 0.4428297504634677 0.7139566889097320
0.6419845451899019 0.4221540588417595 0.6941418532131155
0.6217468744621381 0.5571542588411021 0.2865290891130959
0.2990256106957190 0.6420699672420376 0.5571247608905650
0.7270779273369853 0.6098032597938465 0.5229608842737112
0.5261882885732760 0.6619304567272080 0.6923159007318156
0.5141926415423778 0.7448508785361184 0.4401101952854041
0.4965933072342278 0.4394644472558615 0.5149624286729042
0.7067315579699539 0.6006399624005123 0.6054954542823613
0.7233914804316335 0.6089359679070488 0.6230896477938996

OH/Cu_{309} E_{ads} = −3.06 eV
1.00000000000000
38.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 38.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 38.0000000000000000
Cu O H
309 1 1
Direct
0.4933484884730905 0.4599818461631618 0.4525824546197116

0.5000039616511138	0.4999957868361921	0.5000009804627346
0.4441069223678991	0.4729594063939322	0.4940419816616709
0.5496713631423413	0.4649180917860402	0.4858333734140801
0.4647834151041424	0.5190700148959647	0.4521656119199178
0.4700675285831674	0.4859382736714614	0.5529165565324545
0.5325033516874291	0.4189132482595774	0.5638800929433915
0.5300137838824495	0.5140877433305424	0.4471061276405052
0.4134695346280147	0.5552131335856477	0.4656852887693756
0.5559312232216580	0.5270442964831449	0.5059645722337246
0.5067254026160669	0.5400375424556748	0.5474186160053288
0.5034626740269316	0.5605202301587340	0.4851675090117125
0.4896977387434676	0.3975050879008462	0.4668102449955566
0.4362225958538317	0.4316438855912148	0.4455931377666528
0.4395336246578468	0.4107437752399982	0.5090556148500301
0.5471528940773022	0.4025585823375821	0.5007054934203942
0.5438223040887253	0.4234298394513138	0.4372303273016160
0.4572622943354613	0.4786238012485121	0.4028893419624249
0.4659880072472890	0.4239623160767981	0.5690662723695692
0.4071063038789632	0.4918760765949620	0.4451553352965154
0.4125018845852538	0.4580807968963411	0.5478557390079806
0.5237864080774218	0.4735358472483813	0.3977499693325476
0.5352951992809835	0.4809591033887631	0.5478286100254756
0.3924358936745752	0.5082353091915276	0.5083714380099618
0.5866525056931351	0.4448910888879166	0.5343106442822078
0.5812678184437168	0.4786496691746104	0.4316880958480718
0.5054278622906941	0.4662455149581061	0.6026931592056898
0.4946604992323886	0.5337820660189831	0.3973075540068996
0.4503959865960762	0.5351197008629114	0.5141800571141848
0.4188463338938782	0.5214393792638360	0.5683743826163291
0.6076631837752138	0.4918601167828647	0.4916511919581661
0.4675901991823898	0.5811076383316036	0.4361048207135892
0.4763053766130989	0.5264738091038710	0.6022690609000162
0.5930168452200159	0.5082089315124027	0.5548205827299850
0.5876167208739067	0.5419778434921192	0.4522020794123502
0.5428762784747716	0.5214282691071446	0.5970550927905857
0.5341329487571660	0.5760499849549260	0.4309819677693723
0.4562625771081435	0.5766214197105056	0.5627769320634136
0.4529306865937804	0.5974850436187424	0.4993263327587658
0.5638929597134190	0.5683876539713876	0.5543871887338546
0.5605589658801657	0.5892676657635951	0.4909635342239680
0.5104241287476762	0.6025156759012097	0.5331952578336310
0.4930899056318436	0.3780719287607463	0.5299080364370687
0.4865206088185420	0.4193310038634712	0.4044728787646490
0.3873605852771151	0.4455165419477354	0.4879923048389739
0.6000637968407405	0.4292796149719321	0.4714610310167602
0.4289662481248157	0.5384002550302527	0.4036176406596356
0.4396143506134526	0.4716401733398080	0.6066023143144323
0.5710775792878511	0.4615989510649242	0.5963801655699736
0.5604128569407812	0.5283502141361125	0.3933843335287657
0.3999825886535043	0.5707390632525492	0.5285484357647956
0.6128747700712818	0.5546336142762039	0.5120372425541954
0.5134819358044909	0.5806786677908179	0.5955473737475755
0.5069082171218580	0.6219474627555249	0.4700865350148011
0.4315839399663303	0.3678127623338282	0.4600796709116954
0.5409846254050031	0.3595158688926717	0.4516165619919995
0.3986482723815626	0.4502732733922801	0.3951143433468964
0.4075070006086021	0.3946932034342293	0.5640037352672017
0.5844854790902361	0.3812819183630878	0.5502676049254144

0.5756430271512313	0.4368083025849143	0.3814419072986202
0.4876937844596593	0.4928731771682782	0.3465470589550052
0.5020046786621584	0.4030341192536817	0.6197426003479423
0.3541245768450829	0.5281087022229021	0.4589312374223691
0.3596098123632727	0.4937565837669566	0.5633081467194552
0.6460389566224040	0.4720702696022276	0.5410607823898921
0.6405450861280808	0.5063746959707549	0.4367719519852548
0.5125010593120831	0.5071853283611657	0.6534361294957556
0.4981629900025642	0.5970139223148964	0.3802657865179407
0.4156683075952928	0.6187978563753790	0.4497387460981950
0.4245258189578237	0.5632759545420812	0.6185999051435194
0.6015063220133515	0.5498035797941180	0.6048435016904352
0.5926164972685034	0.6053479773914223	0.4360395525120494
0.4591483576269568	0.6405551082735517	0.5484080249127528
0.5685493684082334	0.6322177573099912	0.5399235678309692
0.4860894707978384	0.3350127541700929	0.4816900369201588
0.4827753803657048	0.3559010134601345	0.4182443118214484
0.4355228717305361	0.3483553245228365	0.5242596331335634
0.4288579863993781	0.3903023201051288	0.3968330297619271
0.5439855594516575	0.3401065320694270	0.5158772358870404
0.5373347751009303	0.3820243422980217	0.3883806577747907
0.3786989309310951	0.4035750626277050	0.4391069602752022
0.3820339484215886	0.3824970211312048	0.5030402484384277
0.3493871787415319	0.4642132694556451	0.4386842533498319
0.4501344900504889	0.4376669216765725	0.3537920771174413
0.3548046688513139	0.4301744234115071	0.5421159078267135
0.4622150382676710	0.3616969858975064	0.5847540290918939
0.5981385507615613	0.3660270107424577	0.4862872276001906
0.5947820580132501	0.3870369861492997	0.4223181912354125
0.5171620389346746	0.4325136822153504	0.3486188109363766
0.5292306003431618	0.3566061773680396	0.5795259029976314
0.3346067949395467	0.4806887587847998	0.5023582034937368
0.4210147781365754	0.4979019262497819	0.3533515017476624
0.4351794850148349	0.4090401529637582	0.6235356824941962
0.3704313486520611	0.5112304629979446	0.3959622724680814
0.3812384258632394	0.4433837817346811	0.6021316389729002
0.6379433032721054	0.4087022951030834	0.5201467442498482
0.6325234651588978	0.4427084236388866	0.4167317465194132
0.5545380079473505	0.4876860953710550	0.3430065869767825
0.5687064995270302	0.3988802414328105	0.6131752417481632
0.6232916238177481	0.4250420177427746	0.5833544624426152
0.6124512309970712	0.4928445734783549	0.3772275481791437
0.4749279468223189	0.4516638127946786	0.6574425968823552
0.4586624365165359	0.5534840176140379	0.3477405715273790
0.6591050031185660	0.4560258665870667	0.4771414561301768
0.3409545030510621	0.5440422551079276	0.5228774034739102
0.3768391792208873	0.5750728240607793	0.4166300068349133
0.5414410975506287	0.4465567068735568	0.6522644859328375
0.3876844115266931	0.5072499899399224	0.6228384608040385
0.5251715913628974	0.5483854873417376	0.3425491973273730
0.3621762560045758	0.5914228294075740	0.4798488988166315
0.3675946520114911	0.5573876927220580	0.5833437156012430
0.4314241961881376	0.6011393806540907	0.3868003199615068
0.4455966806733222	0.5123090854702039	0.6570067959988051
0.6296300702489444	0.4888016184330641	0.6040209965631456
0.6187849805103651	0.5566271545769447	0.3978724104726669
0.6654529197416331	0.5195109899797103	0.4976885058544918
0.5791418391741128	0.5021443232110441	0.6465882606689999

0.5649530789091766	0.5909613819521933	0.3765009232976432
0.6507228620021539	0.5359657132171312	0.5612576318287075
0.4053138758044845	0.6130215861839535	0.5776867192916733
0.6453171883646223	0.5699232801555519	0.4579934244012271
0.4019607250814516	0.6340226038255553	0.5137526600531962
0.4708529279315405	0.6434284582723843	0.4204436199668790
0.4829333190078823	0.5674991268875936	0.6514199701062575
0.5499744211352069	0.5623913659368069	0.6461643824970144
0.5378634140876790	0.6383254491612076	0.4152864800928202
0.4627427396343195	0.6180574478156031	0.6116324383491797
0.4560776323408157	0.6599564412068041	0.4841563193240395
0.6214242859365202	0.5964495711185310	0.5608511046273169
0.6180280067178604	0.6174868560982845	0.4969721218901956
0.5711298689558081	0.6097068312371322	0.6031705705601031
0.5644429905224463	0.6516563698511467	0.4757368758874417
0.5173372749484645	0.6441176548495848	0.5817748951461680
0.4622569066568097	0.7045834490315883	0.5336279650962699
0.4796229097517497	0.3781943416788849	0.3557819426126270
0.4895462402993588	0.3158978148757822	0.5451767137413825
0.3298578763350373	0.4177079113869959	0.4818600406611917
0.6510771143467666	0.3932506077545568	0.4569228102679480
0.3927192032688389	0.5579495843053024	0.3544440722693383
0.4088409305126291	0.4571712369185398	0.6609642831949554
0.6073409686166052	0.4420586778566123	0.6455434323177167
0.5911975915207789	0.5428233776671925	0.3390197990801579
0.3489719474614603	0.6067862223867033	0.5430959360579554
0.6711311098485928	0.5829626516793506	0.5182553639579931
0.5203699491853794	0.6218211579419644	0.6442497459769932
0.5104311182306293	0.6841321994293267	0.4548127544145061
0.4272138162015305	0.3039256335004916	0.4749831485073133
0.4238653302473095	0.3250287296681538	0.4107270597562997
0.5378402194789578	0.2954846992455210	0.4664130879367322
0.5344732373532386	0.3166188549584507	0.4021417898111922
0.3397832666571534	0.4218277002764775	0.3877576836259728
0.3487397519288463	0.3655778667381844	0.5585691652477854
0.5926367053077839	0.3216926741727567	0.4364310421253628
0.3905744963933905	0.4084163197593694	0.3450320444523779
0.4028818300776514	0.3310731473888476	0.5800553854729523
0.3730893449178676	0.3384137069481413	0.4534528749010237
0.5818262761994173	0.3175068114312734	0.5661800004575213
0.5695663856026631	0.3947882117249099	0.3311506876151870
0.3611618583328584	0.4693695177290176	0.3445719228382422
0.3755617319361530	0.3789902184207394	0.6192804368196320
0.6366761239800474	0.3437653686199716	0.5362632709339350
0.4806180931797622	0.4514916669289634	0.2958790014162536
0.4984706841670681	0.3394766831027851	0.6364270553821216
0.6277287673772346	0.3999458792380260	0.3655208938430600
0.2948090544932964	0.5004992535504575	0.4523428364261270
0.3003321493034936	0.4657460159385975	0.5578570278878553
0.6218931447533655	0.3603562185077952	0.6001656512141501
0.6074732847465772	0.4506493476039919	0.3255439671925813
0.4710894562418552	0.3873868315788984	0.6756739708563406
0.4511978663082055	0.5124240911900566	0.2954334387422910
0.5383952736915598	0.3822332729085486	0.6704824916252966
0.5184984084318081	0.5072874835336162	0.2901809092864579
0.3160663868315522	0.5480144855586744	0.4091336841345101
0.3271168214328263	0.4791189289552089	0.6185640147233612
0.3012364334758002	0.5646023880841485	0.4730936702132753

0.3067749182448249	0.5298525110269139	0.5786327207659895
0.6989313881956624	0.4355769029911342	0.5269361276735389
0.6934036065679002	0.4703041604053670	0.4214173615022614
0.6841194991690438	0.4521312493754712	0.5908460334951732
0.6730689372730508	0.5209861772316078	0.3814892523724138
0.4816681340852753	0.4927453376174696	0.7097955744623123
0.4617526722575068	0.6177858961475265	0.3295164498000053
0.5489650089114576	0.4876298563680728	0.7045482243245811
0.3782758596168582	0.6397312316591173	0.3998193127418537
0.5290522385609597	0.6126607772488378	0.3243317529448969
0.3927163809940779	0.5494135059000523	0.6745127215659864
0.7053831937510817	0.4997537393387064	0.5476583813888491
0.6998220671972304	0.5344206889292206	0.4421989658469580
0.3724156686363640	0.6001413490384265	0.6345175416933931
0.3634679536695333	0.6563346453395281	0.4637616883973236
0.5195425555719441	0.5485393037388840	0.7041200397149248
0.5016501187932119	0.6605628569915599	0.3635547800984189
0.6390125455532093	0.5307301993069955	0.6554254986999744
0.6245658014675072	0.6210842162685279	0.3807249535744350
0.4182662182514172	0.6825611928182582	0.4338242341130047
0.4305507712710370	0.6052828179570822	0.6688971293918982
0.6603351768287173	0.5782601944339649	0.6122659324920976
0.4074764853281863	0.6783696020890071	0.5635983231487655
0.6513415349298022	0.6344851705477574	0.4414066593576048
0.6095498781073827	0.5916354318134878	0.6549862179004755
0.5972024065579761	0.6689826991019285	0.4199314279643271
0.4656383451619943	0.6834612459305279	0.5978747501697567
0.5139927479300351	0.6650100630709995	0.5183030779240944
0.6269858577403966	0.6616405155652294	0.5465653031776675
0.5762311544955241	0.6750507260863430	0.5892900615082147
0.5728620499778606	0.6961365660972951	0.5250446460566990
0.4791334425515728	0.2931459746622561	0.4330409310051409
0.3711887416726353	0.3620790217336218	0.3902644551944598
0.3778502409236109	0.3198995382854076	0.5182795145328860
0.5950836098224912	0.3033666423591097	0.5014452341746730
0.5884070729695864	0.3455001223383107	0.3732856600969701
0.3125191839342669	0.4835285525102586	0.3893905578685685
0.3233753930061563	0.4153307629889804	0.5964797599714253
0.4137677546649777	0.4568591317975553	0.3040032110216637
0.4313413079106736	0.3465625207148273	0.6393866066379599
0.5479609082842402	0.4466153715116537	0.2936505580983418
0.5655997935628287	0.3363750832963812	0.6289119901664678
0.2828675736970500	0.5164936009192050	0.5168825011790203
0.6748365505864276	0.3887521756995577	0.5692794725360034
0.6639295490878694	0.4568930770215843	0.3621280211072823
0.5108986628427913	0.4319039970006638	0.7072606210756353
0.4892303453944624	0.5681583622611683	0.2927370333140365
0.3252947439746823	0.6113893143145498	0.4307058344457709
0.3362129860531339	0.5432070699976990	0.6379598742881171
0.7171675482151819	0.4838169720627440	0.4832078598962979
0.4345378330272440	0.6636597315601985	0.3710429743157603
0.4521847520776541	0.5533807564099711	0.7063871335097853
0.6875775736532712	0.5167131009445066	0.6104264805648535
0.6766973046454209	0.5847401120929574	0.4037416740165664
0.5863605090579874	0.5431815080016204	0.6959372582855262
0.5687639569423684	0.6534407819894860	0.3606575431601728
0.4116993753517124	0.6545930700964703	0.6267199410968765
0.4050207040335036	0.6967163055955303	0.4986131577174187

0.6288587559991409	0.6379006088885927	0.6096653259732212
0.6221133424468640	0.6800879794623342	0.4817170034114258
0.5209594962531934	0.7068701438290612	0.5669641229254651
0.5408007766638904	0.2777026021640321	0.5310361580673000
0.5307587043436474	0.3406319039767235	0.3396165764383010
0.3211745768088258	0.3754768931701158	0.4326005430949887
0.3245551144711157	0.3541893493906923	0.4970031325600285
0.4214970329129901	0.3489335551935751	0.3481171465791962
0.5104021181610335	0.3915085136806958	0.2995817803434260
0.5258826343064391	0.2943542778956932	0.5951579571555289
0.4429021541950490	0.3966625101562463	0.3047876902835568
0.4315383233769277	0.2859900537367268	0.5394664739024401
0.4583582076850559	0.2994549208032562	0.6003836322271099
0.2916271818437161	0.4366090601149804	0.4321675487551280
0.2970915642128225	0.4022156857978480	0.5364442017452314
0.4758088832291270	0.3143249436981078	0.3696863243509566
0.2767527027985227	0.4531663425914585	0.4963185698665747
0.6490496079181061	0.3295226355750831	0.4718284811631330
0.4824269160202742	0.2725528473975408	0.4965885771858848
0.6457251574962047	0.3507458666146357	0.4074190416355524
0.3847756364052576	0.5171244613856469	0.3038638575022683
0.4043613833075404	0.3941157288124278	0.6779408109706876
0.3337536424113170	0.5305232887038668	0.3467788984050824
0.6891737386756793	0.3725233013833252	0.5059945346803483
0.6837380745625944	0.4068045869141385	0.4017573068930254
0.3500153988492882	0.4286952093736689	0.6564183396586990
0.5853175947753131	0.5018526917017192	0.2883209712137407
0.6049120704847045	0.3789067959017633	0.6624042987938418
0.7104683842534162	0.4203206724978362	0.4626779277680628
0.4443599722874303	0.4370661130449011	0.7121172034495038
0.4227254393849206	0.5730950940984544	0.2982305973514059
0.6599229384686378	0.4052800537820382	0.6323655331968856
0.6436216427449680	0.5070466544912756	0.3228685913352918
0.3401937023423335	0.5948186658534392	0.3675906389636661
0.3564978042402189	0.4930172890956488	0.6772147092810428
0.5774009465792060	0.4269035378902198	0.7017701566929285
0.5557572427185395	0.5629392112350262	0.2878340366850921
0.2895534608479671	0.5798885784259876	0.5373851632559009
0.3952052188347699	0.6211111463169798	0.3376106844562558
0.4147992395555365	0.4981626494154427	0.7116586688913015
0.3109238545219092	0.6276077283952487	0.4940281253730426
0.3163552801352757	0.5933050340586508	0.5983045632886207
0.6663233318064564	0.4696313406144485	0.6530832726162797
0.6500562961561638	0.5713432809479982	0.3437427164575776
0.6153370150759325	0.4829246379202072	0.6960862214839630
0.5957220994104345	0.6058977697073388	0.3220858965711672
0.7230355873288168	0.5473592831442619	0.5038073729706674
0.3543867314594609	0.6492856331664782	0.5926064970164781
0.3510589034536112	0.6705081190645968	0.5281817923437502
0.7083219324153672	0.5638546973706617	0.5674103632522283
0.7029205605748704	0.5978631846708244	0.4640520628920746
0.4741470871662513	0.7057125393790888	0.4048197734200977
0.4896546398551369	0.6085339033063195	0.7004780307553782
0.5571671875505030	0.6033492318449325	0.6951921016272469
0.5416769792883477	0.7005492239323619	0.3996257742241416
0.4692900904805082	0.6594383523604460	0.6604519555315383
0.4592249026507568	0.7223838314192312	0.4689655723305735
0.6788147498157692	0.6244073628117951	0.5672568255628625

0.6751821257790496	0.6457331517580004	0.5029258341576598
0.5785700326143892	0.6510188764904974	0.6518032360507703
0.5684799446246530	0.7139535286444360	0.4605540904231428
0.5242457546662364	0.6856943934333772	0.6303167974698544
0.5176100186065669	0.7274613800708064	0.5034219770595484
0.4859943218587670	0.2551488120523385	0.5601327584182145
0.4727444720064547	0.3379756811133430	0.3082095228285719
0.2737335852290156	0.3905574369003085	0.4758785447250929
0.7009385350900603	0.3580808776225528	0.4427478411622446
0.3573036744453496	0.5769951471926904	0.3063832283136230
0.3786204365208324	0.4429777854843058	0.7140230829138464
0.6427788887615892	0.4230555931466117	0.6935696342999160
0.6214580310042784	0.5570231999663714	0.2860138838001055
0.2991230729547025	0.6420130316290837	0.5572892615908486
0.7291281861200186	0.6111617195399621	0.5244223889598999
0.5272871658398510	0.6620239985573458	0.6918035435824298
0.5139994217351855	0.7448689289467163	0.4398593034775269
0.4966051405474133	0.4394934515479597	0.5148450850624741
0.7673259252262473	0.6392912941602846	0.5291058684667681
0.7898565003052018	0.6272426420212696	0.5302335111253977

11.7 *H Adsorption

H/Cu_3/Cu(533) $E_{ads} = -0.39$ eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu H

63 1

Selective dynamics

Direct

0.0032853599999996	0.9972806999999975	0.3042624500000031	F	F	F
0.0028217400000017	0.3308767700000033	0.3042691500000032	F	F	F
0.0026800899999984	0.6645640400000019	0.3042978000000005	F	F	F
0.2572489900000008	0.6186597399999982	0.3218759499999990	F	F	F
0.2571973700000001	0.2857762699999995	0.3217927099999969	F	F	F
0.2571614599999990	0.9524293899999989	0.3219123699999997	F	F	F
0.5099116399999986	0.5747781399999994	0.3415763200000015	F	F	F
0.5095861200000016	0.2417833900000019	0.3416938299999970	F	F	F
0.5096986000000001	0.9088501900000026	0.3416314700000029	F	F	F
0.7627858999999972	0.5310134699999978	0.3609394899999998	F	F	F
0.7629538699999969	0.1970798500000015	0.3608490599999996	F	F	F
0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F
0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F

0.0465710325122655 0.2943331709105304 0.4666264213125386 T T T
0.0461757256497029 0.6286920883683758 0.4667868090805133 T T T
0.0466979217380496 0.9611401336533230 0.4666278281394171 T T T
0.3028164004843826 0.2476339757971801 0.4869691016937709 T T T
0.3029503720248160 0.5807385287570305 0.4870480428920563 T T T
0.3031328282783717 0.9143300008413687 0.4870443061150211 T T T
0.5578943117899408 0.2015131258771556 0.5069099276284659 T T T
0.5588446581856977 0.5343850702096333 0.5064983963062129 T T T
0.5584947406870315 0.8683228068292498 0.5067492243847678 T T T
0.8157675469924466 0.1529129925217160 0.5275714560919262 T T T
0.8154028529592436 0.4873937480493319 0.5275996785307687 T T T
0.8146928282943730 0.8214783813643219 0.5278171411608256 T T T
0.0721152071410374 0.1060534183644622 0.5493280132180610 T T T
0.0707635389253924 0.4412292644565336 0.5489992753640648 T T T
0.0716938306320341 0.7742837576245243 0.5496134476500200 T T T
0.3258989255528708 0.0623520578339994 0.5693674866593080 T T T
0.3245841778882084 0.3957403695944233 0.5696310676028147 T T T
0.3266359122771095 0.7278697860013728 0.5690048410969848 T T T
0.5826736075339760 0.0148372080098047 0.5891171304267402 T T T
0.5835857704462811 0.3461014093504497 0.5879425407106014 T T T
0.5837756561187218 0.6812116816188535 0.5880248009608025 T T T
0.8410777988732121 0.6332747588620968 0.6101775694842608 T T T
0.8432446383143686 0.2967251238789138 0.6097402008471866 T T T
0.8420902078255649 0.9650298223477575 0.6104874802881530 T T T
0.0931896847215421 0.5885727794005917 0.6346016650277178 T T T
0.0951558314062236 0.2546304373013949 0.6335763721534958 T T T
0.0972321255617429 0.9193314104432202 0.6356736914716615 T T T
0.3473302099655990 0.5403090875184252 0.6510383029750162 T T T
0.3482918609136805 0.2099729797244146 0.6522499081843472 T T T
0.3479309784827462 0.8809294397975025 0.6511877075448671 T T T
0.6046617693457518 0.4957445113416503 0.6678925567676490 T T T
0.6025239152026493 0.1610079307265616 0.6717730296648085 T T T
0.6023300167096421 0.8351988922551260 0.6718102522572683 T T T
0.8582682816293660 0.4531771893127375 0.6914370669435143 T T T
0.8584418672223676 0.1166911140406140 0.6921743493765666 T T T
0.8535422504887973 0.7888088880266502 0.6929312724352377 T T T
0.6183571166077766 0.6460737162429885 0.7478354195669646 T T T
0.6176827846832015 0.3230390014131278 0.7480111979788078 T T T
0.3664128833873830 0.6950187814084269 0.7281159707996229 T T T
0.4997766007278595 0.5830312305942820 0.7794963028275392 T T T

H/Defected-Cu(533) E_{ads} = −0.38 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu H
59 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F

0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0475924234226156 0.2944234611240937 0.4660846941656991 T T T
0.0474052755794147 0.6275686731868896 0.4658192971891686 T T T
0.0474159949886388 0.9613516365878961 0.4657505201436639 T T T
0.3039619073593027 0.2480247489107295 0.4869226297176386 T T T
0.3051500710385938 0.5803099377992157 0.4864876032131205 T T T
0.3042925841389467 0.9140956869853785 0.4866690911985366 T T T
0.5599469357989777 0.2011715053117235 0.5065977000949704 T T T
0.5602128043376486 0.5352203676540168 0.5066590983248990 T T T
0.5594743028346835 0.8685636554627477 0.5076360825728430 T T T
0.8174114978891253 0.1537214613347137 0.5272533094650317 T T T
0.8166593223884918 0.4883333937757154 0.5274328161902831 T T T
0.8166511942297533 0.8202279712999869 0.5274854959630447 T T T
0.0740497265814472 0.1067510897999830 0.5482527452434194 T T T
0.0723441323687465 0.4415867727376376 0.5487026018517490 T T T
0.0750125945267487 0.7726682049172056 0.5475201411956442 T T T
0.3279046454262067 0.0628028149048358 0.5691330248242858 T T T
0.3294340875550896 0.3949349011737608 0.5691305142475562 T T T
0.3292480343470668 0.7281421219037599 0.5689618609759407 T T T
0.5859185654078806 0.0170236250580381 0.5895449697544561 T T T
0.5868984328168847 0.3470437499807060 0.5881485023521019 T T T
0.5869851406988262 0.6789582320327171 0.5896342233359662 T T T
0.8437319054696353 0.6289441314644991 0.6107865274529740 T T T
0.8456035137633597 0.3016694427700872 0.6094360190256121 T T T
0.8463648217604963 0.9634392581237375 0.6083518544271719 T T T
0.1004459610091272 0.5854429875089701 0.6321020502945457 T T T
0.0970491763155262 0.2547921596768269 0.6334280050993721 T T T
0.0990610120626413 0.9214993916996987 0.6324538765259059 T T T
0.3521543817573535 0.5440008667449372 0.6512551546166880 T T T
0.3531758374920555 0.2095227950405681 0.6519520932322936 T T T
0.3536333139730563 0.8759134318328924 0.6516928637227504 T T T
0.6087572167148355 0.4991559168095302 0.6714798539368177 T T T
0.6061924475158402 0.1663769802298288 0.6736053989106974 T T T
0.6086422512607456 0.8305840690430547 0.6705645641002782 T T T
0.8616456917790258 0.1187213027609000 0.6881205993065527 T T T
0.8635994006939769 0.7828728262567876 0.6881074475473496 T T T
0.6703844472600374 0.2875421026534645 0.7138923805151107 T T T

H/Cu(533) E_{ads} = −0.36 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000

4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu H
60 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0482538579408874 0.2932256527466013 0.4659384015352005 T T T
0.0478866048418478 0.6268892415802670 0.4657963292297597 T T T
0.0480831985897738 0.9599557291417838 0.4659462671194378 T T T
0.3051643916105275 0.2458226169147409 0.4867252311836017 T T T
0.3051582290749482 0.5790204843319121 0.4867698241409309 T T T
0.3056009776741706 0.9119973801929446 0.4867055681953061 T T T
0.5605585587829799 0.2001016914929171 0.5071671423507783 T T T
0.5606163837368012 0.5328702826829413 0.5070285559146368 T T T
0.5608354255099928 0.8655312181729545 0.5071736900557352 T T T
0.8177196134848274 0.1513113277147826 0.5271977083994596 T T T
0.8177236878688289 0.4856627192168534 0.5271757737022654 T T T
0.8178511442271689 0.8186061162252992 0.5277552250938273 T T T
0.0760206343483259 0.1034338304187202 0.5479515671048438 T T T
0.0745775104092905 0.4385436393707868 0.5481225550350121 T T T
0.0749299927375940 0.7705570089259167 0.5481717841347646 T T T
0.3296134420260001 0.0584553320899091 0.5691563059060303 T T T
0.3299044453059761 0.3919918802376741 0.5691794125584220 T T T
0.3299517634455639 0.7252391262921420 0.5692208804456834 T T T
0.5871761756931015 0.0107454339638591 0.5887693862596052 T T T
0.5880476177560404 0.3445610159820319 0.5895413219060820 T T T
0.5880683175824046 0.6757386988184666 0.5895226920151041 T T T
0.8468254098295533 0.6263809094989626 0.6094664571587840 T T T
0.8478699663383722 0.2935543067104265 0.6078607293852929 T T T
0.8467851507337180 0.9624470240043065 0.6094892763735598 T T T
0.1026639201599021 0.5817034571507088 0.6326797130463759 T T T
0.1014928174185626 0.2487063799357778 0.6326815323310673 T T T
0.1015743131377976 0.9155887937516969 0.6326089110349917 T T T
0.3562334034398512 0.5371258774021713 0.6519048718428231 T T T

0.3546437060584089	0.2043312960366861	0.6518301242417817	T	T	T
0.3557877053622096	0.8699140923081692	0.6516896163715381	T	T	T
0.6082824029590576	0.4932804505487052	0.6740244349849331	T	T	T
0.6081451386036585	0.1578130768242627	0.6714833622013123	T	T	T
0.6081259137474226	0.8287282023964125	0.6715545070857043	T	T	T
0.8623714941706777	0.4481218329503612	0.6899057606632512	T	T	T
0.8627510167138002	0.1144190298132110	0.6899301553310929	T	T	T
0.8650621707303745	0.7792023146398760	0.6890037938080257	T	T	T
0.7609378489310227	0.3659089928087359	0.7213561470541581	T	T	T

H/Cu(533) $E_{ads} = -0.33$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu H
60 1
Selective dynamics
Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0466866174857093	0.2945490816379084	0.4659083838337298	T	T	T
0.0467266790452834	0.6275941293182524	0.4660235447680181	T	T	T
0.0469212763238862	0.9610996527149555	0.4659798997591957	T	T	T
0.3028689419270760	0.2478133312824150	0.4869703142884227	T	T	T
0.3027913210030654	0.5810422102752941	0.4868563914376910	T	T	T
0.3028657488814558	0.9139779933835769	0.4869605506959767	T	T	T
0.5578725857288511	0.2013046357984195	0.5065325396355540	T	T	T
0.5578094521673200	0.5357788006606636	0.5065425757479171	T	T	T
0.5580756762746496	0.8681621785111455	0.5072451481352694	T	T	T
0.8148253959951506	0.1542599498279514	0.5274139688220956	T	T	T
0.8140790142207188	0.4883456495951778	0.5276037994411006	T	T	T
0.8142322414981651	0.8214077564237612	0.5275977004901012	T	T	T
0.0698995513300964	0.1085423716029210	0.5482934417117807	T	T	T
0.0700839638590129	0.4417360157252864	0.5482429431589625	T	T	T

0.0698734917469124 0.7752583369006056 0.5482978113354240 T T T
0.3250927207500180 0.0624746789683493 0.5690616706925704 T T T
0.3253870771738806 0.3965261141682437 0.5696537609019987 T T T
0.3254353552442893 0.7279352040556143 0.5696812032730290 T T T
0.5811701766023259 0.0172250412020122 0.5891966113464707 T T T
0.5821042772374164 0.3484077169426024 0.5876100202390956 T T T
0.5812633642903071 0.6810180145115275 0.5892805397453107 T T T
0.8398165613400898 0.6336094993031133 0.6092532585571864 T T T
0.8388572473157704 0.3002905973403192 0.6096016053177424 T T T
0.8385544798383484 0.9684582890055596 0.6095881091316887 T T T
0.0959012861539943 0.5872333753078023 0.6324487301424190 T T T
0.0945128471015947 0.2548277624076470 0.6323843209623908 T T T
0.0959599682323218 0.9197068804623483 0.6322138260489774 T T T
0.3479945518368501 0.5434056269236416 0.6537068207443122 T T T
0.3475332510149794 0.2087500489230104 0.6517026175793303 T T T
0.3474504271860803 0.8788605584985514 0.6517453952971857 T T T
0.6010999818773490 0.4988622052940528 0.6732301672469789 T T T
0.6010466534072511 0.1661682504547853 0.6731975078717580 T T T
0.6019588657210226 0.8317117599660426 0.6716146876538872 T T T
0.8555353971820013 0.4540008303232326 0.6894382215746081 T T T
0.8601959577395214 0.1164477772834285 0.6897679156771191 T T T
0.8558335682424739 0.7864896815429124 0.6893387478452240 T T T
0.4911633014650224 0.4240475207667551 0.7021785794086810 T T T

H/Defected-Cu(533) $E_{ads} = -0.33$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu H
59 1
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F

0.0475804115216742 0.2948527097738687 0.4660418895808225 T T T
0.0476539018719612 0.6276457800310318 0.4659612027243284 T T T
0.0478608758568704 0.9615146516409818 0.4659479878664921 T T T
0.3044085056441694 0.2478239423284168 0.4869101222447622 T T T
0.3055466937351725 0.5801969366135871 0.4865135099044434 T T T
0.3042429361437183 0.9147622838367203 0.4867115558483023 T T T
0.5606289735497016 0.2014564097301441 0.5068667962114040 T T T
0.5606255529990022 0.5345422849186080 0.5071674673129292 T T T
0.5595666217130191 0.8692877957416290 0.5072284994543506 T T T
0.8175581891542381 0.1550229305776540 0.5272414267298062 T T T
0.8170815574018290 0.4882571407514174 0.5277861948954000 T T T
0.8172226211436513 0.8203555188850666 0.5272963633576134 T T T
0.0732541135679071 0.1089261260576083 0.5486113627610638 T T T
0.0731404328773866 0.4409534979949169 0.5486774883807338 T T T
0.0758938117979211 0.7725381503648556 0.5475560280431722 T T T
0.3279329823852876 0.0632846551818219 0.5693618310742838 T T T
0.3299977080816286 0.3948935757441589 0.5690913401609654 T T T
0.3293565654055562 0.7287315399061766 0.5688888610272147 T T T
0.5871366716998019 0.0156534750815139 0.5894606983048056 T T T
0.5879504998235257 0.3461584102516333 0.5893952180810992 T T T
0.5872074957990607 0.6817015181713140 0.5889934853923180 T T T
0.8451209909366572 0.6301751407580463 0.6112544926158360 T T T
0.8453313244992110 0.3026666050416653 0.6108909026704864 T T T
0.8473564552749039 0.9642494950652550 0.6075744241182640 T T T
0.1002383881318633 0.5861620747066709 0.6322035300126023 T T T
0.0966283211482304 0.2570950148639437 0.6340912744935349 T T T
0.0997898026479453 0.9215961580940099 0.6321970866055162 T T T
0.3538296449912622 0.5428675328284924 0.6515622173664040 T T T
0.3533073292425698 0.2103404870433183 0.6520885398671876 T T T
0.3524630126607207 0.8777433514076206 0.6519468747834388 T T T
0.6082128562337947 0.5008663899905290 0.6702317791780488 T T T
0.6061394807591760 0.1664199183604558 0.6743324884955841 T T T
0.6078030501667671 0.8295069073892541 0.6704716588241335 T T T
0.8610661134817805 0.1189695227838009 0.6886461407581548 T T T
0.8618028681650525 0.7894326380714231 0.6887318957747867 T T T
0.7582129045424579 0.0402414774141210 0.7215636425180608 T T T

H/Cu(533) $E_{ads} = -0.32$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu H
60 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F

0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0471114162565009 0.2941727171484775 0.4660273527365634 T T T
0.0469202798219098 0.6275135279827716 0.4659613558511242 T T T
0.0470203864579038 0.9609395978882064 0.4658809694577379 T T T
0.3031493926980929 0.2474127698089258 0.4868331080325904 T T T
0.3036471029963370 0.5804733950167865 0.4867799011174774 T T T
0.3035622458789426 0.9134789792458181 0.4867377848592824 T T T
0.5581292847346133 0.2013947749788290 0.5067717003179292 T T T
0.5579570596472426 0.5352175934900990 0.5068306467762519 T T T
0.5583124799450997 0.8680705214287944 0.5075197729816870 T T T
0.8146844163396476 0.1543571819369915 0.5273383063047684 T T T
0.8143994466488641 0.4881993559736858 0.5273935743565815 T T T
0.8144215461815029 0.8211623478303289 0.5274111680736459 T T T
0.0714149281318762 0.1068737868536940 0.5481459925008645 T T T
0.0706032386240983 0.4413360244382043 0.5483246789239378 T T T
0.0715469721320992 0.7740123737791185 0.5481067177162421 T T T
0.3254350048188355 0.0620105901777445 0.5690122014691466 T T T
0.3255636091685006 0.3956035587168469 0.5691727588803364 T T T
0.3245345241902321 0.7296328177571336 0.5694738806180223 T T T
0.5822986979004129 0.0169306894138195 0.5895778748823347 T T T
0.5823883940327196 0.3482323583475083 0.5886034772232450 T T T
0.5821990463975039 0.6795047808284084 0.5895881781993734 T T T
0.8400490274115406 0.6331904683663535 0.6090817350397303 T T T
0.8410387131986991 0.2991372361022313 0.6087680440590013 T T T
0.8412551605844023 0.9658732534627815 0.6087969145375774 T T T
0.0957316746702017 0.5870232372566898 0.6324802608264166 T T T
0.0962907160190996 0.2527215153826874 0.6324377670676624 T T T
0.0931330724094853 0.9229280030955481 0.6337374686078607 T T T
0.3470683025005691 0.5444135970681636 0.6513669461165611 T T T
0.3490533980375362 0.2091294924611012 0.6515906425149538 T T T
0.3488833680590455 0.8758860272100645 0.6517576924739398 T T T
0.6000533802504296 0.5003121575122789 0.6736219814101257 T T T
0.5998509044739703 0.1666173841725027 0.6736063073097889 T T T
0.6024137664139722 0.8313194512315156 0.6715100120522979 T T T
0.8583274792486355 0.4526643593643372 0.6889485725240284 T T T
0.8537768070283936 0.1218265648936661 0.6899002080151205 T T T
0.8579098355716629 0.7839384813471857 0.6889812619142576 T T T
0.6588356270839038 0.2844127603307238 0.7152375261218841 T T T

H/Cu(533) E_{ads} = −0.32 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu H

60 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0484871991875018 0.2930091548600591 0.4657996143428813 T T T
0.0486313957214451 0.6262252305081999 0.4659938543800889 T T T
0.0484646319891207 0.9595706790031703 0.4659117559851302 T T T
0.3062692498544421 0.2445336671276412 0.4867715864729462 T T T
0.3059102955104564 0.5785229832132736 0.4868831145439814 T T T
0.3063246771812749 0.9115767860025704 0.4868364244845425 T T T
0.5619769223429928 0.1983307586167864 0.5076299494991302 T T T
0.5616173759052580 0.5317965234367433 0.5069233500736285 T T T
0.5614197476759062 0.8657136855812860 0.5069749651961708 T T T
0.8191364699430015 0.1505178685873140 0.5275591028156220 T T T
0.8194602524213588 0.4836963871171523 0.5274754969248220 T T T
0.8191736527525367 0.8175378233326335 0.5275353894418201 T T T
0.0772516456325823 0.1026469623794390 0.5481301042544826 T T T
0.0771399306554396 0.4352817376378046 0.5481722415237164 T T T
0.0762534704172898 0.7700430148391483 0.5483616108366880 T T T
0.3313356166246659 0.0574101150600714 0.5696722641764215 T T T
0.3320627252857147 0.3898589831809761 0.5691682148621156 T T T
0.3322429546793441 0.7233566381237739 0.5693929263797028 T T T
0.5897893214135205 0.0065947354350288 0.5898335239238003 T T T
0.5898188702723869 0.3438980906093628 0.5897996456863839 T T T
0.5896519954323444 0.6755037822610940 0.5887480882102402 T T T
0.8493231927121426 0.6256054367253383 0.6090169919611431 T T T
0.8494942084171511 0.2922377012084897 0.6090494546088608 T T T
0.8484858983227281 0.9596147835100094 0.6094374022062908 T T T
0.1057058465557277 0.5782052913277865 0.6324823865539317 T T T
0.1025400252734085 0.2484522126638316 0.6337318612482713 T T T
0.1051791207166305 0.9125349213813818 0.6325690249791522 T T T
0.3591548145491298 0.5340141688325775 0.6519459967719011 T T T
0.3589944429070877 0.2008690256236955 0.6520817088691795 T T T
0.3568849650333291 0.8695845016131909 0.6517290530637591 T T T
0.6106580373743039 0.4911018174354246 0.6738234117767964 T T T

0.6132573275181467 0.1556342478205543 0.6718646880226062 T T T
0.6108076107017278 0.8247446292885341 0.6738190595846852 T T T
0.8650614546581178 0.4457190112645642 0.6901851573439637 T T T
0.8692594693291006 0.1077661960954457 0.6893693924072802 T T T
0.8696628753066108 0.7765461887662667 0.6893757674454932 T T T
0.6694563654964659 0.6094611855001884 0.7153438756301040 T T T

H/Cu(533) E_{ads} = −0.32 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu H
60 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0464880162666201 0.2944933666679138 0.4660170456519147 T T T
0.0470965678467434 0.6275004725954890 0.4660098225982929 T T T
0.0468983021826458 0.9609471870703032 0.4659616312726693 T T T
0.3026951553200745 0.2475528870323443 0.4866767518437730 T T T
0.3025724003369381 0.5813362986269188 0.4867418972568376 T T T
0.3028552477304554 0.9142146660129251 0.4873612076923392 T T T
0.5580643100855904 0.2016494166427639 0.5067791874827861 T T T
0.5578548351630511 0.5356802182841786 0.5067283416057052 T T T
0.5578286621243747 0.8680358541391374 0.5067532788811109 T T T
0.8145523219112705 0.1545364396170578 0.5275129107882259 T T T
0.8142432002314529 0.4881444509579696 0.5276163700391620 T T T
0.8147374066007091 0.8210538825838232 0.5273998019574745 T T T
0.0707758784383160 0.1075796214003845 0.5482381799984944 T T T
0.0706234260931404 0.4412185385283003 0.5482793816503047 T T T
0.0698485427530687 0.7755086381143430 0.5484586895649176 T T T
0.3254761232378828 0.0641050900245226 0.5697931911937766 T T T
0.3253082103496430 0.3957286921522611 0.5688222552577481 T T T

0.3253240530539928	0.7270285933124301	0.5698405937405201	T	T	T
0.5818798497263797	0.0151329751754126	0.5883580616509841	T	T	T
0.5818295676054464	0.3488229469427711	0.5883965082182517	T	T	T
0.5812929354191413	0.6821946083647072	0.5887706163922701	T	T	T
0.8399624116339772	0.6334728846833126	0.6093207738308263	T	T	T
0.8407744577347338	0.2991199984280747	0.6093382217542878	T	T	T
0.8378071923948486	0.9686259451300946	0.6097438390521799	T	T	T
0.0946373901208186	0.5879766957903142	0.6319038572403051	T	T	T
0.0961839672667008	0.2536904130196406	0.6323823548423720	T	T	T
0.0960127630484785	0.9200823283093202	0.6324580451857844	T	T	T
0.3476367893896627	0.5441465250648279	0.6534925796040985	T	T	T
0.3479294881903037	0.2096469698069454	0.6534348174970380	T	T	T
0.3490573012659803	0.8757314966738484	0.6515986545689052	T	T	T
0.6039472052747620	0.4983866657001700	0.6714021878085336	T	T	T
0.6018019912081630	0.1654372860460441	0.6732185380647553	T	T	T
0.6036245780931611	0.8285362037400229	0.6714066710173368	T	T	T
0.8585381465427439	0.4512010253772171	0.6896296625465466	T	T	T
0.8568364080473739	0.1193180801260927	0.6895515584421090	T	T	T
0.8564745892093425	0.7862235804305958	0.6894880782367491	T	T	T
0.4056408343215387	0.3287119619131493	0.6946437351964481	T	T	T

H/Defected-Cu(533) E_{ads} = −0.32 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu H
59 1
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0462405131622169	0.2948336427985856	0.4660875177614207	T	T	T
0.0461006708587552	0.6279492838412678	0.4660568525400099	T	T	T
0.0465896135271328	0.9615403552151212	0.4659741654472565	T	T	T

0.3021611013421976 0.2485670259388471 0.4870750172182778 T T T
0.3026197008346564 0.5809991133845475 0.4865955704356447 T T T
0.3023036581261939 0.9143672249665283 0.4868866539166095 T T T
0.5579848229120753 0.2013271991158337 0.5063550510185880 T T T
0.5579569409102558 0.5358574262535991 0.5065095649309237 T T T
0.5574420691838655 0.8685113120035532 0.5073166080243543 T T T
0.8150653018221354 0.1545691010076768 0.5274056070046691 T T T
0.8139809300051238 0.4886417064136249 0.5276006818351778 T T T
0.8139359003763922 0.8215070024620267 0.5277047862569177 T T T
0.0693688337220403 0.1093422778821010 0.5486174047474696 T T T
0.0691831038361099 0.4422817672993207 0.5486289311738524 T T T
0.0705390994006350 0.7747135478847190 0.5480482348872668 T T T
0.3242850012789986 0.0629624241142282 0.5690301896854901 T T T
0.3256823668740638 0.3965066498432023 0.5696396752277505 T T T
0.3257135157067746 0.7274876094431078 0.5694419321031967 T T T
0.5814082989212631 0.0171995884099962 0.5888783246526743 T T T
0.5828006537064433 0.3476461018172499 0.5873561689147551 T T T
0.5827585571395465 0.6795423351853759 0.5891820810659847 T T T
0.8397820776360077 0.6299335391047982 0.6106419792357340 T T T
0.8388378947882518 0.3045113640492782 0.6110593198203655 T T T
0.8393516099901592 0.9680182590343271 0.6092293934468671 T T T
0.0956574769913235 0.5865058964799519 0.6321308683333030 T T T
0.0916267869946482 0.2569856094563641 0.6332536125098942 T T T
0.0958749568637587 0.9210836500445094 0.6318006689989401 T T T
0.3474342404210948 0.5434536223408457 0.6539262134279586 T T T
0.3473939289103941 0.2086066888963070 0.6515818918502305 T T T
0.3475925188665177 0.8786386373683799 0.6515674947539544 T T T
0.6029274492649550 0.4975324943987388 0.6712019960598892 T T T
0.6011357590832213 0.1655334653538652 0.6731622640855720 T T T
0.6047421041612113 0.8277731411844483 0.6700119092188900 T T T
0.8604719252046761 0.1146851066585496 0.6886291177650282 T T T
0.8558430333165966 0.7872520424419653 0.6883101760421639 T T T
0.4947703903735437 0.4229870530009847 0.7018540328656188 T T T

H/Cu(533) $E_{ads} = -0.28$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu H
60 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F

0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0463906554881489	0.2950968478735603	0.4661698020360450	T	T	T
0.0463976379591968	0.6280708723046214	0.4661580648595262	T	T	T
0.0465186643444532	0.9609644518659757	0.4661940495704351	T	T	T
0.3026927959943122	0.2472730999457065	0.4865377647926298	T	T	T
0.3026507779206911	0.5814470200401956	0.4864969264797163	T	T	T
0.3028103126885774	0.9145316624249122	0.4870810902363061	T	T	T
0.5580402784259748	0.2017746574933965	0.5068421654808160	T	T	T
0.5574258946435334	0.5356816905265782	0.5069427428338784	T	T	T
0.5577260871067624	0.8683746943939002	0.5069567583380945	T	T	T
0.8135341793178118	0.1552419360359120	0.5276048868178365	T	T	T
0.8136498386974478	0.4887955940522778	0.5275179781293309	T	T	T
0.8133402761309159	0.8220390877852859	0.5275471562214729	T	T	T
0.0700806284891260	0.1083629798042130	0.5480274048126321	T	T	T
0.0708450221304624	0.4417328766660811	0.5487665434318441	T	T	T
0.0703969674383421	0.7741928910766548	0.5486834111378864	T	T	T
0.3243576451215371	0.0641599565391471	0.5694748761882675	T	T	T
0.3249766659610507	0.3960885635295487	0.5680755853906270	T	T	T
0.3246885888115569	0.7282363378676180	0.5694272601133862	T	T	T
0.5799141747746758	0.0172613335629698	0.5890570346011900	T	T	T
0.5802136607612167	0.3494231674088317	0.5890848136935323	T	T	T
0.5812377592111153	0.6825694896522627	0.5889105737012734	T	T	T
0.8406953957843503	0.6331217977995782	0.6093208712021306	T	T	T
0.8395868597124014	0.3005990795532131	0.6092340402376915	T	T	T
0.8403736840635537	0.9658127384272915	0.6093417432938245	T	T	T
0.0952834634400235	0.5877879822031480	0.6343995802354714	T	T	T
0.0949201411998587	0.2524804322279847	0.6323576331856995	T	T	T
0.0950129541398096	0.9230379084060703	0.6321355019120013	T	T	T
0.3486325800739226	0.5434623692853148	0.6533261249135859	T	T	T
0.3485632916225989	0.2092466851660185	0.6532029709445151	T	T	T
0.3494474441782109	0.8754218544460231	0.6515399206537134	T	T	T
0.6017352406920177	0.4985186069270894	0.6718280892998622	T	T	T
0.6042136314172474	0.1637441432818889	0.6720703100022745	T	T	T
0.6014069306831179	0.8321773684624210	0.6717493212578225	T	T	T
0.8550496093828754	0.4542480900493059	0.6894866070918557	T	T	T
0.8565527057474247	0.1199982366337531	0.6894582355476853	T	T	T
0.8536732971508783	0.7880789833335476	0.6901030172123829	T	T	T
0.2395746889989134	0.4665256657544143	0.6815094832723372	T	T	T

H/Cu(533) $E_{ads} = -0.09$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu H
60 1
Selective dynamics
Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0468973618039913	0.2941639392139767	0.4659987385969072	T	T	T
0.0466216812396970	0.6280300770816022	0.4660808795854828	T	T	T
0.0470875014240777	0.9608598857363124	0.4665192184579104	T	T	T
0.3029660242633865	0.2475310084855730	0.4868848674854188	T	T	T
0.3031275430436740	0.5807595018825090	0.4869214429437290	T	T	T
0.3029578829258276	0.9142685796397758	0.4868402098615920	T	T	T
0.5581741447798272	0.2015301060008375	0.5069189518370154	T	T	T
0.5582903523152022	0.5346285693965127	0.5068573035847318	T	T	T
0.5582194284419029	0.8681368686429918	0.5069185888375424	T	T	T
0.8152232139246338	0.1538398148917487	0.5275888500764668	T	T	T
0.8147030149817721	0.4871773561268253	0.5274024681488911	T	T	T
0.8144211350356488	0.8217748187348622	0.5275669206340216	T	T	T
0.0712787208709195	0.1088326225660292	0.5489720993670711	T	T	T
0.0705894640950681	0.4411509546488916	0.5482654426551462	T	T	T
0.0713697615259418	0.7725310691225087	0.5490001568281728	T	T	T
0.3253804232532023	0.0624237398141363	0.5693909722009870	T	T	T
0.3252984765159647	0.3954737935434453	0.5693738506585034	T	T	T
0.3256991035352136	0.7286200677239165	0.5691311731133154	T	T	T
0.5807414776134560	0.0165675233631836	0.5891123151610786	T	T	T
0.5831592518396744	0.3474273997562768	0.5888645637723275	T	T	T
0.5822186164932236	0.6809764429903614	0.5888359946276708	T	T	T
0.8378428804035503	0.6352311599001192	0.6083594311349012	T	T	T
0.8420515872887554	0.2986430288022549	0.6094612211765071	T	T	T
0.8417407348643896	0.9647633342862711	0.6094300923857966	T	T	T
0.0982648382300928	0.5856830138786439	0.6339130871024040	T	T	T
0.0982534534411930	0.2513114297621266	0.6339589382926175	T	T	T
0.0983089771917710	0.9179741464963336	0.6326500721563738	T	T	T
0.3540812757040039	0.5393794431466177	0.6518689664622748	T	T	T
0.3514390083084379	0.2075873558810229	0.6529407814817917	T	T	T
0.3524155326019169	0.8716838897958769	0.6518405318427721	T	T	T
0.6065265065440620	0.4954251687768517	0.6722273939238825	T	T	T
0.6060190140757657	0.1609310169379334	0.6721543820983517	T	T	T
0.6040979607406547	0.8300236445201955	0.6720053818640936	T	T	T
0.8587497780632231	0.4517302167501066	0.6901453541471310	T	T	T

0.8599364933430533 0.1166299400019288 0.6895376580053195 T T T
0.8589033705595542 0.7837980292817311 0.6901687121156933 T T T
0.0781444795218176 0.4351981470887759 0.6780278361163689 T T T

H/Cu(533) E_{ads} = −0.03 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu H
60 1
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0469648714720666 0.2946229032826194 0.4661081544374580 T T T
0.0466558843045636 0.6278629522268510 0.4661005520024832 T T T
0.0466656707578973 0.9608015980204834 0.4661202988746354 T T T
0.3028092421934501 0.2477342517089075 0.4867973969895548 T T T
0.3030559911932343 0.5806963305932393 0.4868083631774749 T T T
0.3030731076631191 0.9141076408173947 0.4869257560980995 T T T
0.5579048837602864 0.2017149856249040 0.5070020482754096 T T T
0.5578535070766427 0.5348448729687221 0.5068384545876932 T T T
0.5580772326171500 0.8684984383914308 0.5069326729488692 T T T
0.8146027312994212 0.1545996643432222 0.5273994156310231 T T T
0.8145525749241609 0.4876408057702711 0.5273364260133286 T T T
0.8147394136817949 0.8208386198057082 0.5276115379785665 T T T
0.0710908919798706 0.1076838535423044 0.5480460819924989 T T T
0.0711073741067111 0.4417355171575249 0.5489113017063312 T T T
0.0712781025805835 0.7729337584959233 0.5489122743105554 T T T
0.3261096317106256 0.0620673432821362 0.5692750715779905 T T T
0.3258663309585715 0.3949851881398586 0.5694846606164454 T T T
0.3255991337742586 0.7283293031826987 0.5691726827681276 T T T
0.5831497559893767 0.0140685243461635 0.5890628532322545 T T T
0.5822595510475944 0.3483927975162389 0.5889399931095566 T T T

0.5824146418682776	0.6812363956000441	0.5887727030476116	T	T	T
0.8409724322357444	0.6313873586002788	0.6089081353521860	T	T	T
0.8422013083282027	0.2983027369720713	0.6093551745202100	T	T	T
0.8408620726877918	0.9667893448674791	0.6088478978066975	T	T	T
0.1011060335354684	0.5824860025993783	0.6339538202787864	T	T	T
0.0987704694987158	0.2493531866584186	0.6323798005869811	T	T	T
0.0985052210430953	0.9197977957120889	0.6322640215694962	T	T	T
0.3538032779331734	0.5395054769249413	0.6522194770118320	T	T	T
0.3535749454810627	0.2043812064807372	0.6521517898790867	T	T	T
0.3530009359905821	0.8726852277080839	0.6519226773438123	T	T	T
0.6053240736453193	0.4959071162170167	0.6721993158195575	T	T	T
0.6072256256524421	0.1595638039194169	0.6722115369704634	T	T	T
0.6072888182923564	0.8285009675082633	0.6722495875110353	T	T	T
0.8597752286652215	0.4491553116146155	0.6897561437988169	T	T	T
0.8593573142488309	0.1184757894924352	0.6896211058255292	T	T	T
0.8637559147530169	0.7803225652236501	0.6902861247184612	T	T	T
0.0643841936045444	0.6132880029545165	0.6945111055733967	T	T	T

H/Cu(111) $E_{ads} = -0.38$ eV

1.00000000000000

7.6579664403000001	0.0000000000000000	0.0000000000000000
3.8289832201000000	6.6319934786000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.5000000000000000

Cu H

45 1

Selective dynamics

Direct

0.8888888887999968	0.2222222223999992	0.3170124957488483	F	F	F
0.2222222221000010	0.2222222223999992	0.3170124957488483	F	F	F
0.5555555553999980	0.2222222223999992	0.3170124957488483	F	F	F
0.8888888890000004	0.5555555553000033	0.3170124957488483	F	F	F
0.2222222222999974	0.5555555553000033	0.3170124957488483	F	F	F
0.5555555556000016	0.5555555553000033	0.3170124957488483	F	F	F
0.8888888891999969	0.8888888882000003	0.3170124957488483	F	F	F
0.2222222225000010	0.8888888882000003	0.3170124957488483	F	F	F
0.5555555557999980	0.8888888882000003	0.3170124957488483	F	F	F
0.0000000000000000	0.0000000000000000	0.3975777759823913	F	F	F
0.3333333332999970	0.0000000000000000	0.3975777759823913	F	F	F
0.6666666666000012	0.0000000000000000	0.3975777759823913	F	F	F
0.0000000002103135	0.3333333328999970	0.3975777759823913	F	F	F
0.3333333335000006	0.3333333328999970	0.3975777759823913	F	F	F
0.6666666668999994	0.3333333328999970	0.3975777759823913	F	F	F
0.9999999996666986	0.6666666672999995	0.3975777759823913	F	F	F
0.3333333329999988	0.6666666672999995	0.3975777759823913	F	F	F
0.6666666663000029	0.6666666672999995	0.3975777759823913	F	F	F
0.1111111113999996	0.1111111104999978	0.4771948603999974	F	F	F
0.4444444447999985	0.1111111104999978	0.4771948603999974	F	F	F
0.7777777781000026	0.1111111104999978	0.4771948603999974	F	F	F
0.1111111108999978	0.4444444449000002	0.4771948603999974	F	F	F
0.4444444442000020	0.4444444449000002	0.4771948603999974	F	F	F
0.7777777774999990	0.4444444449000002	0.4771948603999974	F	F	F
0.1111111111000014	0.7777777777999972	0.4771948603999974	F	F	F
0.4444444443999984	0.7777777777999972	0.4771948603999974	F	F	F
0.7777777777000026	0.7777777777999972	0.4771948603999974	F	F	F
0.8866398228031529	0.2233467553984213	0.5575172935801846	T	T	T
0.2233467550984231	0.2233467553984213	0.5575172935801846	T	T	T
0.5555260773860341	0.2222811784279272	0.5565958930986734	T	T	T

0.8891009548694884	0.5551314235610276	0.5569624523010185	T	T	T
0.2222811783279254	0.5555260772860394	0.5565958930986734	T	T	T
0.5555260775860377	0.5555260772860394	0.5565958930986734	T	T	T
0.8891009550694848	0.8891009540694883	0.5569624523010185	T	T	T
0.2233467554984231	0.8866398222031564	0.5575172935801846	T	T	T
0.5551314240610223	0.8891009540694883	0.5569624523010185	T	T	T
-0.0000438232624977	-0.0000438232624977	0.6374212432632351	T	T	T
0.3334209798249924	-0.0000438232624977	0.6374212432632351	T	T	T
0.6673701544789282	-0.0014069757578540	0.6372300663104501	T	T	T
-0.0000438230521841	0.3334209794249923	0.6374212432632351	T	T	T
0.3334099706839134	0.3334099700839098	0.6391156081678117	T	T	T
0.6665133925321738	0.3334099700839098	0.6391156081678117	T	T	T
0.9985930239088446	0.6673701551789265	0.6372300663104501	T	T	T
0.3334099701839116	0.6665133929321738	0.6391156081678117	T	T	T
0.6673701541789300	0.6673701551789265	0.6372300663104501	T	T	T
0.4444444444444429	0.4444444444444429	0.6754598835121026	T	T	T

H/Cu(111) $E_{ads} = -0.37$ eV

1.00000000000000

7.6579664403000001	0.0000000000000000	0.0000000000000000
3.8289832201000000	6.6319934786000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.5000000000000000

Cu H

45 1

Selective dynamics

Direct

0.8888888887999968	0.2222222223999992	0.3170124957488483	F	F	F
0.2222222221000010	0.2222222223999992	0.3170124957488483	F	F	F
0.5555555553999980	0.2222222223999992	0.3170124957488483	F	F	F
0.8888888890000004	0.5555555553000033	0.3170124957488483	F	F	F
0.2222222222999974	0.5555555553000033	0.3170124957488483	F	F	F
0.5555555556000016	0.5555555553000033	0.3170124957488483	F	F	F
0.8888888891999969	0.8888888882000003	0.3170124957488483	F	F	F
0.2222222225000010	0.8888888882000003	0.3170124957488483	F	F	F
0.5555555557999980	0.8888888882000003	0.3170124957488483	F	F	F
0.0000000000000000	0.0000000000000000	0.3975777759823913	F	F	F
0.3333333332999970	0.0000000000000000	0.3975777759823913	F	F	F
0.6666666666000012	0.0000000000000000	0.3975777759823913	F	F	F
0.0000000002103135	0.3333333328999970	0.3975777759823913	F	F	F
0.3333333335000006	0.3333333328999970	0.3975777759823913	F	F	F
0.6666666668999994	0.3333333328999970	0.3975777759823913	F	F	F
0.9999999996666986	0.6666666672999995	0.3975777759823913	F	F	F
0.3333333329999988	0.6666666672999995	0.3975777759823913	F	F	F
0.6666666663000029	0.6666666672999995	0.3975777759823913	F	F	F
0.1111111113999996	0.1111111104999978	0.4771948603999974	F	F	F
0.4444444447999985	0.1111111104999978	0.4771948603999974	F	F	F
0.7777777781000026	0.1111111104999978	0.4771948603999974	F	F	F
0.1111111108999978	0.4444444449000002	0.4771948603999974	F	F	F
0.4444444442000020	0.4444444449000002	0.4771948603999974	F	F	F
0.7777777774999990	0.4444444449000002	0.4771948603999974	F	F	F
0.1111111111000014	0.7777777777999972	0.4771948603999974	F	F	F
0.4444444443999984	0.7777777777999972	0.4771948603999974	F	F	F
0.7777777777000026	0.7777777777999972	0.4771948603999974	F	F	F
0.8874501517396469	0.2233216512500155	0.5572788594054141	T	T	T
0.2222222221000010	0.2222222223999992	0.5568544354221492	T	T	T
0.5558948636103316	0.2233216512500155	0.5572788594054141	T	T	T
0.8874501519396505	0.5558948635103369	0.5572788594054141	T	T	T

0.2233216511500137 0.5558948635103369 0.5572788594054141 T T T
0.5555555556000016 0.5555555553000033 0.5558035766684605 T T T
0.8888888891999969 0.8888888882000003 0.5569199566740252 T T T
0.2233216513500172 0.8874501511396504 0.5572788594054141 T T T
0.5558948640103316 0.8874501511396504 0.5572788594054141 T T T
-0.0000065769271703 -0.0000065769271703 0.6372703929523630 T T T
0.3323480718056384 0.0019705229887170 0.6374804122353983 T T T
0.6666798204543419 -0.0000065769271703 0.6372703929523630 T T T
0.0019705231990306 0.3323480714056384 0.6374804122353983 T T T
0.3323480720056420 0.3323480714056384 0.6374804122353983 T T T
0.6663306981439187 0.3340052704121586 0.6390192135417547 T T T
-0.0000065772604717 0.6666798211543402 0.6372703929523630 T T T
0.3340052705121603 0.6663306985439187 0.6390192135417547 T T T
0.6663306975439222 0.6663306985439187 0.6390192135417547 T T T
0.5555555555555571 0.5555555555555571 0.6757039139351266 T T T

H/Cu(111) $E_{ads} = -0.25$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
3.8289832201000000 6.6319934786000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu H
45 1
Selective dynamics
Direct
0.8888888887999968 0.2222222223999992 0.3170124957488483 F F F
0.2222222221000010 0.2222222223999992 0.3170124957488483 F F F
0.5555555553999980 0.2222222223999992 0.3170124957488483 F F F
0.8888888890000004 0.5555555553000033 0.3170124957488483 F F F
0.2222222222999974 0.5555555553000033 0.3170124957488483 F F F
0.5555555556000016 0.5555555553000033 0.3170124957488483 F F F
0.8888888891999969 0.8888888882000003 0.3170124957488483 F F F
0.2222222225000010 0.8888888882000003 0.3170124957488483 F F F
0.5555555557999980 0.8888888882000003 0.3170124957488483 F F F
0.0000000000000000 0.0000000000000000 0.3975777759823913 F F F
0.3333333332999970 0.0000000000000000 0.3975777759823913 F F F
0.6666666666000012 0.0000000000000000 0.3975777759823913 F F F
0.0000000002103135 0.3333333328999970 0.3975777759823913 F F F
0.3333333335000006 0.3333333328999970 0.3975777759823913 F F F
0.6666666668999994 0.3333333328999970 0.3975777759823913 F F F
0.9999999996666986 0.6666666672999995 0.3975777759823913 F F F
0.3333333329999988 0.6666666672999995 0.3975777759823913 F F F
0.6666666663000029 0.6666666672999995 0.3975777759823913 F F F
0.1111111113999996 0.1111111104999978 0.4771948603999974 F F F
0.4444444447999985 0.1111111104999978 0.4771948603999974 F F F
0.7777777781000026 0.1111111104999978 0.4771948603999974 F F F
0.1111111108999978 0.4444444449000002 0.4771948603999974 F F F
0.4444444442000020 0.4444444449000002 0.4771948603999974 F F F
0.7777777774999990 0.4444444449000002 0.4771948603999974 F F F
0.1111111111000014 0.7777777777999972 0.4771948603999974 F F F
0.4444444443999984 0.7777777777999972 0.4771948603999974 F F F
0.7777777777000026 0.7777777777999972 0.4771948603999974 F F F
0.8867993652975215 0.2230811542556982 0.5574142528661834 T T T
0.2234528137467773 0.2230811542556982 0.5574142528661834 T T T
0.5555849347640690 0.2221634636718567 0.5560232755724758 T T T
0.8890170116140805 0.5552993100718432 0.5569065150610524 T T T
0.2227409521377706 0.5550064064951596 0.5569174655508984 T T T

0.5555859745670724 0.5550064064951596 0.5569174655508984 T T T
0.8880564648967140 0.8898952692968374 0.5571258417366953 T T T
0.2227130253596150 0.8879072824807720 0.5571428518727688 T T T
0.5553815990064443 0.8898952692968374 0.5571258417366953 T T T
0.0013114154991728 -0.0010071295163130 0.6374402110391225 T T T
0.3330290473171373 -0.0010071295163130 0.6374402110391225 T T T
0.6667361732961460 -0.0001390133922898 0.6378449838198373 T T T
-0.0000460632090164 0.3334254597386569 0.6371360467679585 T T T
0.3337511499533115 0.3327398862264601 0.6390589082538192 T T T
0.6668422971202255 0.3327398862264601 0.6390589082538192 T T T
-0.0008376083121025 0.6671889287701314 0.6372158119552087 T T T
0.3331081988826763 0.6671169355346444 0.6380612538748934 T T T
0.6669820128086721 0.6671889287701314 0.6372158119552087 T T T
0.5001363260990586 0.3330606778018851 0.6806890771854014 T T T

H/Cu(111) $E_{ads} = -0.19$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
3.8289832201000000 6.6319934786000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu H
45 1
Selective dynamics
Direct
0.8888888887999968 0.2222222223999992 0.3170124957488483 F F F
0.2222222221000010 0.2222222223999992 0.3170124957488483 F F F
0.5555555553999980 0.2222222223999992 0.3170124957488483 F F F
0.8888888890000004 0.5555555553000033 0.3170124957488483 F F F
0.2222222222999974 0.5555555553000033 0.3170124957488483 F F F
0.5555555556000016 0.5555555553000033 0.3170124957488483 F F F
0.8888888891999969 0.8888888882000003 0.3170124957488483 F F F
0.2222222225000010 0.8888888882000003 0.3170124957488483 F F F
0.5555555557999980 0.8888888882000003 0.3170124957488483 F F F
0.0000000000000000 0.0000000000000000 0.3975777759823913 F F F
0.3333333332999970 0.0000000000000000 0.3975777759823913 F F F
0.6666666666000012 0.0000000000000000 0.3975777759823913 F F F
0.0000000002103135 0.3333333328999970 0.3975777759823913 F F F
0.3333333335000006 0.3333333328999970 0.3975777759823913 F F F
0.6666666668999994 0.3333333328999970 0.3975777759823913 F F F
0.9999999996666986 0.6666666672999995 0.3975777759823913 F F F
0.3333333329999988 0.6666666672999995 0.3975777759823913 F F F
0.6666666663000029 0.6666666672999995 0.3975777759823913 F F F
0.1111111113999996 0.1111111104999978 0.4771948603999974 F F F
0.4444444447999985 0.1111111104999978 0.4771948603999974 F F F
0.7777777781000026 0.1111111104999978 0.4771948603999974 F F F
0.1111111108999978 0.4444444449000002 0.4771948603999974 F F F
0.4444444442000020 0.4444444449000002 0.4771948603999974 F F F
0.7777777774999990 0.4444444449000002 0.4771948603999974 F F F
0.1111111111000014 0.7777777777999972 0.4771948603999974 F F F
0.4444444443999984 0.7777777777999972 0.4771948603999974 F F F
0.7777777777000026 0.7777777777999972 0.4771948603999974 F F F
0.8887998774522687 0.2224002450954551 0.5571784991213663 T T T
0.2224820447019764 0.2224820450019746 0.5565664549730710 T T T
0.5550359101960471 0.2224820450019746 0.5565664549730710 T T T
0.8897491428182915 0.5551254283908582 0.5570103066991448 T T T
0.2224820449019728 0.5550359100960525 0.5565664549730710 T T T
0.5551254286908565 0.5551254283908582 0.5570103066991448 T T T

0.8887998778522688 0.8887998768522722 0.5571784991213663 T T T
0.2224002451954569 0.8887998768522722 0.5571784991213663 T T T
0.5551254288908529 0.8897491420182915 0.5570103066991448 T T T
-0.0000000000000000 0.0000000000000000 0.6374354529740881 T T T
0.3334161977250601 -0.0003386440474074 0.6376236275529351 T T T
0.6669224462223453 -0.0003386440474074 0.6376236275529351 T T T
-0.0003386438370939 0.3334161973250601 0.6376236275529351 T T T
0.3333333335000006 0.3333333328999970 0.6372877404120828 T T T
0.6669224465223436 0.3334161973250601 0.6376236275529351 T T T
-0.0003386443807086 0.6669224469223436 0.6376236275529351 T T T
0.3334161974250620 0.6669224469223436 0.6376236275529351 T T T
0.6666666663000029 0.6666666672999995 0.6373472059964619 T T T
0.3333333350000061 0.3333333328999970 0.6965785372491520 T T T

H/Cu(100) $E_{ads} = -0.28$ eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu H
45 1
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.3173193249345303 F F F
0.3333333332999970 0.0000000000000000 0.3173193249345303 F F F
0.6666666666000012 0.0000000000000000 0.3173193249345303 F F F
0.0000000000000000 0.3333333332999970 0.3173193249345303 F F F
0.3333333332999970 0.3333333332999970 0.3173193249345303 F F F
0.6666666666000012 0.3333333332999970 0.3173193249345303 F F F
0.0000000000000000 0.6666666666000012 0.3173193249345303 F F F
0.3333333332999970 0.6666666666000012 0.3173193249345303 F F F
0.6666666666000012 0.6666666666000012 0.3173193249345303 F F F
0.1666666667000030 0.1666666667000030 0.3854655552433357 F F F
0.5000000000000000 0.1666666667000030 0.3854655552433357 F F F
0.8333333332999970 0.1666666667000030 0.3854655552433357 F F F
0.1666666667000030 0.5000000000000000 0.3854655552433357 F F F
0.5000000000000000 0.5000000000000000 0.3854655552433357 F F F
0.8333333332999970 0.5000000000000000 0.3854655552433357 F F F
0.1666666667000030 0.8333333332999970 0.3854655552433357 F F F
0.5000000000000000 0.8333333332999970 0.3854655552433357 F F F
0.8333333332999970 0.8333333332999970 0.3854655552433357 F F F
0.0000000000000000 0.0000000000000000 0.4552941175999976 F F F
0.3333333332999970 0.0000000000000000 0.4552941175999976 F F F
0.6666666666000012 0.0000000000000000 0.4552941175999976 F F F
0.0000000000000000 0.3333333332999970 0.4552941175999976 F F F
0.3333333332999970 0.3333333332999970 0.4552941175999976 F F F
0.6666666666000012 0.3333333332999970 0.4552941175999976 F F F
0.0000000000000000 0.6666666666000012 0.4552941175999976 F F F
0.3333333332999970 0.6666666666000012 0.4552941175999976 F F F
0.6666666666000012 0.6666666666000012 0.4552941175999976 F F F
0.1678677220841475 0.1678677220841475 0.5255342423523082 T T T
0.5000000000000000 0.1667325759562782 0.5247965904083661 T T T
0.8321322779158523 0.1678677220841475 0.5255342423523082 T T T
0.1667325759562782 0.5000000000000000 0.5247965904083661 T T T
0.5000000000000000 0.5000000000000000 0.5229750229203731 T T T
0.8332674240437219 0.5000000000000000 0.5247965904083661 T T T
0.1678677220841475 0.8321322779158523 0.5255342423523082 T T T

0.5000000000000000	0.8332674240437219	0.5247965904083661	T	T	T
0.8321322779158523	0.8321322779158523	0.5255342423523082	T	T	T
-0.0000000000000000	-0.0000000000000000	0.5931412445802329	T	T	T
0.3340209629129142	-0.0000000000000000	0.5928974922673421	T	T	T
0.6659790369870838	-0.0000000000000000	0.5928974922673421	T	T	T
-0.0000000000000000	0.3340209629129142	0.5928974922673421	T	T	T
0.3342230951242640	0.3342230951242640	0.5943171606977540	T	T	T
0.6657769047757341	0.3342230951242640	0.5943171606977540	T	T	T
-0.0000000000000000	0.6659790369870838	0.5928974922673421	T	T	T
0.3342230951242640	0.6657769047757341	0.5943171606977540	T	T	T
0.6657769047757341	0.6657769047757341	0.5943171606977540	T	T	T
0.5000000000000000	0.5000000000000000	0.6155136317952784	T	T	T

H/Cu(100) E_{ads} = −0.15 eV
1.00000000000000
7.6579664403000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.5000000000000000
Cu H
45 1
Selective dynamics
Direct

0.0000000000000000	0.0000000000000000	0.3173193249345303	F	F	F
0.3333333332999970	0.0000000000000000	0.3173193249345303	F	F	F
0.6666666666000012	0.0000000000000000	0.3173193249345303	F	F	F
0.0000000000000000	0.3333333332999970	0.3173193249345303	F	F	F
0.3333333332999970	0.3333333332999970	0.3173193249345303	F	F	F
0.6666666666000012	0.3333333332999970	0.3173193249345303	F	F	F
0.0000000000000000	0.6666666666000012	0.3173193249345303	F	F	F
0.3333333332999970	0.6666666666000012	0.3173193249345303	F	F	F
0.6666666666000012	0.6666666666000012	0.3173193249345303	F	F	F
0.1666666667000030	0.1666666667000030	0.3854655552433357	F	F	F
0.5000000000000000	0.1666666667000030	0.3854655552433357	F	F	F
0.8333333332999970	0.1666666667000030	0.3854655552433357	F	F	F
0.1666666667000030	0.5000000000000000	0.3854655552433357	F	F	F
0.5000000000000000	0.5000000000000000	0.3854655552433357	F	F	F
0.8333333332999970	0.5000000000000000	0.3854655552433357	F	F	F
0.1666666667000030	0.8333333332999970	0.3854655552433357	F	F	F
0.5000000000000000	0.8333333332999970	0.3854655552433357	F	F	F
0.8333333332999970	0.8333333332999970	0.3854655552433357	F	F	F
0.0000000000000000	0.0000000000000000	0.4552941175999976	F	F	F
0.3333333332999970	0.0000000000000000	0.4552941175999976	F	F	F
0.6666666666000012	0.0000000000000000	0.4552941175999976	F	F	F
0.0000000000000000	0.3333333332999970	0.4552941175999976	F	F	F
0.3333333332999970	0.3333333332999970	0.4552941175999976	F	F	F
0.6666666666000012	0.3333333332999970	0.4552941175999976	F	F	F
0.0000000000000000	0.6666666666000012	0.4552941175999976	F	F	F
0.3333333332999970	0.6666666666000012	0.4552941175999976	F	F	F
0.6666666666000012	0.6666666666000012	0.4552941175999976	F	F	F
0.1680410990372684	0.1681148679885009	0.5254752922975497	T	T	T
0.5000000000000000	0.1657610189907935	0.5242996308499991	T	T	T
0.8319589009627315	0.1681148679885009	0.5254752922975497	T	T	T
0.1680410990372684	0.4985517987115021	0.5254752922975497	T	T	T
0.5000000000000000	0.5009056477092094	0.5242996308499991	T	T	T
0.8319589009627315	0.4985517987115021	0.5254752922975497	T	T	T
0.1664356809303681	0.8333333332999970	0.5251760936719171	T	T	T
0.5000000000000000	0.8333333332999970	0.5250205338244555	T	T	T

0.8335643190696319	0.8333333332999970	0.5251760936719171	T	T	T
0.0000000000000000	0.0010083226964896	0.5932757162840799	T	T	T
0.3327791628431840	-0.0012833889807971	0.5932805254564079	T	T	T
0.6672208370568140	-0.0012833889807971	0.5932805254564079	T	T	T
0.0000000000000000	0.3333333332999970	0.5929917769430746	T	T	T
0.3349106496934491	0.3333333332999970	0.5957178332050553	T	T	T
0.6650893502065491	0.3333333332999970	0.5957178332050553	T	T	T
0.0000000000000000	0.6656583439035114	0.5932757162840799	T	T	T
0.3327791628431840	0.6679500555807981	0.5932805254564079	T	T	T
0.6672208370568140	0.6679500555807981	0.5932805254564079	T	T	T
0.5000000000000000	0.3333333332999970	0.6367886676839118	T	T	T

H/Cu(100) E_{ads} = 0.34 eV

1.00000000000000

7.6579664403000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.6579664403000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.5000000000000000

Cu H

45 1

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.3173193249345303	F	F	F
0.3333333332999970	0.0000000000000000	0.3173193249345303	F	F	F
0.6666666666000012	0.0000000000000000	0.3173193249345303	F	F	F
0.0000000000000000	0.3333333332999970	0.3173193249345303	F	F	F
0.3333333332999970	0.3333333332999970	0.3173193249345303	F	F	F
0.6666666666000012	0.3333333332999970	0.3173193249345303	F	F	F
0.0000000000000000	0.6666666666000012	0.3173193249345303	F	F	F
0.3333333332999970	0.6666666666000012	0.3173193249345303	F	F	F
0.6666666666000012	0.6666666666000012	0.3173193249345303	F	F	F
0.1666666667000030	0.1666666667000030	0.3854655552433357	F	F	F
0.5000000000000000	0.1666666667000030	0.3854655552433357	F	F	F
0.8333333332999970	0.1666666667000030	0.3854655552433357	F	F	F
0.1666666667000030	0.5000000000000000	0.3854655552433357	F	F	F
0.5000000000000000	0.5000000000000000	0.3854655552433357	F	F	F
0.8333333332999970	0.5000000000000000	0.3854655552433357	F	F	F
0.1666666667000030	0.8333333332999970	0.3854655552433357	F	F	F
0.5000000000000000	0.8333333332999970	0.3854655552433357	F	F	F
0.8333333332999970	0.8333333332999970	0.3854655552433357	F	F	F
0.0000000000000000	0.0000000000000000	0.4552941175999976	F	F	F
0.3333333332999970	0.0000000000000000	0.4552941175999976	F	F	F
0.6666666666000012	0.0000000000000000	0.4552941175999976	F	F	F
0.0000000000000000	0.3333333332999970	0.4552941175999976	F	F	F
0.3333333332999970	0.3333333332999970	0.4552941175999976	F	F	F
0.6666666666000012	0.3333333332999970	0.4552941175999976	F	F	F
0.0000000000000000	0.6666666666000012	0.4552941175999976	F	F	F
0.3333333332999970	0.6666666666000012	0.4552941175999976	F	F	F
0.6666666666000012	0.6666666666000012	0.4552941175999976	F	F	F
0.1671858341119213	0.1671858341119213	0.5248475093959325	T	T	T
0.4994808325880817	0.1671858341119213	0.5248475093959325	T	T	T
0.8333333332999970	0.1680203333596455	0.5258103342643998	T	T	T
0.1671858341119213	0.4994808325880817	0.5248475093959325	T	T	T
0.4994808325880817	0.4994808325880817	0.5248475093959325	T	T	T
0.8333333332999970	0.4986463333403575	0.5258103342643998	T	T	T
0.1680203333596455	0.8333333332999970	0.5258103342643998	T	T	T
0.4986463333403575	0.8333333332999970	0.5258103342643998	T	T	T
0.8333333332999970	0.8333333332999970	0.5246593176993881	T	T	T

-0.0004562286290088	-0.0004562286290088	0.5932773568086529	T	T	T
0.3333333332999970	0.0012844922623037	0.5945748860474136	T	T	T
0.6671228952290100	-0.0004562286290088	0.5932773568086529	T	T	T
0.0012844922623037	0.3333333332999970	0.5945748860474136	T	T	T
0.3333333332999970	0.3333333332999970	0.5949471830435571	T	T	T
0.6653821743376975	0.3333333332999970	0.5945748860474136	T	T	T
-0.0004562286290088	0.6671228952290100	0.5932773568086529	T	T	T
0.3333333332999970	0.6653821743376975	0.5945748860474136	T	T	T
0.6671228952290100	0.6671228952290100	0.5932773568086529	T	T	T
0.3333333332999970	0.3333333332999970	0.6543262697821496	T	T	T

H/Cu(211) $E_{ads} = -0.33$ eV
1.00000000000000
6.2527034153000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.6579664403000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.3164343000000009
Cu H
45 1
Selective dynamics
Direct

0.0061862950247047	0.1666666667000030	0.3120745335338029	F	F	F
0.0061862950247047	0.5000000000000000	0.3120745335338029	F	F	F
0.0061862950247047	0.8333333332999970	0.3120745335338029	F	F	F
0.3355456677560653	0.0000000000000000	0.3354619372229379	F	F	F
0.3355456677560653	0.3333333332999970	0.3354619372229379	F	F	F
0.3355456677560653	0.6666666666000012	0.3354619372229379	F	F	F
0.6630854692850079	0.1666666667000030	0.3607350091654666	F	F	F
0.6630854692850079	0.5000000000000000	0.3607350091654666	F	F	F
0.6630854692850079	0.8333333332999970	0.3607350091654666	F	F	F
0.9944057463905267	0.0000000000000000	0.3915351276171819	F	F	F
0.9944057463905267	0.3333333332999970	0.3915351276171819	F	F	F
0.9944057463905267	0.6666666666000012	0.3915351276171819	F	F	F
0.3330656692422309	0.1666666667000030	0.4179888222780335	F	F	F
0.3330656692422309	0.5000000000000000	0.4179888222780335	F	F	F
0.3330656692422309	0.8333333332999970	0.4179888222780335	F	F	F
0.6656564241704075	0.0000000000000000	0.4448469552356400	F	F	F
0.6656564241704075	0.3333333332999970	0.4448469552356400	F	F	F
0.6656564241704075	0.6666666666000012	0.4448469552356400	F	F	F
0.0003515212697778	0.1666666667000030	0.4732099031121066	F	F	F
0.0003515212697778	0.5000000000000000	0.4732099031121066	F	F	F
0.0003515212697778	0.8333333332999970	0.4732099031121066	F	F	F
0.3333333329999988	0.0000000000000000	0.5000000000000000	F	F	F
0.3333333329999988	0.3333333332999970	0.5000000000000000	F	F	F
0.3333333329999988	0.6666666666000012	0.5000000000000000	F	F	F
0.6663151448302216	0.1666666667000030	0.5267900968878934	F	F	F
0.6663151448302216	0.5000000000000000	0.5267900968878934	F	F	F
0.6663151448302216	0.8333333332999970	0.5267900968878934	F	F	F
0.0004764890106055	-0.0004520286665911	0.5550345557769796	T	T	T
0.0010887330110503	0.3333333332999970	0.5547653722195123	T	T	T
0.0004764890106055	0.6671186952665923	0.5550345557769796	T	T	T
0.3331757387897274	0.1681821906669863	0.5825413251767717	T	T	T
0.3331757387897274	0.4984844760330165	0.5825413251767717	T	T	T
0.3315354527270334	0.8333333332999970	0.5818294941504877	T	T	T
0.6701891776861125	0.0017905934815645	0.6086298742056280	T	T	T
0.6724142833091548	0.3333333332999970	0.6073842714211443	T	T	T
0.6701891776861125	0.6648760731184367	0.6086298742056280	T	T	T
0.0012058191227569	0.1673749941841325	0.6389556089875524	T	T	T

0.0012058191227569	0.4992916725158705	0.6389556089875524	T	T	T
-0.0018734284817517	0.8333333332999970	0.6390185663532825	T	T	T
0.3263998987535431	-0.0018617613661684	0.6641841125896709	T	T	T
0.3270518443070954	0.3333333332999970	0.6670418969919848	T	T	T
0.3263998987535431	0.6685284279661697	0.6641841125896709	T	T	T
0.6579091803353461	0.1669461869723029	0.6885132939439396	T	T	T
0.6579091803353461	0.4997204797277001	0.6885132939439396	T	T	T
0.6567194868007564	0.8333333332999970	0.6876896419627370	T	T	T
0.5191631211993661	0.3333333333333357	0.7174259351680757	T	T	T

H/Cu(211) $E_{ads} = -0.26$ eV

1.00000000000000

6.2527034153000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.6579664403000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.3164343000000009

Cu H

45 1

Selective dynamics

Direct

0.0061862950247047	0.1666666667000030	0.3120745335338029	F	F	F
0.0061862950247047	0.5000000000000000	0.3120745335338029	F	F	F
0.0061862950247047	0.8333333332999970	0.3120745335338029	F	F	F
0.3355456677560653	0.0000000000000000	0.3354619372229379	F	F	F
0.3355456677560653	0.3333333332999970	0.3354619372229379	F	F	F
0.3355456677560653	0.6666666666000012	0.3354619372229379	F	F	F
0.6630854692850079	0.1666666667000030	0.3607350091654666	F	F	F
0.6630854692850079	0.5000000000000000	0.3607350091654666	F	F	F
0.6630854692850079	0.8333333332999970	0.3607350091654666	F	F	F
0.9944057463905267	0.0000000000000000	0.3915351276171819	F	F	F
0.9944057463905267	0.3333333332999970	0.3915351276171819	F	F	F
0.9944057463905267	0.6666666666000012	0.3915351276171819	F	F	F
0.3330656692422309	0.1666666667000030	0.4179888222780335	F	F	F
0.3330656692422309	0.5000000000000000	0.4179888222780335	F	F	F
0.3330656692422309	0.8333333332999970	0.4179888222780335	F	F	F
0.6656564241704075	0.0000000000000000	0.4448469552356400	F	F	F
0.6656564241704075	0.3333333332999970	0.4448469552356400	F	F	F
0.6656564241704075	0.6666666666000012	0.4448469552356400	F	F	F
0.0003515212697778	0.1666666667000030	0.4732099031121066	F	F	F
0.0003515212697778	0.5000000000000000	0.4732099031121066	F	F	F
0.0003515212697778	0.8333333332999970	0.4732099031121066	F	F	F
0.3333333329999988	0.0000000000000000	0.5000000000000000	F	F	F
0.3333333329999988	0.3333333332999970	0.5000000000000000	F	F	F
0.3333333329999988	0.6666666666000012	0.5000000000000000	F	F	F
0.6663151448302216	0.1666666667000030	0.5267900968878934	F	F	F
0.6663151448302216	0.5000000000000000	0.5267900968878934	F	F	F
0.6663151448302216	0.8333333332999970	0.5267900968878934	F	F	F
-0.0017961033252065	0.0000000000000000	0.5550288357314237	T	T	T
-0.0012645121847303	0.3334472692668528	0.5549862403266772	T	T	T
-0.0012645121847303	0.6665527306331457	0.5549862403266772	T	T	T
0.3279984244383635	0.1687089316850480	0.5826005165161711	T	T	T
0.3275096200923395	0.5000000000000000	0.5818819772464667	T	T	T
0.3279984244383635	0.8312910683149519	0.5826005165161711	T	T	T
0.6644921878087388	0.0000000000000000	0.6080175129516585	T	T	T
0.6653691158228228	0.3332581550938636	0.6078234197846414	T	T	T
0.6653691158228228	0.6667418448061344	0.6078234197846414	T	T	T
-0.0058001775049479	0.1672284418529086	0.6388578157504681	T	T	T
-0.0117248701821582	0.5000000000000000	0.6392636287940194	T	T	T

-0.0058001775049479	0.8327715581470914	0.6388578157504681	T	T	T
0.3213330145258635	0.0000000000000000	0.6640879042168247	T	T	T
0.3163628831458614	0.3331860942879660	0.6664957160741225	T	T	T
0.3163628831458614	0.6668139056120317	0.6664957160741225	T	T	T
0.6524970066499486	0.1652032953371339	0.6873153539704874	T	T	T
0.6475832348287833	0.5000000000000000	0.6879252268614774	T	T	T
0.6524970066499486	0.8347967046628664	0.6873153539704874	T	T	T
0.3866563272873985	0.5000000000000000	0.7086593559316667	T	T	T

11.8 *CO_2 Adsorption

CO_2/Cu(533)	E_{ads} = −0.28 eV				
1.00000000000000					
10.3878408006999994	0.0000000000000000	0.0000000000000000			
4.5828709415000004	6.0103788927000004	0.0000000000000000			
0.0000000000000000	0.0000000000000000	26.5000000000000000			
Cu C O					
60 1 2					
Selective dynamics					
Direct					
0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0469768822945769	0.2943176707704073	0.4659981669821640	T	T	T
0.0469646729222529	0.6276303619521507	0.4660213975936221	T	T	T
0.0469462139787994	0.9609637147755942	0.4660013560190434	T	T	T
0.3034081512920671	0.2472430305411672	0.4868385893074947	T	T	T
0.3033287132861705	0.5806170854480039	0.4868401893525545	T	T	T
0.3034449908294059	0.9138677670171321	0.4867832607150457	T	T	T
0.5585107888692606	0.2013075166169708	0.5068998634191058	T	T	T
0.5586756497475563	0.5345328899359869	0.5068959083039468	T	T	T
0.5587357154230538	0.8677369713350720	0.5068868064573621	T	T	T
0.8152298832885092	0.1540274720237422	0.5275820370255710	T	T	T
0.8153536104009235	0.4871484711738492	0.5275965428647291	T	T	T
0.8152702819610883	0.8206443104305139	0.5275870853453043	T	T	T

0.0718399174954448 0.1069911825433070 0.5482443739742351 T T T
0.0718595091192664 0.4403316217927313 0.5483105364127375 T T T
0.0717631003060747 0.7737221365928123 0.5483337444706202 T T T
0.3267877468644237 0.0610954312914311 0.5691770083174822 T T T
0.3264533763940935 0.3948563988198026 0.5692850965021652 T T T
0.3266597653029142 0.7280255415021919 0.5692042980234994 T T T
0.5835904584247252 0.0138632926955081 0.5889395221712989 T T T
0.5835369393881524 0.3472895624008956 0.5889219582114189 T T T
0.5836148239187530 0.6805031569333611 0.5889822894786100 T T T
0.8426699460591471 0.6310527671472198 0.6093548245828623 T T T
0.8427932576749625 0.2977622137637379 0.6094900675003088 T T T
0.8424964740911334 0.9649735322266205 0.6093706291726260 T T T
0.0978330236433324 0.5855526361956325 0.6327944614988442 T T T
0.0983571189420099 0.2516375759651105 0.6325523829554111 T T T
0.0981780847488414 0.9186351947833040 0.6326200025996114 T T T
0.3514549605943008 0.5409576425498390 0.6518074622882516 T T T
0.3514519533704293 0.2072758120815195 0.6517528052806183 T T T
0.3513497088113013 0.8740285927853918 0.6519801703984492 T T T
0.6048154387313381 0.4962516716674524 0.6720712074670073 T T T
0.6037855893610228 0.1641016043722808 0.6721077837809493 T T T
0.6040330722717761 0.8299973253030902 0.6720961209033507 T T T
0.8593320864494434 0.4510876923466541 0.6897229224332665 T T T
0.8589787939583334 0.1174560286442050 0.6897773092866081 T T T
0.8568824354325368 0.7862510552542935 0.6893847431525352 T T T
0.2046428766811887 0.4923493231789211 0.7705174349932248 T T T
0.2059460363233691 0.6464813515299305 0.7706184498116391 T T T
0.2027446901684455 0.3387304627883861 0.7708034180898540 T T T

CO_2/Cu(533) E_{ads} = −0.27 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 2
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F

0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0474521541038687 0.2938742453189714 0.4659542055529251 T T T
0.0475682316299507 0.6271071908773832 0.4659263940126804 T T T
0.0475430153871073 0.9604698111499304 0.4659333646466671 T T T
0.3043714548608681 0.2463723781976958 0.4867571417973147 T T T
0.3044435508557424 0.5796796447439693 0.4867457395065754 T T T
0.3043356978805689 0.9131112984754978 0.4867628878072454 T T T
0.5600285154655906 0.2000053364986857 0.5068520567039946 T T T
0.5599494979046981 0.5335085258842936 0.5068755644154075 T T T
0.5599713295006156 0.8666310732920499 0.5068672595822302 T T T
0.8170882401571935 0.1524388058632774 0.5275521673003668 T T T
0.8169380451924551 0.4858394371406157 0.5276081059221746 T T T
0.8171691803996930 0.8189748548801670 0.5275544923016277 T T T
0.0738726368612592 0.1052991251574914 0.5482507958959936 T T T
0.0739161337996028 0.4385700279171580 0.5482504901217673 T T T
0.0740238783518967 0.7718117802956385 0.5482182188478034 T T T
0.3290076866250826 0.0592508868272860 0.5691311865428147 T T T
0.3290125512311245 0.3926182077098637 0.5690989723215604 T T T
0.3289715331391585 0.7260179521235376 0.5691421008094656 T T T
0.5863562446875705 0.0114565532477971 0.5887914126280640 T T T
0.5862876377699401 0.3450366549620049 0.5887990564818394 T T T
0.5861147327448502 0.6783791558730689 0.5889598549747760 T T T
0.8455673444735037 0.6287733759988914 0.6094029171277285 T T T
0.8455753296061937 0.2953975302218305 0.6094507937892307 T T T
0.8457455873636135 0.9619893597964608 0.6093351151560218 T T T
0.1013694240529479 0.5824708603782900 0.6326732983498972 T T T
0.1013856007368986 0.2491619896366220 0.6326038084052733 T T T
0.1013562679408529 0.9158090355785030 0.6326067056113037 T T T
0.3549106891030801 0.5378620053351457 0.6516043925503218 T T T
0.3549643544859356 0.2042725109501818 0.6515431391988767 T T T
0.3546328034547119 0.8712867553900464 0.6518603904364199 T T T
0.6080926409912739 0.4933478107092398 0.6719783462364615 T T T
0.6082886307421319 0.1600095231227581 0.6716762209536407 T T T
0.6079362922979296 0.8269247045708086 0.6719672740873905 T T T
0.8625308487716422 0.4481588096003249 0.6896905820169372 T T T
0.8625384409761232 0.1144762778963252 0.6897164757927159 T T T
0.8621581547577857 0.7817220165923137 0.6896393117788606 T T T
0.2903413284299638 0.4212474730826005 0.7745354784876938 T T T
0.2878758777646422 0.5785222714694476 0.7747764141222626 T T T
0.2925202690220980 0.2642136766435944 0.7746350225641371 T T T

CO_2/Cu(533) E_{ads} = −0.27 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 2
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F

0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0472917071107192	0.2940654722597381	0.4659681419597689	T	T	T
0.0473544897590758	0.6273512409948375	0.4659588992830017	T	T	T
0.0473068604176683	0.9607089788010013	0.4659295196003740	T	T	T
0.3040335971720075	0.2467143203507424	0.4867085357612473	T	T	T
0.3040315328473727	0.5801480401573620	0.4867228056492095	T	T	T
0.3039754545118726	0.9134509745586219	0.4867215762181105	T	T	T
0.5596732069095567	0.2004242403062798	0.5068135894704296	T	T	T
0.5596372581904970	0.5337795326885998	0.5068498731388539	T	T	T
0.5596184294987829	0.8670967494853121	0.5068542049019072	T	T	T
0.8166446224925387	0.1529198321122576	0.5275793916169552	T	T	T
0.8165029716412655	0.4864180681060579	0.5276094164565217	T	T	T
0.8166468640461668	0.8195868508075208	0.5275774991627408	T	T	T
0.0732367577080479	0.1059027228262402	0.5482607700760848	T	T	T
0.0733340768632593	0.4392478486983453	0.5482787926737299	T	T	T
0.0733432761690425	0.7726641856660731	0.5482554579986778	T	T	T
0.3284094882642153	0.0598468748862951	0.5690266195491495	T	T	T
0.3285222074083995	0.3932664094448974	0.5689460508861174	T	T	T
0.3284663787644176	0.7268164536590308	0.5690391702668414	T	T	T
0.5858422025607264	0.0122185104357149	0.5887619643878993	T	T	T
0.5859038229497009	0.3455884701898894	0.5888051770609246	T	T	T
0.5855740654912350	0.6791617193771418	0.5888913733572447	T	T	T
0.8450530195039179	0.6296686095702401	0.6094988440458802	T	T	T
0.8449904698358868	0.2963369240964996	0.6094643288062636	T	T	T
0.8451225376097155	0.9628310289284334	0.6094704599357745	T	T	T
0.1010852445603018	0.5832463621025558	0.6325693744284245	T	T	T
0.1008665626875325	0.2499187675564392	0.6325642868417741	T	T	T
0.1010691888535371	0.9164679448465806	0.6327108012143887	T	T	T
0.3545126756254182	0.5387438265232317	0.6513693040061824	T	T	T
0.3545700457389589	0.2049627603433897	0.6513411312372747	T	T	T
0.3541623235929922	0.8722726381708186	0.6519303118407069	T	T	T
0.6074329129177479	0.4946935656941751	0.6719415778488788	T	T	T
0.6076765615015335	0.1608790510784995	0.6717584677389894	T	T	T
0.6074226893171212	0.8280219228817575	0.6719987013935139	T	T	T
0.8618979291002423	0.4490989270662620	0.6897127530190231	T	T	T
0.8620827288500393	0.1157068245769807	0.6896733546034702	T	T	T
0.8621069125171446	0.7823746071674740	0.6897759773859888	T	T	T
0.3147182010547254	0.3886940424625063	0.7773884958307697	T	T	T
0.1932833347146706	0.4125790756229425	0.7709891280635244	T	T	T

0.4358898930560532 0.3650807084302718 0.7841520898333165 T T T

CO_2/Cu(533) E_{ads} = −0.27 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 2
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0473802020235252 0.2938607370848333 0.4659932630332138 T T T
0.0472901001733107 0.6272773743617366 0.4660479832002071 T T T
0.0475137527231503 0.9604349726206435 0.4659799052894135 T T T
0.3039647153334247 0.2465986506316983 0.4867735071728955 T T T
0.3041284993126291 0.5798588161691116 0.4867538223766026 T T T
0.3041624315196572 0.9132733033362986 0.4867618059392865 T T T
0.5596946377854924 0.2001751467042294 0.5068364541884028 T T T
0.5598969108116389 0.5334229999752074 0.5068080857678625 T T T
0.5596566447311626 0.8668934787571523 0.5068874831985773 T T T
0.8170325777265415 0.1522721894343114 0.5275788904966128 T T T
0.8167550719647508 0.4859253497761226 0.5276438488711545 T T T
0.8165485382953239 0.8193944978134183 0.5276664224680292 T T T
0.0735379936179194 0.1054767998716439 0.5483512463434396 T T T
0.0732039412521541 0.4389618850229476 0.5484154750162816 T T T
0.0735197443683691 0.7721377993276196 0.5483839537570132 T T T
0.3283524208810035 0.0598477766967106 0.5692193215292325 T T T
0.3283402817827683 0.3927659665505761 0.5690277779575623 T T T
0.3286446421069402 0.7264444037106246 0.5689699898046514 T T T
0.5854330724894358 0.0121962130419242 0.5888593006345180 T T T
0.5861933720528534 0.3449263901498053 0.5886471182158320 T T T
0.5857291127445478 0.6787305420193274 0.5888804153491689 T T T
0.8447797082588925 0.6294936242212634 0.6096148181859689 T T T

0.8451016338115284 0.2957514528564370 0.6094891123995707 T T T
0.8451257611869099 0.9623267681869772 0.6095383542733714 T T T
0.1005760261114167 0.5830497346330263 0.6327818829058119 T T T
0.1006310294109772 0.2497435078101573 0.6328872301136452 T T T
0.1009489556536053 0.9161321460944147 0.6328039291030682 T T T
0.3545840542453034 0.5379118924801619 0.6509395567083769 T T T
0.3538427526906062 0.2053822095393901 0.6520020618268199 T T T
0.3539310849241707 0.8718908526975312 0.6518204629928104 T T T
0.6069189600976187 0.4942635072751723 0.6718382880045526 T T T
0.6071264409409538 0.1608555004301975 0.6717830164161029 T T T
0.6068706342315281 0.8279384063464539 0.6720428113353860 T T T
0.8611131454741286 0.4490564008431867 0.6898057451264692 T T T
0.8613449394821306 0.1156696489302981 0.6897375000113319 T T T
0.8612576353958276 0.7824149906867564 0.6899624121530679 T T T
0.3203532012071871 0.5752062492354318 0.7798607361315267 T T T
0.2067792238565240 0.5798363671099210 0.7729297451928666 T T T
0.4336134460976925 0.5708906724635956 0.7871268140447913 T T T

CO_2/Cu(533) E_{ads} = −0.26 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 2
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0472175465736673 0.2940908971764550 0.4659474528666174 T T T
0.0473226874652759 0.6273131300816495 0.4659459203760496 T T T
0.0473887096062562 0.9605880165369833 0.4659283171706423 T T T
0.3041039061524777 0.2464853344433511 0.4867047840155034 T T T
0.3041936765508904 0.5799034806716689 0.4866742822473319 T T T
0.3041229930551099 0.9135062684465164 0.4867037344478459 T T T

0.5598520472373855 0.2001228134212372 0.5067952529899584 T T T
0.5598465134027969 0.5336124079144882 0.5067993261460516 T T T
0.5596772427043861 0.8670501308677753 0.5069127476343578 T T T
0.8170389318057901 0.1524999802043205 0.5275467818171901 T T T
0.8166138667639744 0.4862502789359316 0.5276272817494710 T T T
0.8167238418093982 0.8194069100649287 0.5276396020029658 T T T
0.0736368712757764 0.1056202002603426 0.5482612268213544 T T T
0.0735911852893650 0.4388347328551996 0.5482797805091321 T T T
0.0737756295253968 0.7720280843733864 0.5482518425505887 T T T
0.3287457318826153 0.0596371465663190 0.5692716344849104 T T T
0.3288029827137072 0.3924162074151242 0.5688599509925591 T T T
0.3287770261876408 0.7267661763764576 0.5688604135834676 T T T
0.5859258294214205 0.0120459195072759 0.5889665904472204 T T T
0.5866145755239349 0.3447998662904355 0.5886196276380234 T T T
0.5858887014483888 0.6786927923178335 0.5889786429740689 T T T
0.8452325917836923 0.6291896872158064 0.6094975922712640 T T T
0.8454369981344750 0.2956933723152530 0.6094537808001338 T T T
0.8454423276758389 0.9623456850382179 0.6094494522983953 T T T
0.1012018594395956 0.5828464115097669 0.6326991928406038 T T T
0.1010784552025855 0.2495497618669232 0.6327267334061234 T T T
0.1011913487942516 0.9159922988799182 0.6326864454376662 T T T
0.3554409707331621 0.5374791473231110 0.6504809276862333 T T T
0.3543639846777703 0.2051791087580157 0.6519346599987250 T T T
0.3543581499181823 0.8716245930192452 0.6519359201859163 T T T
0.6077099236504641 0.4936399858651160 0.6719492316658938 T T T
0.6076971509489587 0.1608490278306554 0.6719550807728948 T T T
0.6075291023011722 0.8274555169673918 0.6720764619869797 T T T
0.8619145984495843 0.4486815167787675 0.6897405652308063 T T T
0.8620578025350892 0.1151622976154716 0.6897694332789717 T T T
0.8620096431072645 0.7820710208058789 0.6897275604541894 T T T
0.2999403555467495 0.5781666275096721 0.7763839953282851 T T T
0.2998520958407960 0.7334535892348769 0.7765501780419690 T T T
0.3001763113513752 0.4227642259844687 0.7766091300882324 T T T

CO_2/Cu(533) E_{ads} = −0.26 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 2
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F

0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0476094085755027	0.2937153028066112	0.4659323700671552	T	T	T
0.0475292872087389	0.6270454548238923	0.4660285341406323	T	T	T
0.0475515882219092	0.9604233996057224	0.4659601225600954	T	T	T
0.3042960796121504	0.2463711172190581	0.4867649736470369	T	T	T
0.3043544171402858	0.5797884806049436	0.4867514378705421	T	T	T
0.3042546816027518	0.9131555204949443	0.4867517236212187	T	T	T
0.5599470016957293	0.1999911687731378	0.5067642627342028	T	T	T
0.5601067466654095	0.5332757562676229	0.5067878962967362	T	T	T
0.5599280525072947	0.8666177652103598	0.5068321609931122	T	T	T
0.8173312061401139	0.1519365665281436	0.5276018719697867	T	T	T
0.8171960520078472	0.4854426243780486	0.5276082067301617	T	T	T
0.8170168240638277	0.8189498060676136	0.5276187719686970	T	T	T
0.0738866165299898	0.1052193471148044	0.5483391963566223	T	T	T
0.0737267237176472	0.4384738420066686	0.5483648590673464	T	T	T
0.0740505249346273	0.7716971891425024	0.5483393094367166	T	T	T
0.3288147514854768	0.0594640655786936	0.5692075217903456	T	T	T
0.3289171394300366	0.3924555895349560	0.5690431427157298	T	T	T
0.3291065487894185	0.7261825736683737	0.5690315283449517	T	T	T
0.5860134952798380	0.0116145564586340	0.5887178105656121	T	T	T
0.5865971848637365	0.3446180409345282	0.5885748313410286	T	T	T
0.5863105090824845	0.6783920811253339	0.5887937127440884	T	T	T
0.8453612246682123	0.6288933007041296	0.6095415769759164	T	T	T
0.8457477649936158	0.2952244600636514	0.6095007813956358	T	T	T
0.8459549541038883	0.9615958685539771	0.6094762745711774	T	T	T
0.1013193093475881	0.5823230311556233	0.6326674072510111	T	T	T
0.1013453744519274	0.2491488754456519	0.6328508165207228	T	T	T
0.1017730503186384	0.9154799669075034	0.6327889022672281	T	T	T
0.3552970909529337	0.5374084396665100	0.6511450755853789	T	T	T
0.3547443689730836	0.2046255595446222	0.6518917912191141	T	T	T
0.3547957353453850	0.8712069220023092	0.6518596039916974	T	T	T
0.6080646670845592	0.4934335738536520	0.6715682310488776	T	T	T
0.6084611361888038	0.1594568224221109	0.6713760809615952	T	T	T
0.6076907416615676	0.8271133623441254	0.6720133498368129	T	T	T
0.8620043227459969	0.4484034057336043	0.6898041895607099	T	T	T
0.8623498315842943	0.1147056335484593	0.6897199120615455	T	T	T
0.8622654246089129	0.7814629092744199	0.6898385014023393	T	T	T
0.3829371924926080	0.5099298941706927	0.7816237869452883	T	T	T
0.2679811091197732	0.5194015481638790	0.7732534512464206	T	T	T
0.4975601818175211	0.5007880105503594	0.7903253196533706	T	T	T

CO_2/Defected-Cu(533) E_{ads} = −0.25 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
59 1 2

Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0470591126808044 0.2940220890032911 0.4660562801086972 T T T
0.0471446328785489 0.6270216526004078 0.4660164085778123 T T T
0.0471581906957623 0.9608806479621881 0.4659662764099856 T T T
0.3037502222043406 0.2467057045499800 0.4868532653486559 T T T
0.3043485396109067 0.5794386936318872 0.4865296585192719 T T T
0.3036378513524405 0.9136225450982226 0.4867093256812356 T T T
0.5600937611140160 0.1997923111796906 0.5067568789533692 T T T
0.5601175429881086 0.5332673615252682 0.5068725629579246 T T T
0.5593330777497544 0.8666855830619226 0.5070281021655368 T T T
0.8172426700603480 0.1521305659919092 0.5277195805436651 T T T
0.8167757809042183 0.4857100844331610 0.5277942043160123 T T T
0.8168476225283430 0.8186940521592193 0.5277502230214552 T T T
0.0728824606195946 0.1060537376932279 0.5486962912597485 T T T
0.0725802294787464 0.4389117997516745 0.5487291813130150 T T T
0.0740339368273673 0.7714779521826928 0.5480229857108853 T T T
0.3277310534859032 0.0599546912676401 0.5693175266316057 T T T
0.3288932588646907 0.3923800163896787 0.5690018199529930 T T T
0.3289962287237950 0.7259121850837920 0.5688106623740118 T T T
0.5857635233258802 0.0116321286065021 0.5886592289406856 T T T
0.5865872128152234 0.3442615924303849 0.5885331201134910 T T T
0.5868971798437974 0.6774971543696355 0.5891096303552956 T T T
0.8447763696613921 0.6252344259401040 0.6109728170372163 T T T
0.8451461549886226 0.2989437068682957 0.6108652221733361 T T T
0.8458364432148687 0.9613305059145993 0.6092770331585809 T T T
0.1008580035598390 0.5814619421412881 0.6323864441721990 T T T
0.0975708816096494 0.2517021379916658 0.6336993443482396 T T T
0.1010486222205009 0.9165349125848347 0.6323724567706179 T T T
0.3543047047379126 0.5378620314896377 0.6513051185783427 T T T
0.3535654692239694 0.2049709378795459 0.6520875310768713 T T T
0.3537950181569062 0.8716671572957113 0.6520688392325565 T T T
0.6095057941065923 0.4926343891121122 0.6704365277860458 T T T
0.6078442133556042 0.1596784597048675 0.6715613147376475 T T T

0.6092313660022751 0.8246893894267675 0.6706152975026388 T T T
0.8621986031261487 0.1133551450047500 0.6886820832084382 T T T
0.8619314945450794 0.7823402387550193 0.6887992318782820 T T T
0.3959144127443289 0.5148721762767314 0.7837012794532725 T T T
0.2864797994287869 0.5104436839511475 0.7765731161028980 T T T
0.5051191553191098 0.5195683222254593 0.7912321289129752 T T T

CO_2/Cu(533) E_{ads} = −0.24 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 2
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0473726751757608 0.2939609222645574 0.4659162204843121 T T T
0.0474372365818161 0.6272099371051033 0.4659430734157655 T T T
0.0474280988390694 0.9605595026844258 0.4659254705201239 T T T
0.3041479911727875 0.2464877380722757 0.4867555889069019 T T T
0.3042004902798914 0.5799075276750880 0.4867193700266832 T T T
0.3041646931445348 0.9133606970543194 0.4867346844207895 T T T
0.5597348167046655 0.2002127174395769 0.5068009062354845 T T T
0.5597517561223476 0.5336654482452292 0.5068082449029085 T T T
0.5596668939006640 0.8669946975268482 0.5068915152030335 T T T
0.8168976191137614 0.1526005244089452 0.5275146557242588 T T T
0.8166198826313391 0.4862111932182205 0.5275502345998276 T T T
0.8166677708067959 0.8194339750773370 0.5275615307989686 T T T
0.0735736336133415 0.1056263339275414 0.5482193305672426 T T T
0.0734051936825938 0.4389541774642257 0.5482502222815314 T T T
0.0736488850730611 0.7721173560777845 0.5482241863974910 T T T
0.3285429790733039 0.0597485900437326 0.5692094871225832 T T T
0.3285636490725065 0.3927756991495207 0.5690048597573669 T T T

0.3285684273473486	0.7266023322543892	0.5690076707302991	T	T	T
0.5857262002927635	0.0120835177010031	0.5888564226981642	T	T	T
0.5860813023794311	0.3451632788147224	0.5886153006836706	T	T	T
0.5857187005615121	0.6787915605757959	0.5888667394799401	T	T	T
0.8451795146408950	0.6292027038468813	0.6094043895868867	T	T	T
0.8454798470085894	0.2956234820406314	0.6093249190433816	T	T	T
0.8454783406377163	0.9622413889266824	0.6093245819572883	T	T	T
0.1012717896117684	0.5826485201559579	0.6326836961305655	T	T	T
0.1011974336220659	0.2494214774562524	0.6326759004233118	T	T	T
0.1012472459842627	0.9159286032124764	0.6326918470723850	T	T	T
0.3548574292282924	0.5378999590408975	0.6511702995490796	T	T	T
0.3544760634387692	0.2049295653781769	0.6519301546743437	T	T	T
0.3543900108307000	0.8716559743487460	0.6519136670187208	T	T	T
0.6080236779638110	0.4935677356633689	0.6716371782471051	T	T	T
0.6080867481715131	0.1602832033693788	0.6716128800944787	T	T	T
0.6079044640203703	0.8269911343711860	0.6719331886210539	T	T	T
0.8622735159520214	0.4482583850765411	0.6896393856572089	T	T	T
0.8619638702597230	0.1152820523844053	0.6896423491068376	T	T	T
0.8622322174379304	0.7818787442133409	0.6896547241316878	T	T	T
0.3965621821479752	0.5017151751203835	0.7833299059107752	T	T	T
0.3928759074551141	0.6599687346676288	0.7832415428562959	T	T	T
0.4001082770499236	0.3435728006326523	0.7837468213455412	T	T	T

CO_2/DefectedCu(533) E_{ads} = −0.24 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
59 1 2
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0470006268934226	0.2941189186946993	0.4661132369999939	T	T	T

0.0471428797194573	0.6270648142853008	0.4660649267096535	T	T	T
0.0472231903325530	0.9608339947434954	0.4660066870490753	T	T	T
0.3037999423864572	0.2466791656035671	0.4868994922236828	T	T	T
0.3044108477399422	0.5794803833021192	0.4865732572759812	T	T	T
0.3036802805586918	0.9137442197020063	0.4867518903457480	T	T	T
0.5602203182258148	0.1998060411678506	0.5067969799300748	T	T	T
0.5602356930683661	0.5333800121219044	0.5069138558924983	T	T	T
0.5593881360414176	0.8668423126082616	0.5071154130713635	T	T	T
0.8173531955914072	0.1521877404919917	0.5277871976001001	T	T	T
0.8167404381859713	0.4859446448345642	0.5279029495314357	T	T	T
0.8169000365991119	0.8187445254238417	0.5278484638641966	T	T	T
0.0728783800994998	0.1061639886660092	0.5487913238582878	T	T	T
0.0726316567448426	0.4389962926583417	0.5488414925505488	T	T	T
0.0740276838790177	0.7715531360817334	0.5481345359769706	T	T	T
0.3277519160962397	0.0600767151591341	0.5694395225234917	T	T	T
0.3288998887657072	0.3924928209673073	0.5690255350548888	T	T	T
0.3290102354535093	0.7261610134286164	0.5688535341218890	T	T	T
0.5857365208689093	0.0120396351791746	0.5888040839179618	T	T	T
0.5865715936878162	0.3446092269161308	0.5885762373633813	T	T	T
0.5868373686542714	0.6778200048115548	0.5892461564492204	T	T	T
0.8448213409606800	0.6255213421669362	0.6111403498882915	T	T	T
0.8450612844738767	0.2993256328615607	0.6109796986271212	T	T	T
0.8456501181920569	0.9618025639510726	0.6093959133817968	T	T	T
0.1007200618389924	0.5818792608758865	0.6326322659634525	T	T	T
0.0974189168326466	0.2519688321973760	0.6338147964645816	T	T	T
0.1008105391051028	0.9168414426089279	0.6325208036394310	T	T	T
0.3540985047210484	0.5383516871932903	0.6512423320479706	T	T	T
0.3532155974484658	0.2056411620756615	0.6521558240574513	T	T	T
0.3535029890518109	0.8721975293682191	0.6522050809692288	T	T	T
0.6093892093449551	0.4930771437264486	0.6705624035921283	T	T	T
0.6074485944718550	0.1606419919414010	0.6717514157202564	T	T	T
0.6091155806068891	0.8252444029066728	0.6706789751583269	T	T	T
0.8617514696850955	0.1141919767267029	0.6888733862644610	T	T	T
0.8615442881232280	0.7833809580711435	0.6889656445927944	T	T	T
0.4062566436382526	0.4952829980973515	0.7838701753797384	T	T	T
0.4415057708505951	0.6162478683899254	0.7852503287157163	T	T	T
0.3708841929436630	0.3745048418703873	0.7828896614301941	T	T	T

CO_2/Cu(533) E_{ads} = −0.23 eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O

60 1 2

Selective dynamics

Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F

0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0471224957205088	0.2941322503146097	0.4659888238919234	T	T	T
0.0472890967016161	0.6272771031509027	0.4659832393252940	T	T	T
0.0472303918560619	0.9606532483678558	0.4659484852180680	T	T	T
0.3036674911386447	0.2470122268668893	0.4868607531719156	T	T	T
0.3039190214114999	0.5801607556456216	0.4868182972264932	T	T	T
0.3036923230699524	0.9137044430426033	0.4868182562514814	T	T	T
0.5592332468178579	0.2006300971955896	0.5068166366073520	T	T	T
0.5592712181745128	0.5341395087303379	0.5067791748964294	T	T	T
0.5590122374094486	0.8676259313911951	0.5068451021554601	T	T	T
0.8163816612723767	0.1529819180648976	0.5274783501825110	T	T	T
0.8160456076837527	0.4866541864660889	0.5275377751398292	T	T	T
0.8161925369927692	0.8198577251806654	0.5275652554483093	T	T	T
0.0730218644367006	0.1060453762887314	0.5482992423667015	T	T	T
0.0726333152460481	0.4396284672754679	0.5483962963494560	T	T	T
0.0731314488438089	0.7725527264498772	0.5482785301591223	T	T	T
0.3274348944489286	0.0607887060404895	0.5693438786423143	T	T	T
0.3276157821422169	0.3938069083555434	0.5692924112253652	T	T	T
0.3280613294621783	0.7269343975262067	0.5692125236790825	T	T	T
0.5846618605597476	0.0129276200443867	0.5887558071691970	T	T	T
0.5850453312932555	0.3460950308260731	0.5885611188057580	T	T	T
0.5846753722097192	0.6800202889043850	0.5887534210575032	T	T	T
0.8439368230838603	0.6302618944126704	0.6093736937168407	T	T	T
0.8442971520378800	0.2967289027191986	0.6092183398576076	T	T	T
0.8444382226656455	0.9631186887949718	0.6092580908671800	T	T	T
0.0997890109262680	0.5840006329827840	0.6328965899074710	T	T	T
0.0996497136743432	0.2506902420195402	0.6329372626013507	T	T	T
0.1001437113304789	0.9169500381529762	0.6325903501147914	T	T	T
0.3534202502609999	0.5393641716092668	0.6518462560339956	T	T	T
0.3529570633757326	0.2063413888518049	0.6520600364733581	T	T	T
0.3530324441555648	0.8728880078409078	0.6520348795750147	T	T	T
0.6066633829825138	0.4949762416163268	0.6713593501067635	T	T	T
0.6066052725070920	0.1614124742820393	0.6712727545109851	T	T	T
0.6058758258185489	0.8287992432893950	0.6719994304675622	T	T	T
0.8600283412853028	0.4504309656971362	0.6896284022655381	T	T	T
0.8611472760800312	0.1161043346839771	0.6893895720273718	T	T	T
0.8600253278327498	0.7835380495211989	0.6896274740244096	T	T	T
0.6021611318062071	0.3193896100993946	0.7972152623751282	T	T	T
0.4623104795630887	0.4271539294023570	0.7901558991963561	T	T	T
0.7420519204959062	0.2115873088966294	0.8046724568610241	T	T	T

CO_2/Cu(533) E_{ads} = −0.22 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000

4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 2
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0472778009005698 0.2940057206137314 0.4659741830923882 T T T
0.0472195024764177 0.6273651610966352 0.4659908206793750 T T T
0.0473312798272801 0.9605849234814969 0.4659738667607776 T T T
0.3038373857024878 0.2467903491135764 0.4868157276439362 T T T
0.3039099511327431 0.5800206146178907 0.4868221990599494 T T T
0.3039548768059023 0.9133419038939172 0.4868084594730582 T T T
0.5593536859389928 0.2003510955108697 0.5068189860885681 T T T
0.5594250959111037 0.5337276177651109 0.5068146088674697 T T T
0.5593121043154645 0.8672714337588424 0.5068497537447016 T T T
0.8163967436116477 0.1528422531337054 0.5275554097030637 T T T
0.8163383103084905 0.4862952376258131 0.5275623859443597 T T T
0.8162081762481703 0.8196102123826279 0.5276364420362248 T T T
0.0731170734313230 0.1058040558526409 0.5482957071498145 T T T
0.0728219253345000 0.4393383386442876 0.5483549519565893 T T T
0.0729656184711638 0.7725431854084355 0.5483292174123617 T T T
0.3276912491759932 0.0603177667790002 0.5692598854721036 T T T
0.3277599734927122 0.3933646111406383 0.5692461533023825 T T T
0.3279731175514438 0.7266553672214321 0.5692236110814558 T T T
0.5847851658454450 0.0126160458475640 0.5888925233292815 T T T
0.5849156253969907 0.3454068131536117 0.5886148489064805 T T T
0.5848691303499209 0.6795086076892167 0.5886364351661689 T T T
0.8440108048116606 0.6297329692673512 0.6095225163681226 T T T
0.8445682472911131 0.2960847165613359 0.6092980321595834 T T T
0.8441314736334928 0.9629188133088832 0.6093924230629263 T T T
0.0996437809149021 0.5836904833918565 0.6327760399496195 T T T
0.0996544354480262 0.2503811440397065 0.6328810664710569 T T T
0.0999373599469094 0.9167856712196989 0.6326978754875094 T T T
0.3529690014496575 0.5389305440216124 0.6518762848882085 T T T

0.3529251734236850 0.2058136886329470 0.6520338088280154 T T T
0.3529722043567184 0.8725311827558591 0.6519394825785803 T T T
0.6065951003440673 0.4942039494996241 0.6707374696955768 T T T
0.6062021947741001 0.1612822624754489 0.6719543061099170 T T T
0.6059180775424062 0.8281488339586904 0.6719173267381195 T T T
0.8600989759131639 0.4494984765628367 0.6897963718005545 T T T
0.8604957576522421 0.1158152637938738 0.6895440385381421 T T T
0.8602013420122968 0.7829610069410061 0.6897946316165047 T T T
0.5968571736928421 0.5173280218732791 0.7973167555520557 T T T
0.4697554395388321 0.5596104067548431 0.7897036156247064 T T T
0.7239347846630941 0.4750379476391729 0.8053243994443158 T T T

CO_2/Cu(533) E_{ads} = −0.22 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 2
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0472974317413352 0.2939375282887898 0.4659509137921113 T T T
0.0472145921515649 0.6273056874796422 0.4659457252527412 T T T
0.0472514187855414 0.9605641903384586 0.4659413312307765 T T T
0.3038541005830746 0.2467900239410540 0.4867601382780328 T T T
0.3038738812382384 0.5800544840269252 0.4867716355494784 T T T
0.3039211276959913 0.9133311919963870 0.4867349149504216 T T T
0.5592430095563105 0.2005795519487306 0.5068197461160168 T T T
0.5594023808140558 0.5338370499338668 0.5067968356029258 T T T
0.5592692107169517 0.8673707653299425 0.5068176177128194 T T T
0.8162602273868390 0.1530846084226334 0.5274954940106663 T T T
0.8162774825832806 0.4864974105305044 0.5274830018679850 T T T
0.8160980302809131 0.8197958880641715 0.5275575526573586 T T T

0.0731248955397678	0.1057196711019757	0.5481736839910687	T	T	T
0.0728488532972093	0.4393626028950189	0.5482703967669297	T	T	T
0.0729171949626733	0.7724757815717878	0.5482423696766462	T	T	T
0.3278042698099107	0.0602428246267441	0.5691287494256324	T	T	T
0.3276406020788504	0.3936008008737539	0.5691966913711682	T	T	T
0.3280625237361279	0.7266118337727128	0.5691175619984890	T	T	T
0.5846508306966166	0.0130190411347417	0.5888449091173383	T	T	T
0.5848743728833786	0.3458625021725587	0.5886746264374314	T	T	T
0.5848719523374205	0.6796737736199523	0.5886576567156324	T	T	T
0.8440151990933995	0.6301780075454851	0.6093862514462137	T	T	T
0.8444226643448957	0.2967284690345533	0.6091333387129783	T	T	T
0.8440342719651960	0.9632686282693238	0.6092088869115704	T	T	T
0.0995477701449350	0.5838844999341690	0.6327662737448053	T	T	T
0.0999226366388216	0.2502594696848867	0.6325944037490966	T	T	T
0.1000778517107249	0.9168669321924158	0.6324524179244136	T	T	T
0.3529290013699332	0.5393488788886512	0.6518420138507097	T	T	T
0.3529250290285710	0.2060822123402952	0.6519272099516511	T	T	T
0.3531017936288944	0.8726126951562041	0.6518590315571275	T	T	T
0.6064848518803824	0.4949338432212579	0.6711344919289813	T	T	T
0.6061431385766393	0.1619895963756734	0.6719262934754481	T	T	T
0.6060724317796800	0.8285263949949985	0.6718660805539082	T	T	T
0.8608443483433940	0.4499101851038915	0.6894932031784208	T	T	T
0.8609914309377706	0.1158203565275191	0.6890822854286752	T	T	T
0.8600544385684534	0.7839607212914759	0.6896807679520540	T	T	T
0.6770626415358163	0.4317181205972685	0.8007973348510511	T	T	T
0.5476373668171072	0.4762710798673774	0.7997764319481006	T	T	T
0.8069065546722088	0.3868692456890633	0.8021886591008750	T	T	T

CO_2/Defected-Cu(533) E_{ads} = −0.22 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
59 1 2
Selective dynamics
Direct

0.0033480000000026	0.9974660000000029	0.3038949999999971	F	F	F
0.0030229999999989	0.3308680000000024	0.3037470000000013	F	F	F
0.0028649999999999	0.6641070000000013	0.3038379999999989	F	F	F
0.2572189999999992	0.6189010000000010	0.3215059999999994	F	F	F
0.2573160000000030	0.2854460000000003	0.3213999999999970	F	F	F
0.2573659999999975	0.9523849999999996	0.3214630000000014	F	F	F
0.5101849999999999	0.5748710000000017	0.3417460000000005	F	F	F
0.5102159999999998	0.2413540000000012	0.3418539999999979	F	F	F
0.5104720000000000	0.9080429999999993	0.3417389999999969	F	F	F
0.7634449999999973	0.5304860000000033	0.3608040000000017	F	F	F
0.7634180000000015	0.1971289999999968	0.3608270000000005	F	F	F
0.7633700000000019	0.8637719999999973	0.3608990000000034	F	F	F
0.0192890000000006	0.4838880000000003	0.3841249999999974	F	F	F
0.0193859999999972	0.1505420000000015	0.3841350000000006	F	F	F
0.0193610000000035	0.8170920000000024	0.3841170000000034	F	F	F
0.2784880000000030	0.4343569999999985	0.4044999999999987	F	F	F
0.2786070000000009	0.1011620000000022	0.4046140000000022	F	F	F
0.2783230000000003	0.7678590000000014	0.4045160000000010	F	F	F
0.5354340000000022	0.3872569999999982	0.4245429999999999	F	F	F
0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F

0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0466868342182401	0.2944397290380333	0.4660312934863907	T	T	T
0.0468172318860783	0.6273180919829422	0.4659124842654065	T	T	T
0.0467678773267661	0.9613248604997188	0.4659308805053696	T	T	T
0.3031314192465864	0.2473604464445442	0.4868073683301341	T	T	T
0.3036708269290511	0.5800450846239703	0.4864612523134424	T	T	T
0.3029726959542907	0.9141679587507680	0.4866486639836092	T	T	T
0.5592228826146965	0.2005627622727035	0.5066018246128027	T	T	T
0.5591529729782081	0.5340768261078194	0.5067237927551369	T	T	T
0.5584690202323974	0.8674833205630524	0.5067932452118775	T	T	T
0.8161333566995941	0.1532214766141062	0.5275638890312943	T	T	T
0.8157261404028349	0.4866134653312368	0.5276452972944959	T	T	T
0.8159098407403879	0.8196827479499057	0.5276064032058042	T	T	T
0.0716637099876032	0.1071522403144862	0.5485892893285959	T	T	T
0.0713266210971701	0.4401724648600315	0.5486278383485923	T	T	T
0.0727044342722165	0.7726148939279016	0.5478595590481724	T	T	T
0.3261913892443946	0.0612775158213255	0.5691406435231713	T	T	T
0.3272651175410368	0.3939820098822652	0.5689758191805129	T	T	T
0.3273568026017913	0.7271344733372141	0.5687934358510701	T	T	T
0.5840358532276688	0.0129790107842429	0.5883024923202569	T	T	T
0.5845273660401673	0.3458484489168281	0.5881999185170463	T	T	T
0.5849789278994474	0.6793613478120945	0.5886591785104778	T	T	T
0.8427578422532427	0.6268692370948280	0.6106097986170205	T	T	T
0.8433314487811145	0.3004801820562852	0.6106133116339600	T	T	T
0.8439001949386450	0.9633336570694766	0.6090781708862211	T	T	T
0.0985675293449884	0.5835241521083492	0.6323629591907576	T	T	T
0.0953492145511146	0.2536222820993119	0.6335064454551508	T	T	T
0.0987376713883094	0.9184012787024853	0.6321918774712236	T	T	T
0.3516153326282144	0.5400728772791613	0.6517323812518654	T	T	T
0.3510707825927470	0.2069983248239840	0.6518402842243620	T	T	T
0.3513065692853625	0.8738120292292813	0.6519224551432840	T	T	T
0.6068075005243535	0.4951368697440264	0.6694903592595868	T	T	T
0.6049865412511333	0.1617996497941050	0.6709221685935021	T	T	T
0.6065735150976918	0.8265628051396081	0.6702816454675764	T	T	T
0.8598027842230264	0.1155830767964381	0.6884871379609100	T	T	T
0.8586653532168997	0.7842819493509440	0.6883367763375918	T	T	T
0.6276283241549622	0.3181758053718964	0.7944171105426943	T	T	T
0.4878133865264209	0.4116101695141434	0.7973318801340464	T	T	T
0.7682173834185611	0.2242454008704998	0.7918956848831891	T	T	T

CO_2/Cu(533) E_{ads} = −0.22 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 2
Selective dynamics
Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F

0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0475330642004225	0.2938415219998453	0.4659221393920650	T	T	T
0.0475358337107247	0.6271332163078185	0.4659224091369634	T	T	T
0.0475639621543139	0.9604626995221534	0.4659078322189774	T	T	T
0.3042891267603266	0.2464664298643895	0.4867262240448271	T	T	T
0.3043687176992453	0.5797321322149338	0.4866997742895942	T	T	T
0.3043509283391466	0.9131436314116915	0.4867038032804261	T	T	T
0.5599211235556248	0.2000827531614994	0.5067685332845920	T	T	T
0.5599740338123158	0.5334330700986613	0.5067545406984489	T	T	T
0.5598769714114941	0.8668326962125049	0.5067812970188325	T	T	T
0.8170962545102999	0.1524239394611357	0.5274377823279530	T	T	T
0.8170004929020215	0.4859616761860005	0.5274634695579060	T	T	T
0.8169958743184317	0.8190769485657409	0.5274640961234495	T	T	T
0.0739309898799627	0.1052922449036430	0.5481686603303839	T	T	T
0.0737763240607259	0.4387258879952005	0.5482370837251783	T	T	T
0.0739564852676990	0.7718606030964578	0.5481678177780651	T	T	T
0.3287771950010799	0.0595237100160803	0.5690749145558432	T	T	T
0.3288550657265873	0.3927396377643680	0.5690329260103510	T	T	T
0.3290090910474661	0.7260123182898155	0.5689895553491080	T	T	T
0.5859826030039620	0.0117589731049404	0.5886363916468144	T	T	T
0.5861612931113590	0.3450907515790090	0.5885365185431409	T	T	T
0.5860250130469844	0.6786448486508928	0.5886473490006674	T	T	T
0.8454403084537631	0.6289234329311005	0.6093220629236750	T	T	T
0.8457153507014004	0.2955350786509275	0.6091290642789767	T	T	T
0.8457541484547825	0.9618422535264355	0.6091130529526320	T	T	T
0.1015550237489080	0.5824434738329670	0.6325896953917567	T	T	T
0.1014547584813050	0.2491110472734093	0.6325918990639189	T	T	T
0.1018231871799964	0.9154549132554713	0.6324328966366835	T	T	T
0.3549546520512918	0.5377439077096120	0.6516593668424985	T	T	T
0.3546472594920953	0.2047295234340553	0.6517684854611134	T	T	T
0.3547138074663174	0.8712813342525090	0.6517439817954573	T	T	T
0.6084633060496923	0.4932507031909391	0.6712252676479236	T	T	T
0.6084998706115395	0.1596680872930277	0.6711787358753017	T	T	T
0.6080575191019213	0.8268344568150042	0.6716341403033762	T	T	T
0.8625436473667952	0.4479735275784601	0.6895058104516339	T	T	T
0.8631072350733262	0.1142340327131111	0.6891607034245424	T	T	T
0.8626044321857136	0.7814592521502735	0.6894878917459469	T	T	T
0.5531504312613900	0.3681570467163670	0.7924676489747935	T	T	T
0.5530394750600424	0.5234813591884538	0.7926354703010006	T	T	T
0.5533103074569486	0.2127811611400341	0.7926084478251806	T	T	T

CO_2/Defected-Cu(533) E_{ads} = −0.21 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
59 1 2
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0469938149327885 0.2942791257492751 0.4660018361886422 T T T
0.0469731289347335 0.6272013871738455 0.4659330985904158 T T T
0.0470995655852768 0.9610300488810986 0.4659081752661715 T T T
0.3035431581600873 0.2471626018362799 0.4868449040175298 T T T
0.3041338368475006 0.5797414241551017 0.4864818125287994 T T T
0.3035551037185773 0.9138224265850863 0.4866299814534545 T T T
0.5597786497558941 0.2002828940916409 0.5066840467308985 T T T
0.5599179371200601 0.5336714034558345 0.5067837987042693 T T T
0.5590893813310435 0.8673075313107594 0.5068970993640501 T T T
0.8168613827535898 0.1526691614321719 0.5275565727094848 T T T
0.8165286733046744 0.4863386655807470 0.5276348114688579 T T T
0.8165405786258391 0.8194762688742991 0.5277769915295395 T T T
0.0727551562111282 0.1064750095015644 0.5484735084082991 T T T
0.0722262893187483 0.4396563177675608 0.5486801502099293 T T T
0.0735602960565588 0.7720007768754679 0.5478804548297764 T T T
0.3273451049249657 0.0606337190315860 0.5692055729293051 T T T
0.3283694489601530 0.3933346827810015 0.5690589544378405 T T T
0.3287905768644306 0.7262093002199084 0.5687601316769435 T T T
0.5853342977738478 0.0125986920015604 0.5885797181220956 T T T
0.5858038984758052 0.3449844693364124 0.5883454709415125 T T T
0.5864078718186364 0.6787493033787364 0.5887552828392780 T T T
0.8442115928506334 0.6261217615390037 0.6108129046890760 T T T
0.8447547969291805 0.2996577429111882 0.6104212940184575 T T T
0.8452344513217387 0.9629643954404643 0.6093470181758066 T T T
0.1001304158495687 0.5825682379202299 0.6324426650143177 T T T

0.0968807613603352 0.2525852941804571 0.6334816893459828 T T T
0.1009303130341184 0.9170414888029490 0.6319114866502841 T T T
0.3532802680347611 0.5389754497127256 0.6518371385973717 T T T
0.3529336269713643 0.2060365508017923 0.6519666793502553 T T T
0.3531099925788299 0.8729025431336962 0.6519774789718042 T T T
0.6082476055866318 0.4942406681830271 0.6694162806842999 T T T
0.6072164691536029 0.1612314580937688 0.6716682626280144 T T T
0.6086069763652232 0.8254912747367111 0.6704651580585237 T T T
0.8635333322258715 0.1141508119035785 0.6884549036612599 T T T
0.8607355586378261 0.7837565917530791 0.6886097243657114 T T T
0.7059186088450439 0.3352736556928873 0.7932837778068654 T T T
0.5728502323315814 0.4141566060356187 0.8052439536415380 T T T
0.8403894132559906 0.2550575476208101 0.7815441892864703 T T T

CO_2/Defected-Cu(533) E_{ads} = −0.21 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
59 1 2
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0470593609974843 0.2942757807944270 0.4660614872856879 T T T
0.0472019042533961 0.6271937443247273 0.4660020067712059 T T T
0.0471519440160274 0.9610805738255734 0.4659543027542956 T T T
0.3037309461107839 0.2469293020466702 0.4869092539017954 T T T
0.3043248334049475 0.5795821302273623 0.4865696846397579 T T T
0.3036054694629203 0.9137387210576053 0.4867191554199610 T T T
0.5600488967715928 0.2000360188117297 0.5067611584673160 T T T
0.5600867878664294 0.5334677682724542 0.5068744140120056 T T T
0.5592680563635234 0.8669170352499348 0.5070045161569213 T T T
0.8172249355597018 0.1525369698979568 0.5276638907108568 T T T

0.8168032585111696 0.4861972751606430 0.5277513044385115 T T T
0.8169381248708556 0.8188652390178209 0.5276715325925234 T T T
0.0729913579064055 0.1063853507310862 0.5486714626688242 T T T
0.0726797881923396 0.4393747711808176 0.5487934927459135 T T T
0.0741379238960753 0.7717391968919769 0.5480283542379872 T T T
0.3278051192324380 0.0600975893988445 0.5693249943877875 T T T
0.3289538706735370 0.3927866446439302 0.5691626617570914 T T T
0.3292142269194289 0.7258589808216562 0.5689101929847241 T T T
0.5858832472144689 0.0116906765042961 0.5886083677288417 T T T
0.5864896414087094 0.3446045227559636 0.5885582324303974 T T T
0.5869680375572430 0.6776615280460586 0.5890716910291263 T T T
0.8450532968219263 0.6254521026872067 0.6109887500730866 T T T
0.8454458131130391 0.2993044719603450 0.6106650614448579 T T T
0.8459862972874420 0.9614173645513906 0.6090936727447459 T T T
0.1011339281153868 0.5818212651066934 0.6326434954776473 T T T
0.0977779809420153 0.2519466242728498 0.6337339293158212 T T T
0.1016257340595018 0.9165212976243583 0.6322462602248275 T T T
0.3544312627367390 0.5381134853607776 0.6519194213275258 T T T
0.3536917658437810 0.2051263261935675 0.6521038424756045 T T T
0.3540737247331635 0.8717909886480215 0.6521677840350183 T T T
0.6101826527923526 0.4924271221371072 0.6703051478524497 T T T
0.6080485126247114 0.1597590737350709 0.6714057988120608 T T T
0.6095673827889426 0.8245756206131410 0.6705078579214051 T T T
0.8631907780822770 0.1128075238208338 0.6882514268435594 T T T
0.8619504465526658 0.7829303300002486 0.6887689608866626 T T T
0.5751330583226570 0.3637637969884462 0.7953917056169048 T T T
0.5923372010220849 0.5030255813838614 0.7915920526133438 T T T
0.5581345355860714 0.2246151663751226 0.7995570872402815 T T T

CO_2/Defected-Cu(533) E_{ads} = −0.21 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
59 1 2
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F

0.5353589999999997	0.0536609999999982	0.4246529999999993	F	F	F
0.5353720000000024	0.7203889999999973	0.4245549999999980	F	F	F
0.7901030000000020	0.3414780000000022	0.4452939999999970	F	F	F
0.7902539999999973	0.0081070000000025	0.4453010000000006	F	F	F
0.7900119999999973	0.6749369999999999	0.4453510000000023	F	F	F
0.0470530579549297	0.2940341379365963	0.4659373978411293	T	T	T
0.0469891434307087	0.6271650093380557	0.4659016181545820	T	T	T
0.0470813840837607	0.9609289606757411	0.4658552962446313	T	T	T
0.3035141643184371	0.2470658206245346	0.4867641924732116	T	T	T
0.3040610640816409	0.5797220340421282	0.4864631411620962	T	T	T
0.3035694787816393	0.9136625175876472	0.4865795314914996	T	T	T
0.5596845043334950	0.2002405222475498	0.5066071170989090	T	T	T
0.5598208046984284	0.5336415409962050	0.5066965146710714	T	T	T
0.5590559423843040	0.8672637106847504	0.5068405426553197	T	T	T
0.8168613734604995	0.1525445731349435	0.5275166967369503	T	T	T
0.8166014492642418	0.4861324627248307	0.5275401815483874	T	T	T
0.8164614994449449	0.8192608191486727	0.5276176020656516	T	T	T
0.0727833189568602	0.1062141135182683	0.5484094763805112	T	T	T
0.0721589269538897	0.4394982837998077	0.5485398404054167	T	T	T
0.0734468363195677	0.7720388135041117	0.5478525649600922	T	T	T
0.3272488601158896	0.0605292196309021	0.5690684724498992	T	T	T
0.3282131114883082	0.3932411576690109	0.5689452655550449	T	T	T
0.3285176501399280	0.7262639362177308	0.5687270654418243	T	T	T
0.5851324663445620	0.0125626498106196	0.5884788843822617	T	T	T
0.5856247309299535	0.3447981345319391	0.5881464054738810	T	T	T
0.5863097428856205	0.6785985378469575	0.5885499609150054	T	T	T
0.8440457541767493	0.6260333997773582	0.6107095505326664	T	T	T
0.8449051778749100	0.2993095864634899	0.6102664866431551	T	T	T
0.8449271233707154	0.9623395697648010	0.6090932962892132	T	T	T
0.0999439992696726	0.5824296137078265	0.6322541840138564	T	T	T
0.0968129046387863	0.2524357817345039	0.6333254300116036	T	T	T
0.1002781092498833	0.9173609812299390	0.6320499885340536	T	T	T
0.3530940631645338	0.5389843896757335	0.6516582772548574	T	T	T
0.3525804774360017	0.2060022824597090	0.6518421967530658	T	T	T
0.3530351134711616	0.8726215285990085	0.6518303396298778	T	T	T
0.6089217644644790	0.4932798144040667	0.6689368852001629	T	T	T
0.6066933686730831	0.1611605916321315	0.6715859208690543	T	T	T
0.6081930496622202	0.8256679810270201	0.6701847681334523	T	T	T
0.8612819102122787	0.1150873362455682	0.6882817819710831	T	T	T
0.8606463778884832	0.7837192114699003	0.6885372146219858	T	T	T
0.5875472355269760	0.5218913287636671	0.7907476983967423	T	T	T
0.4619981904069089	0.5546819992146336	0.7928789477382121	T	T	T
0.7134902755848449	0.4889358488886157	0.7890939572037312	T	T	T

CO_2/Cu(533) E_{ads} = −0.21 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 2
Selective dynamics
Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F

0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0475355298081969	0.2938663032133066	0.4659342194134425	T	T	T
0.0474317322302900	0.6272492677324158	0.4659529382544784	T	T	T
0.0475753148268675	0.9604529948001498	0.4659307804934519	T	T	T
0.3041853817838596	0.2466157384696147	0.4867576873010583	T	T	T
0.3042242020971826	0.5798566431658921	0.4867431614475166	T	T	T
0.3043483401459379	0.9131512876520834	0.4867278723963465	T	T	T
0.5597711163725526	0.2001459032791625	0.5067996837495904	T	T	T
0.5598733776712963	0.5335087094604314	0.5067762398553008	T	T	T
0.5598266242589233	0.8670778449553752	0.5067951527241245	T	T	T
0.8170232343468344	0.1524548585466000	0.5274745674118014	T	T	T
0.8169825281778960	0.4859824391126758	0.5274682730614423	T	T	T
0.8167802620047844	0.8193864956366701	0.5275435224393323	T	T	T
0.0738965011099504	0.1053329208468047	0.5481949978846496	T	T	T
0.0736207931416752	0.4389180640274992	0.5482684190413392	T	T	T
0.0736546223853389	0.7721910075718981	0.5482660891395374	T	T	T
0.3286852360782714	0.0597443624145228	0.5691111970050355	T	T	T
0.3285855311582828	0.3930594054400347	0.5691268351651194	T	T	T
0.3287526530751653	0.7262641591727677	0.5690636667838350	T	T	T
0.5857858017077114	0.0121641290951321	0.5888802223101026	T	T	T
0.5858644747267139	0.3450066118598377	0.5885213672955144	T	T	T
0.5858908690416901	0.6791370497237421	0.5885163412449163	T	T	T
0.8451742633314402	0.6292890677486271	0.6093616027589513	T	T	T
0.8456974254777900	0.2954970481965435	0.6091180433614188	T	T	T
0.8451748723316050	0.9625543715866546	0.6093444985946687	T	T	T
0.1009641515254912	0.5829966973554258	0.6326696203015407	T	T	T
0.1011268555082319	0.2495114254970310	0.6326203852399066	T	T	T
0.1011893591092793	0.9161123879121366	0.6326303676202532	T	T	T
0.3542921103013851	0.5385540707995985	0.6517738307958399	T	T	T
0.3541768687529316	0.2052806643209260	0.6518557561102366	T	T	T
0.3543485605299281	0.8716817294044300	0.6517676713450005	T	T	T
0.6083240235634202	0.4934985151619181	0.6705605060847882	T	T	T
0.6074289105750748	0.1610144277848110	0.6718426181032523	T	T	T
0.6073944511562860	0.8275285914012388	0.6718367258638908	T	T	T
0.8619634926653340	0.4484914474962421	0.6894964643554863	T	T	T
0.8620329090583356	0.1155805470302297	0.6894648549731186	T	T	T
0.8618254189652913	0.7821689432201989	0.6896106126260858	T	T	T
0.5597225379698535	0.5274104748006191	0.7966750839692160	T	T	T
0.5599335136947705	0.6824407089305212	0.7968606855194177	T	T	T

0.5595584970727095 0.3723490698341062 0.7968376279964557 T T T

CO_2/Defected-Cu(533) E_{ads} = −0.20 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
59 1 2
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0471095370118046 0.2943354787758462 0.4661101026751520 T T T
0.0470671760769820 0.6272462546153945 0.4660338087120147 T T T
0.0469862928702520 0.9612855978280896 0.4660248448433270 T T T
0.3034638539260021 0.2475069274491391 0.4868566200396231 T T T
0.3038360293477909 0.5803251331965440 0.4865015434672124 T T T
0.3033665259828937 0.9141654389345240 0.4866721936248929 T T T
0.5596532330912137 0.2010186112193652 0.5067238148944777 T T T
0.5597708701025343 0.5341931780153666 0.5068667237190242 T T T
0.5590235679280703 0.8677161786711869 0.5068815435649445 T T T
0.8163910770968945 0.1536777575506531 0.5275751984581111 T T T
0.8162294691195445 0.4871453568678637 0.5276017398782993 T T T
0.8163232134603797 0.8203341402857903 0.5277200939845565 T T T
0.0725085154016092 0.1072319669803224 0.5486010206165739 T T T
0.0721917202729562 0.4403122029381774 0.5487920477606588 T T T
0.0733720347776942 0.7727390391204718 0.5480143533515420 T T T
0.3271072506522700 0.0614515505517406 0.5691249144256796 T T T
0.3281661703622847 0.3942685239138268 0.5690137493971633 T T T
0.3284144248697717 0.7270778346673149 0.5687819314606987 T T T
0.5851847973534547 0.0135158706763848 0.5884896619101140 T T T
0.5856082444947138 0.3461667523605632 0.5886062194539340 T T T
0.5860770505198328 0.6797086418405904 0.5888736644507949 T T T
0.8436164192560691 0.6277348970355383 0.6106738243759298 T T T

0.8436594711165690 0.3017704920033588 0.6104397619283656 T T T
0.8445857458853562 0.9645408051543402 0.6093655265159500 T T T
0.0998862439158469 0.5837383998885574 0.6325741394157445 T T T
0.0961124971407258 0.2542117732121479 0.6335183635329896 T T T
0.1001238711942508 0.9185907866083463 0.6320032142625333 T T T
0.3526325657676937 0.5404564934145389 0.6518287004361031 T T T
0.3524427774132252 0.2071690028436560 0.6517788368495403 T T T
0.3521616168858152 0.8745885801605221 0.6518727788043565 T T T
0.6071708552371993 0.4963564632488019 0.6700455207508550 T T T
0.6064036737640872 0.1623967189300544 0.6717404873643530 T T T
0.6081342251257589 0.8269303059902211 0.6704094612970231 T T T
0.8613686747776059 0.1177640784465956 0.6883650637757976 T T T
0.8603618158304057 0.7847663446306417 0.6884779818563590 T T T
0.8825579495762645 0.0486764564123763 0.8046668762656889 T T T
0.8945699472497116 0.1651255205231014 0.7789266854750770 T T T
0.8705240568976055 0.9329410504261832 0.8300552976846874 T T T

CO_2/Defected-Cu(533) E_{ads} = −0.20 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
59 1 2
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0469314034703068 0.2943174118679023 0.4660007208043294 T T T
0.0470876476005864 0.6272025788905791 0.4659287135336829 T T T
0.0471105402621782 0.9609982889208637 0.4658964132014889 T T T
0.3034535495321161 0.2471020838761261 0.4868059952561140 T T T
0.3041488021231071 0.5797014646457490 0.4864767993942579 T T T
0.3034315316279335 0.9137990422130197 0.4866370399229318 T T T
0.5598005753539033 0.1999401007103307 0.5066665001510930 T T T

0.5598300718409215 0.5336999891716683 0.5067486216869060 T T T
0.5589913870756473 0.8674098093678110 0.5068949127160169 T T T
0.8169391566073793 0.1526197867196010 0.5275794290011121 T T T
0.8165237139607574 0.4863105400525721 0.5276334241564468 T T T
0.8164936665138950 0.8191484121187268 0.5276287853447772 T T T
0.0726275639784736 0.1064231681604409 0.5485260170023235 T T T
0.0721411356014786 0.4395984600979738 0.5486309048610527 T T T
0.0736091693894389 0.7720788984954308 0.5478775735777267 T T T
0.3272295385862741 0.0606070758727037 0.5691360656064444 T T T
0.3283602038583749 0.3930851103462175 0.5689320964529556 T T T
0.3286256718306538 0.7261756126026602 0.5687343823647250 T T T
0.5852328676558117 0.0124275206863962 0.5886174979897389 T T T
0.5857031657376732 0.3447653798069630 0.5881380582295307 T T T
0.5862673581043298 0.6787967233806104 0.5886177523197759 T T T
0.8440570128709451 0.6261787353359547 0.6108766884645616 T T T
0.8448640793420724 0.2996540598678987 0.6103905045784674 T T T
0.8449275404383128 0.9622427200801429 0.6090509626568930 T T T
0.1000765662179558 0.5824184933235476 0.6323385131440458 T T T
0.0968401593083459 0.2525569373587060 0.6335156997521868 T T T
0.1004218870793380 0.9172676026576949 0.6321045507554830 T T T
0.3531217898518603 0.5391004420459080 0.6516798983827349 T T T
0.3527055269926064 0.2059240219391221 0.6518759038062015 T T T
0.3530008924356612 0.8725467679234931 0.6518392575322731 T T T
0.6090474028227172 0.4930755606672677 0.6691118226348343 T T T
0.6066119178671295 0.1614469199749398 0.6717384652833528 T T T
0.6083588230146733 0.8256247622713013 0.6704078402742342 T T T
0.8613801847220344 0.1148441686835130 0.6882027136268781 T T T
0.8610203758349331 0.7838101312884608 0.6886010504708424 T T T
0.5916747138806702 0.5149775452989157 0.7943963027957153 T T T
0.6215143058997156 0.6409858760972751 0.7893851623261208 T T T
0.5621727850056583 0.3890015740736287 0.7997757571703866 T T T

CO_2/Defected-Cu(533) E_{ads} = −0.20 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
59 1 2
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F

0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0472011918821913 0.2942663578667304 0.4659722525840527 T T T
0.0471987463865765 0.6271017999278409 0.4658956680655376 T T T
0.0472855689643045 0.9609918673023762 0.4658840125217824 T T T
0.3039631724024943 0.2469688763185690 0.4868449368135859 T T T
0.3045137087006088 0.5795573239154331 0.4864564592993046 T T T
0.3039088089572867 0.9136991733739134 0.4866096634184360 T T T
0.5602784397755284 0.2000847028276724 0.5067482151814261 T T T
0.5604486207727740 0.5333768553833080 0.5068256641152326 T T T
0.5595618727932826 0.8669933797847902 0.5069373032048458 T T T
0.8173725825913170 0.1525023031660851 0.5275313996016524 T T T
0.8170848257943704 0.4860047334239101 0.5276257840190800 T T T
0.8171582586185304 0.8191712268779744 0.5277505166807155 T T T
0.0733873098369257 0.1063127542914834 0.5483904300915384 T T T
0.0729903745376356 0.4393037420946871 0.5486252482418760 T T T
0.0742861049546484 0.7716028824449468 0.5477845855986743 T T T
0.3282012351244192 0.0602046322250133 0.5691862883348624 T T T
0.3292022787669427 0.3930176847798895 0.5690428463647189 T T T
0.3297748170136182 0.7256680029554965 0.5686560902544258 T T T
0.5862147875983178 0.0122077202514652 0.5885964982751927 T T T
0.5867261713079808 0.3447472852033092 0.5885247993091139 T T T
0.5873298626611532 0.6779398486898169 0.5889145135853389 T T T
0.8451328955600217 0.6255258892765262 0.6106607775267192 T T T
0.8455337790846892 0.2993187702754779 0.6104618376348971 T T T
0.8461521452938396 0.9626787079392607 0.6092663085494493 T T T
0.1011610924778505 0.5822745286744033 0.6324235989296918 T T T
0.0979124227561285 0.2521374792075740 0.6334097554551585 T T T
0.1024259545434448 0.9162100296428902 0.6315674010632412 T T T
0.3545447651581714 0.5384798770305497 0.6518483805244741 T T T
0.3539534990049253 0.2056965180084910 0.6519398591622059 T T T
0.3542821115735121 0.8721807385249839 0.6519415774187606 T T T
0.6100086002792093 0.4930405464252893 0.6701663241829917 T T T
0.6085289416690969 0.1606138953211878 0.6718355656675574 T T T
0.6094889321355899 0.8251579065870996 0.6704606207114490 T T T
0.8657414795086376 0.1125025770387514 0.6882768010519354 T T T
0.8616111750357635 0.7824376184117676 0.6883522198974159 T T T
0.8261738260392846 0.1416184320417524 0.8016339694132708 T T T
0.7294571896851697 0.1494000503359850 0.8261866027681104 T T T
0.9238554487802353 0.1335218168333759 0.7767904904476663 T T T

CO_2/Cu(533) E_{ads} = −0.19 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 2
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F

0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0468721505101990	0.2943679387622327	0.4658047565856508	T	T	T
0.0469089847725900	0.6276430317173275	0.4658098204497767	T	T	T
0.0468708584798162	0.9609921391702922	0.4658042950035007	T	T	T
0.3031720423000990	0.2473853495756068	0.4866473417577512	T	T	T
0.3031695807061232	0.5807282884668025	0.4866427428626216	T	T	T
0.3031614054819008	0.9140644834537094	0.4866363798557714	T	T	T
0.5582969564775258	0.2014784559466312	0.5066611438285823	T	T	T
0.5583274255335340	0.5347692223395941	0.5066674806994911	T	T	T
0.5583153157020689	0.8680894933973822	0.5066608030840560	T	T	T
0.8149600015271705	0.1542618906185803	0.5272672076977527	T	T	T
0.8149628465220673	0.4875094736985851	0.5272632180392094	T	T	T
0.8149375526969276	0.8208712066584187	0.5272152099196699	T	T	T
0.0714521364653870	0.1072913892334656	0.5479382536976801	T	T	T
0.0714231420005685	0.4406336816229715	0.5479688038434932	T	T	T
0.0714214759535061	0.7740116616054055	0.5479612411516024	T	T	T
0.3259871526192858	0.0617731470794274	0.5689243711364120	T	T	T
0.3258908365360322	0.3952415791204072	0.5689486405116064	T	T	T
0.3260161143148312	0.7284385052905820	0.5689211902555288	T	T	T
0.5825072716782822	0.0147298073919523	0.5884440775400327	T	T	T
0.5826453519482929	0.3479565680381896	0.5884844933912305	T	T	T
0.5826855802359852	0.6812258315759298	0.5884847876873228	T	T	T
0.8416497109065280	0.6322226920556613	0.6087410588922448	T	T	T
0.8418017875947266	0.2986286401585120	0.6088043344144691	T	T	T
0.8416203843102009	0.9651714839807817	0.6086969154208156	T	T	T
0.0969878422783826	0.5862032406750725	0.6322957876170451	T	T	T
0.0972770182240445	0.2524839881474845	0.6322528604310943	T	T	T
0.0973072435849109	0.9192864317355632	0.6322615062053383	T	T	T
0.3499990235386721	0.5419106137988612	0.6516021344386476	T	T	T
0.3497464553637163	0.2087090593763495	0.6515972001294678	T	T	T
0.3500677785181906	0.8750590393760370	0.6515993232857151	T	T	T
0.6031236262162839	0.4975736334423939	0.6714509586363379	T	T	T
0.6026315823087618	0.1644724048432043	0.6713687392140842	T	T	T
0.6026966143111012	0.8313664118834713	0.6713713097676223	T	T	T
0.8570350526901942	0.4533763758951897	0.6885302081592939	T	T	T
0.8568693919725797	0.1185240090432015	0.6884263924787980	T	T	T

0.8569869634212146 0.7860165273750822 0.6888625953849040 T T T
0.9403508770418143 0.2152228610380783 0.7975027583005716 T T T
0.9406253741991183 0.3702868400145721 0.7967836094325851 T T T
0.9400222676386832 0.0602535400883539 0.7983047087274262 T T T

CO_2/Defected-Cu(533) E_{ads} = −0.19 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
59 1 2
Selective dynamics
Direct
0.0033480000000026 0.9974660000000029 0.3038949999999971 F F F
0.0030229999999989 0.3308680000000024 0.3037470000000013 F F F
0.0028649999999999 0.6641070000000013 0.3038379999999989 F F F
0.2572189999999992 0.6189010000000010 0.3215059999999994 F F F
0.2573160000000030 0.2854460000000003 0.3213999999999970 F F F
0.2573659999999975 0.9523849999999996 0.3214630000000014 F F F
0.5101849999999999 0.5748710000000017 0.3417460000000005 F F F
0.5102159999999998 0.2413540000000012 0.3418539999999979 F F F
0.5104720000000000 0.9080429999999993 0.3417389999999969 F F F
0.7634449999999973 0.5304860000000033 0.3608040000000017 F F F
0.7634180000000015 0.1971289999999968 0.3608270000000005 F F F
0.7633700000000019 0.8637719999999973 0.3608990000000034 F F F
0.0192890000000006 0.4838880000000003 0.3841249999999974 F F F
0.0193859999999972 0.1505420000000015 0.3841350000000006 F F F
0.0193610000000035 0.8170920000000024 0.3841170000000034 F F F
0.2784880000000030 0.4343569999999985 0.4044999999999987 F F F
0.2786070000000009 0.1011620000000022 0.4046140000000022 F F F
0.2783230000000003 0.7678590000000014 0.4045160000000010 F F F
0.5354340000000022 0.3872569999999982 0.4245429999999999 F F F
0.5353589999999997 0.0536609999999982 0.4246529999999993 F F F
0.5353720000000024 0.7203889999999973 0.4245549999999980 F F F
0.7901030000000020 0.3414780000000022 0.4452939999999970 F F F
0.7902539999999973 0.0081070000000025 0.4453010000000006 F F F
0.7900119999999973 0.6749369999999999 0.4453510000000023 F F F
0.0470155943446237 0.2938003235029929 0.4660779526079604 T T T
0.0470799134111989 0.6267258054831750 0.4660079566367343 T T T
0.0470403592254904 0.9606214812702130 0.4659618992952793 T T T
0.3036217775086218 0.2465168081955896 0.4869029542187834 T T T
0.3041886936673625 0.5792146445999620 0.4865461074768710 T T T
0.3035473893152059 0.9132879223374383 0.4867156288757920 T T T
0.5598606811292990 0.1995473959231261 0.5068098702490266 T T T
0.5599214768128499 0.5330346987895860 0.5068896794510749 T T T
0.5591080344213989 0.8665687406769611 0.5070262312469436 T T T
0.8168731033128058 0.1520205305535205 0.5277271688997256 T T T
0.8165771050839683 0.4855294194399155 0.5278061148564177 T T T
0.8165600791514559 0.8183871066465976 0.5277062109347899 T T T
0.0726675816901725 0.1056408320417227 0.5486511526006767 T T T
0.0722821951935009 0.4386931518882701 0.5488234428282974 T T T
0.0736816682035048 0.7710786225546460 0.5480009681525611 T T T
0.3272823488385499 0.0597301643464592 0.5693198509894110 T T T
0.3284728943265302 0.3923845936950913 0.5691397487467820 T T T
0.3286994718950759 0.7253616371637058 0.5689032782038098 T T T
0.5853756314828801 0.0114148496693234 0.5887583384967816 T T T

0.5859266571958260	0.3440877524516335	0.5885798934692263	T	T	T
0.5864131025868474	0.6774974726560482	0.5890213769058971	T	T	T
0.8442945920277983	0.6249341047811758	0.6110307955488803	T	T	T
0.8449001810225295	0.2986036896174071	0.6107380272293061	T	T	T
0.8452528879809349	0.9606105762737501	0.6091344764430803	T	T	T
0.1004429262756594	0.5812103900401902	0.6326265384074781	T	T	T
0.0970341709873424	0.2514103582069025	0.6338058880301815	T	T	T
0.1008694029975568	0.9159227387110394	0.6322129008819779	T	T	T
0.3535960738535863	0.5378084607401480	0.6519816311300505	T	T	T
0.3530268447006842	0.2047544229210366	0.6520662329842886	T	T	T
0.3532723664398916	0.8714368984740264	0.6520887167251576	T	T	T
0.6092834199819348	0.4919980692447199	0.6700462283275943	T	T	T
0.6069456584566184	0.1600290713626532	0.6718486823700992	T	T	T
0.6085243751154983	0.8246094064915263	0.6706225625654748	T	T	T
0.8625304476996757	0.1114576835521664	0.6881115456703476	T	T	T
0.8612364698298085	0.7817370015382865	0.6888177663871278	T	T	T
0.7070131826538043	0.3820771022493262	0.7984597793355953	T	T	T
0.6668147033282559	0.5623859940442867	0.7914517324398703	T	T	T
0.7477170177289356	0.2015432074165658	0.8057073359790199	T	T	T

CO_2/Cu(533) E_{ads} = −0.19 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 2
Selective dynamics
Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0470554582440919	0.2942262271836358	0.4658897115631245	T	T	T
0.0469978885373213	0.6276122634258565	0.4658984337143576	T	T	T
0.0470263782626078	0.9608740222867980	0.4658831681027802	T	T	T
0.3034370660039912	0.2471812737085601	0.4866913726604686	T	T	T

0.3034721748848701 0.5804860704436684 0.4867151603979573 T T T
0.3035125778615862 0.9137525271576794 0.4866952415089028 T T T
0.5587165008875472 0.2010623859999240 0.5067681086708019 T T T
0.5587721467968165 0.5343751090979878 0.5067364476051270 T T T
0.5587676457828538 0.8677874125639060 0.5067584184820025 T T T
0.8155921740881209 0.1536413912562957 0.5273978954822791 T T T
0.8156085035150914 0.4870483489107602 0.5273967063742697 T T T
0.8155256887069149 0.8204646992458575 0.5273968279363765 T T T
0.0722004451167280 0.1066549090810876 0.5480899416411070 T T T
0.0720590682984212 0.4401720871633356 0.5481415497961950 T T T
0.0720741883643736 0.7734561389357021 0.5481575827343174 T T T
0.3269186878541363 0.0610188498349998 0.5690253414972030 T T T
0.3267923862906240 0.3944581743904833 0.5690683277007381 T T T
0.3269167832841515 0.7276831511157669 0.5690231615127137 T T T
0.5836328493319300 0.0137689913452518 0.5886945360307018 T T T
0.5836726223803331 0.3468618776607945 0.5885655927419084 T T T
0.5837224711217472 0.6805213376972060 0.5885583154024189 T T T
0.8428123425777919 0.6313509480494425 0.6090603395682165 T T T
0.8430951901869321 0.2974896979182734 0.6089508510004626 T T T
0.8428377538581674 0.9642227855521676 0.6090941616096318 T T T
0.0985084635482615 0.5849729494379600 0.6325743699342541 T T T
0.0988522347247468 0.2512718835255149 0.6324186321882939 T T T
0.0988261669834101 0.9179956606786775 0.6324332639445425 T T T
0.3517067556958116 0.5405301426944018 0.6517739243157339 T T T
0.3516230692184711 0.2072155969850429 0.6517613601990925 T T T
0.3517679867119715 0.8737044904250850 0.6517589508066118 T T T
0.6050833370794686 0.4959528120452471 0.6711173368360951 T T T
0.6046699785782165 0.1629946521532650 0.6716430590285339 T T T
0.6046564147943896 0.8296680560590991 0.6716368114391866 T T T
0.8595711856938987 0.4506212466380053 0.6888658198269578 T T T
0.8595641344534044 0.1171758110118913 0.6889641556440851 T T T
0.8589742435622952 0.7843368319423604 0.6893094159315021 T T T
0.7271143441697132 0.3954660201006837 0.8039483805197863 T T T
0.7210403742865998 0.5556011552796042 0.8044504703638848 T T T
0.7337911308105918 0.2348147984062453 0.8036976756831541 T T T

CO_2/Cu(533) E_{ads} = −0.19 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 2
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F

0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0470767743827251	0.2940789661745868	0.4659300545943453	T	T	T
0.0470416016597536	0.6274685753313024	0.4659197562112451	T	T	T
0.0470827977113099	0.9606917607245535	0.4659259228668916	T	T	T
0.3035586519461673	0.2469224111524788	0.4867328330469953	T	T	T
0.3035786263790696	0.5802040890572491	0.4867492149321367	T	T	T
0.3036252927028017	0.9134994934605281	0.4867251394068378	T	T	T
0.5588477122572301	0.2007823411840620	0.5068335160857058	T	T	T
0.5589205943944386	0.5340262863914539	0.5068344727341677	T	T	T
0.5589397354260411	0.8674100136883696	0.5068303086005398	T	T	T
0.8156151878335497	0.1534410871567841	0.5274898566264686	T	T	T
0.8156029477573364	0.4868286907881112	0.5274594433874504	T	T	T
0.8155728158236388	0.8199304157071734	0.5274622860925851	T	T	T
0.0723021447420519	0.1062416289477129	0.5481295011060089	T	T	T
0.0722462339319421	0.4397523354007065	0.5481777545807757	T	T	T
0.0723117454543784	0.7728834870798656	0.5481933994579321	T	T	T
0.3271835864208711	0.0603999429186921	0.5690646628374286	T	T	T
0.3270082735525707	0.3939235492550628	0.5691470846910966	T	T	T
0.3270900310816612	0.7271882113131934	0.5691186452199959	T	T	T
0.5838540295118673	0.0131398801955311	0.5888286399153264	T	T	T
0.5839576396178856	0.3464346957381809	0.5888310727846219	T	T	T
0.5839407066551677	0.6797699838664227	0.5887974973105655	T	T	T
0.8431597418452775	0.6302923096651188	0.6093002188670581	T	T	T
0.8431787979126369	0.2973643394630802	0.6091086394567499	T	T	T
0.8430261808775621	0.9633252655499638	0.6089888716915318	T	T	T
0.0986733951962979	0.5843203353378944	0.6326528588387359	T	T	T
0.0991346063289270	0.2505930137350735	0.6323245116985902	T	T	T
0.0988230734232327	0.9176240614025125	0.6325053746303579	T	T	T
0.3517914106017505	0.5400458263439003	0.6518558490872313	T	T	T
0.3517610536052393	0.2064956610727499	0.6518363193239325	T	T	T
0.3519512785085015	0.8731001027107135	0.6518563816506137	T	T	T
0.6051844350654471	0.4955480647529838	0.6718903122374082	T	T	T
0.6044878839031770	0.1624983200888421	0.6719034646745172	T	T	T
0.6051380065304655	0.8285725713479577	0.6718946201115145	T	T	T
0.8603728129229246	0.4494445416570503	0.6893263605167645	T	T	T
0.8586745546433754	0.1163905105759801	0.6887112346878060	T	T	T
0.8590210924426754	0.7842436930079917	0.6894551153243145	T	T	T
0.8641205157232019	0.2889839681970954	0.8068686847675923	T	T	T
0.7763084998096693	0.2511363454798082	0.8210496163387120	T	T	T
0.9524192782378026	0.3269452331387915	0.7927437239815478	T	T	T

CO_2/Cu(533) E_{ads} = −0.18 eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O
60 1 2
Selective dynamics
Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F
0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0475513388307257	0.2939145885483636	0.4658476913523275	T	T	T
0.0475456577216824	0.6273327972682411	0.4658277619918511	T	T	T
0.0475209396769515	0.9605937123098287	0.4658285641685959	T	T	T
0.3043843157761800	0.2465788825040632	0.4866429884507942	T	T	T
0.3043075798257434	0.5800356196222428	0.4866807189453274	T	T	T
0.3044119079850523	0.9131786682600533	0.4866452754336304	T	T	T
0.5597690976817854	0.2004976451848635	0.5067435059814107	T	T	T
0.5599237503096176	0.5335925618220799	0.5067823159698384	T	T	T
0.5599692367448943	0.8669316601293670	0.5067413522781807	T	T	T
0.8170281219849815	0.1526700511173547	0.5274025353586573	T	T	T
0.8170672123557042	0.4860846170470605	0.5273272424874468	T	T	T
0.8169455942519112	0.8196424920686444	0.5273565527343531	T	T	T
0.0741898385003125	0.1052266632395394	0.5479913978018930	T	T	T
0.0741073622339369	0.4389138879171436	0.5479664347709285	T	T	T
0.0738729734108140	0.7723467629174575	0.5481071070347376	T	T	T
0.3293507415772903	0.0593778081172700	0.5689232100036912	T	T	T
0.3288775669417630	0.3932222924701073	0.5690379141696802	T	T	T
0.3290106778799893	0.7263002456647110	0.5690600269112042	T	T	T
0.5859804945753589	0.0123885308119264	0.5886490618429057	T	T	T
0.5860423541551971	0.3454844527379164	0.5887085449282878	T	T	T
0.5862283012306306	0.6786988231021223	0.5886547367707430	T	T	T
0.8455492661761298	0.6296598175228048	0.6088682303774766	T	T	T
0.8456313037816953	0.2957115051509144	0.6088810364901568	T	T	T
0.8453732345527702	0.9627331541656217	0.6091435157912851	T	T	T
0.1011909376054980	0.5831501846776797	0.6324459074500105	T	T	T
0.1019280220128948	0.2492853229771836	0.6319792587436236	T	T	T
0.1011991965898129	0.9165939606230508	0.6324912102275765	T	T	T
0.3544270351498055	0.5388206432065559	0.6517720012524615	T	T	T
0.3545759253761482	0.2052859756578779	0.6516999461159476	T	T	T
0.3546810919722113	0.8718774946306050	0.6517028044786687	T	T	T

0.6080346202403183 0.4942414572693193 0.6716970153001450 T T T
0.6076327574059676 0.1610726826733681 0.6717454691592768 T T T
0.6080026868802022 0.8273911988136780 0.6716323552407502 T T T
0.8632343930602578 0.4480701120204738 0.6884977462971356 T T T
0.8618379839473319 0.1160673034718929 0.6892674107618808 T T T
0.8619300766439798 0.7826841525363231 0.6892751717273167 T T T
0.8404850845995663 0.4555162732161505 0.8120605456489076 T T T
0.7210351646823796 0.4892585033403563 0.8266926387085248 T T T
0.9605400304644932 0.4215055284224297 0.7974743402689765 T T T

$CO_2/Cu_3/Cu(533)$ $E_{ads} = -0.18$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
63 1 2
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F
0.2571614599999990 0.9524293899999989 0.3219123699999997 F F F
0.5099116399999986 0.5747781399999994 0.3415763200000015 F F F
0.5095861200000016 0.2417833900000019 0.3416938299999970 F F F
0.5096986000000001 0.9088501900000026 0.3416314700000029 F F F
0.7627858999999972 0.5310134699999978 0.3609394899999998 F F F
0.7629538699999969 0.1970798500000015 0.3608490599999996 F F F
0.7629705100000024 0.8638077299999978 0.3608832600000014 F F F
0.0188077500000006 0.4844866199999984 0.3845455499999986 F F F
0.0188649600000019 0.1508076399999965 0.3844206699999972 F F F
0.0189457299999987 0.8174492599999965 0.3845321800000008 F F F
0.2777182000000025 0.4350678200000004 0.4051130599999979 F F F
0.2779364200000032 0.1018241299999971 0.4049400600000013 F F F
0.2778532499999997 0.7683188099999967 0.4050370400000034 F F F
0.5346647900000008 0.3873898000000011 0.4243529600000002 F F F
0.5347255300000029 0.0542446099999978 0.4245416400000011 F F F
0.5343893300000033 0.7214487199999979 0.4243017399999971 F F F
0.7896143700000025 0.3418778500000030 0.4451831499999983 F F F
0.7893677400000030 0.0085227100000012 0.4452920299999974 F F F
0.7895473399999986 0.6754118300000016 0.4453449800000016 F F F
0.0464369972115201 0.2945376084436330 0.4663750365294022 T T T
0.0459723504446650 0.6288058451099662 0.4666664059055486 T T T
0.0465781875411020 0.9612357139692732 0.4663799156625270 T T T
0.3024890334622227 0.2478406977788393 0.4869587965233605 T T T
0.3026731679781432 0.5812849691213133 0.4870322848599977 T T T
0.3026293866677672 0.9147869141617189 0.4869944685930476 T T T
0.5579028918714057 0.2023755103839551 0.5066694899366787 T T T
0.5584814981710856 0.5349188168085914 0.5061746310058806 T T T
0.5581375381443504 0.8682660223938324 0.5065895996125883 T T T
0.8154356355457522 0.1537209297243630 0.5272953746306311 T T T
0.8149050720387812 0.4880647512696902 0.5273853630420794 T T T
0.8143973952408144 0.8220250872260844 0.5277299806256806 T T T
0.0709295233526129 0.1076162318817616 0.5488979630838826 T T T
0.0703307770301431 0.4417343226729834 0.5486846608417499 T T T

0.0710301679769736 0.7751568700561594 0.5491313881454901 T T T
0.3256907043988805 0.0623895800064975 0.5690990026133959 T T T
0.3244690780239648 0.3963184252143278 0.5691135506374337 T T T
0.3264943171788946 0.7287746170291374 0.5689616044091177 T T T
0.5819649858731226 0.0162023231500873 0.5882184918859006 T T T
0.5833829667323660 0.3483933778976163 0.5879446774569862 T T T
0.5831138766113400 0.6812228729758049 0.5879538378872785 T T T
0.8408194226515183 0.6338211801535995 0.6098353168408057 T T T
0.8414755419457298 0.2990956385225296 0.6094933200651843 T T T
0.8411913008968459 0.9670217421615852 0.6100941272764207 T T T
0.0931378641611751 0.5892907673318608 0.6339417410685626 T T T
0.0954547361387104 0.2549786651202779 0.6327682545969947 T T T
0.0974190214378776 0.9200231935577456 0.6338835831750048 T T T
0.3469241915373804 0.5403639039006672 0.6504021554466253 T T T
0.3477380403947114 0.2110257323474643 0.6518432013907794 T T T
0.3475622629924259 0.8820411609478447 0.6513711446840684 T T T
0.6040877704581489 0.4975092889198588 0.6691195105278168 T T T
0.6024367410192849 0.1616221549206293 0.6705807102976512 T T T
0.6025491212237413 0.8366860670363353 0.6702245781223033 T T T
0.8617315229514300 0.4514988273653540 0.6906947935216796 T T T
0.8634483546657598 0.1136832585433510 0.6913225876657481 T T T
0.8543358601994576 0.7894775785856908 0.6921203850072574 T T T
0.6212739238214713 0.6485813168957483 0.7464523720525104 T T T
0.6249542891726541 0.3150292448881412 0.7468617653429513 T T T
0.3694780451922234 0.6882701491177521 0.7274141970957795 T T T
0.6435175753106427 0.5864184288396680 0.8596274934632053 T T T
0.6261412316144124 0.7282491764332494 0.8344742725708018 T T T
0.6608916679721401 0.4455923590079589 0.8844566086546185 T T T

CO_2/Cu(533) $E_{ads} = -0.17$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 2
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F

0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F
0.0470725657237430 0.2942144227859178 0.4658614633312877 T T T
0.0470773363195854 0.6276393623896240 0.4659280368676315 T T T
0.0470048940587383 0.9609173262563179 0.4659308771419906 T T T
0.3035832349634300 0.2470523078444448 0.4867148500450951 T T T
0.3033731674983349 0.5806295040349718 0.4868241221428410 T T T
0.3036168147971647 0.9136848144042375 0.4867417662355634 T T T
0.5586703527825678 0.2012289151025220 0.5068435332274460 T T T
0.5587856288014555 0.5343839672447400 0.5068288367678520 T T T
0.5590155149440661 0.8676338928422261 0.5068017661991299 T T T
0.8154450715866494 0.1536721286975359 0.5274554888864867 T T T
0.8156527284111049 0.4870170714779489 0.5274203270137929 T T T
0.8155420355149546 0.8207424442583899 0.5274463859718128 T T T
0.0722856909717353 0.1066226070734883 0.5481017167097888 T T T
0.0721921522145193 0.4401376312397732 0.5481034438011202 T T T
0.0719784174883366 0.7736211695695528 0.5483158316733384 T T T
0.3271600433893761 0.0609093361336933 0.5690677094223013 T T T
0.3266693239608418 0.3945549578973943 0.5691661345439482 T T T
0.3268171209120769 0.7278711513859588 0.5692048252030238 T T T
0.5837061288860037 0.0138718665654221 0.5888176622575040 T T T
0.5835043893576087 0.3472105970707035 0.5888256942168389 T T T
0.5838445622656988 0.6802899185244878 0.5887625886052382 T T T
0.8428643504663593 0.6318734078883458 0.6089503952494618 T T T
0.8428657325720522 0.2971185661674822 0.6089553065510059 T T T
0.8427871934069754 0.9646232261441638 0.6094757862373691 T T T
0.0983659152563750 0.5850209761964860 0.6327156332525107 T T T
0.0987033537291219 0.2515456192138700 0.6323045431753396 T T T
0.0984643149542825 0.9184137840398739 0.6326772606360103 T T T
0.3514804027687305 0.5406886693283954 0.6518853502591198 T T T
0.3515179465526632 0.2073726288415854 0.6518759816112464 T T T
0.3514161362630539 0.8742984002021092 0.6518867610226133 T T T
0.6043694794432736 0.4966900787155774 0.6718470228664477 T T T
0.6046318491191991 0.1631452095030532 0.6719393899600796 T T T
0.6044646982802925 0.8299024710744308 0.6718218964108347 T T T
0.8587237263837268 0.4513728443880543 0.6881475589474148 T T T
0.8590293765214045 0.1181192054643813 0.6896511384032398 T T T
0.8588662400525205 0.7843605756797991 0.6896553587829845 T T T
0.8757970550374820 0.4331292709451409 0.8094623392310499 T T T
0.8712744422201069 0.5920466496277786 0.8102200831341437 T T T
0.8809111260913181 0.2737202585703178 0.8089162083971732 T T T

CO_2/Cu_3/Cu(533) E_{ads} = −0.15 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
63 1 2
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F

0.2572489900000008	0.6186597399999982	0.3218759499999990	F	F	F
0.2571973700000001	0.2857762699999995	0.3217927099999969	F	F	F
0.2571614599999990	0.9524293899999989	0.3219123699999997	F	F	F
0.5099116399999986	0.5747781399999994	0.3415763200000015	F	F	F
0.5095861200000016	0.2417833900000019	0.3416938299999970	F	F	F
0.5096986000000001	0.9088501900000026	0.3416314700000029	F	F	F
0.7627858999999972	0.5310134699999978	0.3609394899999998	F	F	F
0.7629538699999969	0.1970798500000015	0.3608490599999996	F	F	F
0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F
0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0466295784859473	0.2942308890310409	0.4663632766625865	T	T	T
0.0460331435946214	0.6287890567102572	0.4666452891797748	T	T	T
0.0465510688284326	0.9611687464316025	0.4664075896646047	T	T	T
0.3026440626984828	0.2479551120579834	0.4868760823492304	T	T	T
0.3027032770177108	0.5810088232816576	0.4870836475488428	T	T	T
0.3026723433108349	0.9143389604824406	0.4869597524323185	T	T	T
0.5579430892309593	0.2019112973576215	0.5067187505902495	T	T	T
0.5585147936341163	0.5346452193330591	0.5061547841213081	T	T	T
0.5585820662648732	0.8674330568136083	0.5063817028661455	T	T	T
0.8156264844841770	0.1532337333764280	0.5273135078801204	T	T	T
0.8154807724888063	0.4871665784130249	0.5273599774217560	T	T	T
0.8147558769934085	0.8215249591311922	0.5276897757417280	T	T	T
0.0713218574341011	0.1065529634329391	0.5490054997571107	T	T	T
0.0706785732143579	0.4415215098708672	0.5485727394558884	T	T	T
0.0714270505375940	0.7746726941402184	0.5492919249451700	T	T	T
0.3262546896875838	0.0621130065158079	0.5684610553760975	T	T	T
0.3250447642625749	0.3958894739801890	0.5694763279681180	T	T	T
0.3264079212022271	0.7276705586919706	0.5691068840506766	T	T	T
0.5825763212413673	0.0134124685451462	0.5880319825644468	T	T	T
0.5834484384152261	0.3476139696394124	0.5877503493233421	T	T	T
0.5839767467405114	0.6799548203630715	0.5878236026849867	T	T	T
0.8410444831981840	0.6331176640097679	0.6097877844375941	T	T	T
0.8419024721528168	0.2977100454994291	0.6095527322356468	T	T	T
0.8423738923068855	0.9655011975758693	0.6100865106945652	T	T	T
0.0941484827506169	0.5879651541492611	0.6340244915294899	T	T	T
0.0964164780502342	0.2541586098819065	0.6321423802912437	T	T	T
0.0966281904599595	0.9202067548559558	0.6350699926987328	T	T	T
0.3474758921094577	0.5399397939954310	0.6517071759849425	T	T	T
0.3484947696593532	0.2094878124955256	0.6517436508333786	T	T	T
0.3479909021462265	0.8823669384849024	0.6497320782410927	T	T	T
0.6035219519684372	0.4972549422453765	0.6686898124394781	T	T	T
0.6034627272659964	0.1571798602422017	0.6690269998727860	T	T	T
0.6029261842720184	0.8332635653957789	0.6714135119787369	T	T	T
0.8653012400998125	0.4475690919982231	0.6901873261574442	T	T	T
0.8580788367239988	0.1175250935473918	0.6920606071029025	T	T	T
0.8551199287676141	0.7876518019696446	0.6920121479184501	T	T	T
0.6319941570186822	0.6299955130546140	0.7469731205093711	T	T	T

0.6081892334777331	0.3202210368020261	0.7449515282106388	T	T	T
0.3672726334321191	0.7052404047137283	0.7270678093052054	T	T	T
0.6292148232015243	0.4729679414180093	0.8567282182988242	T	T	T
0.5844664905625069	0.3653383140697779	0.8640092970359053	T	T	T
0.6742600748138771	0.5809816983571640	0.8497277758107775	T	T	T

$CO_2/Cu_3/Cu(533)$ E_{ads} = −0.01 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
63 1 2
Selective dynamics
Direct

0.0032853599999996	0.9972806999999975	0.3042624500000031	F	F	F
0.0028217400000017	0.3308767700000033	0.3042691500000032	F	F	F
0.0026800899999984	0.6645640400000019	0.3042978000000005	F	F	F
0.2572489900000008	0.6186597399999982	0.3218759499999990	F	F	F
0.2571973700000001	0.2857762699999995	0.3217927099999969	F	F	F
0.2571614599999990	0.9524293899999989	0.3219123699999997	F	F	F
0.5099116399999986	0.5747781399999994	0.3415763200000015	F	F	F
0.5095861200000016	0.2417833900000019	0.3416938299999970	F	F	F
0.5096986000000001	0.9088501900000026	0.3416314700000029	F	F	F
0.7627858999999972	0.5310134699999978	0.3609394899999998	F	F	F
0.7629538699999969	0.1970798500000015	0.3608490599999996	F	F	F
0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F
0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0465744794685139	0.2942628588114094	0.4663817412383314	T	T	T
0.0459639222632286	0.6287901107517049	0.4666780876070683	T	T	T
0.0465868258341295	0.9612180465666481	0.4664441762099605	T	T	T
0.3027350954102405	0.2476748063880919	0.4868716136440579	T	T	T
0.3027387854683291	0.5810497111260911	0.4870209034212635	T	T	T
0.3029994850755182	0.9143442133987192	0.4869477672674092	T	T	T
0.5580580685096387	0.2021017564336812	0.5067575818713191	T	T	T
0.5587540686369821	0.5343979314486680	0.5062642570345897	T	T	T
0.5585593752010906	0.8676914708936125	0.5066180135186719	T	T	T
0.8155421541915848	0.1532266752800079	0.5273931759324201	T	T	T
0.8154471595290440	0.4871709390409135	0.5273535382520150	T	T	T
0.8144074673332578	0.8217708774665254	0.5278354807828850	T	T	T
0.0716872783187506	0.1064272713340876	0.5489415711908032	T	T	T
0.0708146186611872	0.4412102928656732	0.5486296194399386	T	T	T
0.0713650410977496	0.7745469905505383	0.5492833695478921	T	T	T
0.3265542940058383	0.0618351193935584	0.5688308346135732	T	T	T
0.3249231976822879	0.3955348960272991	0.5691713103958757	T	T	T
0.3271348448919749	0.7276652652637566	0.5688471250577285	T	T	T

0.5823964229416293 0.0155342828934501 0.5885519830945695 T T T
0.5839769005242128 0.3474541504705266 0.5882875879926106 T T T
0.5841855597026855 0.6797725727268714 0.5881385399868984 T T T
0.8412261011995120 0.6329774758365145 0.6097208357303766 T T T
0.8422134296134971 0.2978249754769159 0.6094002286425728 T T T
0.8415004246945750 0.9659114370939396 0.6101921555262007 T T T
0.0935830062531119 0.5884563320059685 0.6341735415125532 T T T
0.0964019583647221 0.2539583330739926 0.6324816603697397 T T T
0.0982038171951745 0.9190371058759925 0.6343348403910457 T T T
0.3481454509983680 0.5387503616396856 0.6502874645561735 T T T
0.3486079255429085 0.2101781109590672 0.6519372147896002 T T T
0.3490393431344123 0.8813206142521748 0.6502949086110411 T T T
0.6048474247888288 0.4964919121419293 0.6701176887936512 T T T
0.6025014040491500 0.1621525129531740 0.6716928303869401 T T T
0.6026788139044927 0.8357620119182881 0.6709268229037145 T T T
0.8627768940822744 0.4499604665901751 0.6900895994770118 T T T
0.8619596541744037 0.1137837848476419 0.6909952366345331 T T T
0.8536346165260048 0.7889032572756812 0.6921571936119099 T T T
0.6261264676291576 0.6487057381521107 0.7478415321484412 T T T
0.6249474084911809 0.3185800722407915 0.7491344189660625 T T T
0.3655054193041437 0.6960036098784530 0.7259629480588520 T T T
0.6297161100376242 0.4615369788680590 0.8181398205553591 T T T
0.6343973012137587 0.6155331235063733 0.8284226472950155 T T T
0.6326397284537953 0.3085854027456563 0.8344576871019916 T T T

$CO_2/Cu_3/Cu(533)$ $E_{ads} = -0.01$ eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
63 1 2
Selective dynamics
Direct
0.0032853599999996 0.9972806999999975 0.3042624500000031 F F F
0.0028217400000017 0.3308767700000033 0.3042691500000032 F F F
0.0026800899999984 0.6645640400000019 0.3042978000000005 F F F
0.2572489900000008 0.6186597399999982 0.3218759499999990 F F F
0.2571973700000001 0.2857762699999995 0.3217927099999969 F F F
0.2571614599999990 0.9524293899999989 0.3219123699999997 F F F
0.5099116399999986 0.5747781399999994 0.3415763200000015 F F F
0.5095861200000016 0.2417833900000019 0.3416938299999970 F F F
0.5096986000000001 0.9088501900000026 0.3416314700000029 F F F
0.7627858999999972 0.5310134699999978 0.3609394899999998 F F F
0.7629538699999969 0.1970798500000015 0.3608490599999996 F F F
0.7629705100000024 0.8638077299999978 0.3608832600000014 F F F
0.0188077500000006 0.4844866199999984 0.3845455499999986 F F F
0.0188649600000019 0.1508076399999965 0.3844206699999972 F F F
0.0189457299999987 0.8174492599999965 0.3845321800000008 F F F
0.2777182000000025 0.4350678200000004 0.4051130599999979 F F F
0.2779364200000032 0.1018241299999971 0.4049400600000013 F F F
0.2778532499999997 0.7683188099999967 0.4050370400000034 F F F
0.5346647900000008 0.3873898000000011 0.4243529600000002 F F F
0.5347255300000029 0.0542446099999978 0.4245416400000011 F F F
0.5343893300000033 0.7214487199999979 0.4243017399999971 F F F
0.7896143700000025 0.3418778500000030 0.4451831499999983 F F F
0.7893677400000030 0.0085227100000012 0.4452920299999974 F F F

0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0467564296397837	0.2940960847727238	0.4663725574276189	T	T	T
0.0462919022515335	0.6286554182915489	0.4667226621321313	T	T	T
0.0467242815853006	0.9610080822783300	0.4664774535495215	T	T	T
0.3034933927139339	0.2471545958502854	0.4868072645159363	T	T	T
0.3030299349095341	0.5808367984360350	0.4870915168743707	T	T	T
0.3033779634235050	0.9136441077365262	0.4869692298391889	T	T	T
0.5587483318511063	0.2012733430176096	0.5067328544530052	T	T	T
0.5593057179858115	0.5339865648163741	0.5063123697229999	T	T	T
0.5593913738147526	0.8674286057629744	0.5065280991915394	T	T	T
0.8165185768923454	0.1521154052251785	0.5275961328038483	T	T	T
0.8163077022815091	0.4862810014338333	0.5274465037480509	T	T	T
0.8156556436926269	0.8211470323985101	0.5277904572285377	T	T	T
0.0724808446446619	0.1052326786731192	0.5491413356184882	T	T	T
0.0720793391373671	0.4401618188334381	0.5485370654633974	T	T	T
0.0720873671230680	0.7743794968538440	0.5497269551137980	T	T	T
0.3276745439390115	0.0606863839884982	0.5685328738463385	T	T	T
0.3260328581472829	0.3945256898843191	0.5690107730587837	T	T	T
0.3272158873649648	0.7274487036276407	0.5689935203475945	T	T	T
0.5841090607409731	0.0139630665935002	0.5885191882019066	T	T	T
0.5853159055793115	0.3465041745824922	0.5880763485364900	T	T	T
0.5853093917866493	0.6793812283129572	0.5878740007440798	T	T	T
0.8432307176229189	0.6320397226218494	0.6094764869000757	T	T	T
0.8435354174877581	0.2956998995288794	0.6097452822430612	T	T	T
0.8436295853652621	0.9645199543321873	0.6108632368066865	T	T	T
0.0950733554001870	0.5866020735013155	0.6344092628998919	T	T	T
0.0981476224919968	0.2521495768858082	0.6322818920514145	T	T	T
0.0980560897816425	0.9189894404945728	0.6369492112880323	T	T	T
0.3505500655593146	0.5364282251660765	0.6496788047848775	T	T	T
0.3503703283517667	0.2076477745326651	0.6514294312311689	T	T	T
0.3499541422935317	0.8800135625871738	0.6502690937383109	T	T	T
0.6032307682357418	0.5023110390045575	0.6698491276708192	T	T	T
0.6040779092073303	0.1593683601450418	0.6707573044597794	T	T	T
0.6051200554008961	0.8324193221351869	0.6708350669903661	T	T	T
0.8657489367122116	0.4470154832747317	0.6896609531651490	T	T	T
0.8541443487957537	0.1213402793137865	0.6930009335323732	T	T	T
0.8551231660119376	0.7867551505833403	0.6927352515662907	T	T	T
0.6452327424692456	0.6435444573971136	0.7489050432151259	T	T	T
0.5983015534801486	0.3371877079737614	0.7464552659239891	T	T	T
0.3469489161290885	0.7067877123574460	0.7262573153321763	T	T	T
0.4355349380015802	0.6208074585462809	0.7993437119582623	T	T	T
0.3234296068227722	0.6413941968745972	0.8210372816579657	T	T	T
0.5433966905015574	0.6429973167830065	0.8124199674661410	T	T	T

$CO_2/Cu_3/Cu(533)$ E_{ads} = 0.05 eV

1.00000000000000

10.3878408006999994	0.0000000000000000	0.0000000000000000
4.5828709415000004	6.0103788927000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.5000000000000000

Cu C O

63 1 2

Selective dynamics

Direct

0.0032853599999996	0.9972806999999975	0.3042624500000031	F	F	F
0.0028217400000017	0.3308767700000033	0.3042691500000032	F	F	F
0.0026800899999984	0.6645640400000019	0.3042978000000005	F	F	F
0.2572489900000008	0.6186597399999982	0.3218759499999990	F	F	F

0.2571973700000001	0.2857762699999995	0.3217927099999969	F	F	F
0.2571614599999990	0.9524293899999989	0.3219123699999997	F	F	F
0.5099116399999986	0.5747781399999994	0.3415763200000015	F	F	F
0.5095861200000016	0.2417833900000019	0.3416938299999970	F	F	F
0.5096986000000001	0.9088501900000026	0.3416314700000029	F	F	F
0.7627858999999972	0.5310134699999978	0.3609394899999998	F	F	F
0.7629538699999969	0.1970798500000015	0.3608490599999996	F	F	F
0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F
0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0465669434970339	0.2942140852871729	0.4664711229416851	T	T	T
0.0463038644946141	0.6283846543645127	0.4666578976158924	T	T	T
0.0464781847697484	0.9613138978240356	0.4664937121643093	T	T	T
0.3029059112066614	0.2473423073724455	0.4869905889486585	T	T	T
0.3028679146343970	0.5809978858061294	0.4871072100207932	T	T	T
0.3027858262375792	0.9144030554412538	0.4870995827501405	T	T	T
0.5581235804593081	0.2021326755318044	0.5065081028019434	T	T	T
0.5584971480722863	0.5347059677731838	0.5062524012079664	T	T	T
0.5581934009464945	0.8675713749340968	0.5064345138351416	T	T	T
0.8157149795283408	0.1532296681029416	0.5275014439911125	T	T	T
0.8154951032958354	0.4870954524117429	0.5275456487660829	T	T	T
0.8153085290072090	0.8208333477863271	0.5276074435968732	T	T	T
0.0716399051282985	0.1064476215178077	0.5493149508803056	T	T	T
0.0713990622053043	0.4404722503252184	0.5488619032400534	T	T	T
0.0719954210749220	0.7740615555730518	0.5493713381255656	T	T	T
0.3257597427884171	0.0618800059975229	0.5691631445419368	T	T	T
0.3251232272947515	0.3955345204551569	0.5692269476080190	T	T	T
0.3263035199356666	0.7282972686336314	0.5692217130684141	T	T	T
0.5830395688780826	0.0143654156357948	0.5873183792713486	T	T	T
0.5839742189836995	0.3479916881738799	0.5878625878874342	T	T	T
0.5841007154899879	0.6789680975862203	0.5880055668767702	T	T	T
0.8425233140696594	0.6318527926218304	0.6097638001168499	T	T	T
0.8424448800257320	0.2974335881169267	0.6099128364024824	T	T	T
0.8433817323968921	0.9641858267618422	0.6099545058732175	T	T	T
0.0934355167876961	0.5883705589367658	0.6346067567973734	T	T	T
0.0943094790552202	0.2550492877664162	0.6338226096541922	T	T	T
0.0967356464214194	0.9198796199621321	0.6359269244701387	T	T	T
0.3481602685580945	0.5396084998858531	0.6506132224720005	T	T	T
0.3479329085924069	0.2099175284210770	0.6514230665970098	T	T	T
0.3486297399314378	0.8797169205767063	0.6508565618395843	T	T	T
0.6024885985371660	0.4975963724804846	0.6708170729088269	T	T	T
0.6030415149711582	0.1595419358230383	0.6685104771392995	T	T	T
0.6030849188503922	0.8356578773206963	0.6687250561791391	T	T	T
0.8550389435306274	0.4560285291285252	0.6913536193321425	T	T	T
0.8553595953203337	0.1189679996156479	0.6919253686416529	T	T	T
0.8518585483174383	0.7905194688462959	0.6926233410715158	T	T	T
0.6126879739659510	0.6773450172641948	0.7471108189998383	T	T	T
0.6134720418244441	0.2984768055228154	0.7471555552158046	T	T	T

0.3549584433573485	0.7031367467315812	0.7284445020625978	T	T	T
0.4649538555019080	0.6123374012431781	0.7973375341347867	T	T	T
0.4898431364899503	0.7437304800564748	0.8149511117893240	T	T	T
0.4903471015982551	0.4382565031184804	0.8144532177786518	T	T	T

$CO_2/Cu_3/Cu(533)$ E_{ads} = 0.18 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
63 1 2
Selective dynamics
Direct

0.0032853599999996	0.9972806999999975	0.3042624500000031	F	F	F
0.0028217400000017	0.3308767700000033	0.3042691500000032	F	F	F
0.0026800899999984	0.6645640400000019	0.3042978000000005	F	F	F
0.2572489900000008	0.6186597399999982	0.3218759499999990	F	F	F
0.2571973700000001	0.2857762699999995	0.3217927099999969	F	F	F
0.2571614599999990	0.9524293899999989	0.3219123699999997	F	F	F
0.5099116399999986	0.5747781399999994	0.3415763200000015	F	F	F
0.5095861200000016	0.2417833900000019	0.3416938299999970	F	F	F
0.5096986000000001	0.9088501900000026	0.3416314700000029	F	F	F
0.7627858999999972	0.5310134699999978	0.3609394899999998	F	F	F
0.7629538699999969	0.1970798500000015	0.3608490599999996	F	F	F
0.7629705100000024	0.8638077299999978	0.3608832600000014	F	F	F
0.0188077500000006	0.4844866199999984	0.3845455499999986	F	F	F
0.0188649600000019	0.1508076399999965	0.3844206699999972	F	F	F
0.0189457299999987	0.8174492599999965	0.3845321800000008	F	F	F
0.2777182000000025	0.4350678200000004	0.4051130599999979	F	F	F
0.2779364200000032	0.1018241299999971	0.4049400600000013	F	F	F
0.2778532499999997	0.7683188099999967	0.4050370400000034	F	F	F
0.5346647900000008	0.3873898000000011	0.4243529600000002	F	F	F
0.5347255300000029	0.0542446099999978	0.4245416400000011	F	F	F
0.5343893300000033	0.7214487199999979	0.4243017399999971	F	F	F
0.7896143700000025	0.3418778500000030	0.4451831499999983	F	F	F
0.7893677400000030	0.0085227100000012	0.4452920299999974	F	F	F
0.7895473399999986	0.6754118300000016	0.4453449800000016	F	F	F
0.0467839726230798	0.2948782824835299	0.4661552479056044	T	T	T
0.0461557527529711	0.6286820951396150	0.4665106103676936	T	T	T
0.0467246873746500	0.9615579507787881	0.4662760536984292	T	T	T
0.3031640410039602	0.2478675765705731	0.4871990057263207	T	T	T
0.3030915640283030	0.5815000551828474	0.4870019277413814	T	T	T
0.3032184692492937	0.9149326120090375	0.4869599142929697	T	T	T
0.5582965979231010	0.2024867942898499	0.5067211740171370	T	T	T
0.5593268742325457	0.5352083605391115	0.5061744245208734	T	T	T
0.5583289917862194	0.8690951373764709	0.5068615702533361	T	T	T
0.8160817418086596	0.1540054241170006	0.5274090087991117	T	T	T
0.8156878837626343	0.4883601413343092	0.5272389621572110	T	T	T
0.8146736307784574	0.8218527781209157	0.5276766586423574	T	T	T
0.0720128673888412	0.1080469739746871	0.5483773500476861	T	T	T
0.0711091046902795	0.4417956219664157	0.5485652531054339	T	T	T
0.0715437960368660	0.7749273442785585	0.5487139613585110	T	T	T
0.3266749716926544	0.0620639648560225	0.5695947744142680	T	T	T
0.3254302456025082	0.3965707959739249	0.5693544785761034	T	T	T
0.3286285362678286	0.7281946626824681	0.5688514079184268	T	T	T
0.5825493221241071	0.0180176974389636	0.5888210963209467	T	T	T

0.5846062805492395 0.3481643745937977 0.5878613229676757 T T T
0.5845031464349281 0.6814332837453122 0.5882090508195319 T T T
0.8422603204116961 0.6330239426396281 0.6100906638926622 T T T
0.8428907825598331 0.3006648542822737 0.6093055755623729 T T T
0.8410218508172044 0.9664875903068070 0.6095303000468040 T T T
0.0942149097267366 0.5895042685744981 0.6339331111491601 T T T
0.0965639866626503 0.2544998230639606 0.6326743801095018 T T T
0.1008601814548072 0.9183537256983089 0.6318123103798589 T T T
0.3489067077562150 0.5406448454954462 0.6503473148514279 T T T
0.3484886875979860 0.2117413494259529 0.6520915087178433 T T T
0.3500754615892775 0.8800125086089241 0.6526123913023036 T T T
0.6076925710182245 0.4946349916580336 0.6692298418399985 T T T
0.6017184577120342 0.1677290984095722 0.6730611217690857 T T T
0.6037577430218689 0.8391084377006613 0.6698437038328821 T T T
0.8649138915720593 0.4506817447215883 0.6918394363132769 T T T
0.8709337217932418 0.1065880503439085 0.6882696418144592 T T T
0.8550021690955040 0.7926305165393978 0.6918750274074972 T T T
0.6249202481946314 0.6596663911377950 0.7465921105707676 T T T
0.6494181866759190 0.2973095463364986 0.7494277411581874 T T T
0.3821083118618576 0.6712021999894632 0.7282974732109393 T T T
0.8358626732600903 0.4194754452480356 0.7846531014681372 T T T
0.7813185186304910 0.3230023389385797 0.8035167002274469 T T T
0.9528197117683439 0.4168119870953019 0.7907132837371501 T T T

CO_2/Cu(533) E_{ads} = 0.41 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 2
Selective dynamics
Direct
0.0028167898171247 0.9976489200151235 0.3039441514165659 F F F
0.0028168126308827 0.3309822584785778 0.3039441467559953 F F F
0.0028166948928572 0.6643157218161591 0.3039441885103784 F F F
0.2574744155189990 0.6187501937377888 0.3215671923011243 F F F
0.2574743459681059 0.2854169557851023 0.3215672127806215 F F F
0.2574743968137767 0.9520835415233222 0.3215672125015629 F F F
0.5105906574178505 0.5744865754527027 0.3419001422873720 F F F
0.5105905876198378 0.2411532791391480 0.3419001792932548 F F F
0.5105906483272449 0.9078198903871950 0.3419001573355089 F F F
0.7636894606504967 0.5301109644673829 0.3610473030755728 F F F
0.7636894407361865 0.1967776805852210 0.3610473058847674 F F F
0.7636894167226558 0.8634443753729286 0.3610473732197121 F F F
0.0195132785813925 0.4837611278234846 0.3840689485058775 F F F
0.0195133508624821 0.1504277547768567 0.3840689230531780 F F F
0.0195133330193613 0.8170944694876141 0.3840689446337322 F F F
0.2788346320849726 0.4342671477263238 0.4046315537572127 F F F
0.2788346371584254 0.1009338234076012 0.4046315502992286 F F F
0.2788346581162955 0.7676004559074485 0.4046315435029300 F F F
0.5357270031477697 0.3868634222981058 0.4245696545963042 F F F
0.5357269405365486 0.0535301389338798 0.4245696700534936 F F F
0.5357269752515279 0.7201967655408623 0.4245696478064147 F F F
0.7903599325221791 0.3412600279625764 0.4453948406040951 F F F
0.7903598818119377 0.0079267544482065 0.4453948506937095 F F F
0.7903598896628807 0.6745933372964998 0.4453948584338505 F F F

0.0475493035426039	0.2937964140278475	0.4658477497657097	T	T	T
0.0470388532595805	0.6274668382741235	0.4660534609869738	T	T	T
0.0468305281959709	0.9603980561486836	0.4660750969305528	T	T	T
0.3038194471933964	0.2470790734084926	0.4867474802806349	T	T	T
0.3040383898707919	0.5794994191971461	0.4868784876018846	T	T	T
0.3045515586957306	0.9118416190650197	0.4867955141880812	T	T	T
0.5596944617578956	0.1999794301115028	0.5068938750592331	T	T	T
0.5594608866000699	0.5330081500634115	0.5067117350864566	T	T	T
0.5601278935536800	0.8662331208387085	0.5067596794561534	T	T	T
0.8159775100776226	0.1521250840823397	0.5280150556343089	T	T	T
0.8170860979605462	0.4854486294532395	0.5274299156695239	T	T	T
0.8164609208910000	0.8190560767977548	0.5276393004855526	T	T	T
0.0733817215216532	0.1048126106792988	0.5476019073702905	T	T	T
0.0735680149162138	0.4396146737143964	0.5488072319888118	T	T	T
0.0729913869956385	0.7702664107068812	0.5489175635830724	T	T	T
0.3286693524994507	0.0588095892556588	0.5683298959949855	T	T	T
0.3277186612185876	0.3938829619218873	0.5698306278990327	T	T	T
0.3280847572544012	0.7240456273859132	0.5697086244707833	T	T	T
0.5847966147447483	0.0121711033090389	0.5886054652815657	T	T	T
0.5832415756510372	0.3465187062145549	0.5890897971905262	T	T	T
0.5853480730679623	0.6779971864290644	0.5882269666700634	T	T	T
0.8445139596546376	0.6295295829797158	0.6094979543351391	T	T	T
0.8448036510313381	0.2957742364984471	0.6090546555226454	T	T	T
0.8451151630945580	0.9590731568233942	0.6099465455290072	T	T	T
0.1026957599123673	0.5794993381195584	0.6367124292400024	T	T	T
0.1007685166900718	0.2464395755851956	0.6312504236987717	T	T	T
0.0994639529074840	0.9179475503344003	0.6312442949376219	T	T	T
0.3588989022528992	0.5365543455311370	0.6542989539645725	T	T	T
0.3547445976598157	0.1987530868940413	0.6509091922844941	T	T	T
0.3549870939423382	0.8710461650626035	0.6511150243727497	T	T	T
0.6103331413854876	0.4928453262877681	0.6711743388238756	T	T	T
0.6117550475881538	0.1537841508987532	0.6705935820937227	T	T	T
0.6081811828980336	0.8252946096816086	0.6710801110916158	T	T	T
0.8630210298297002	0.4439100073666517	0.6894595310175157	T	T	T
0.8616136800700656	0.1167570063228293	0.6890837236149884	T	T	T
0.8557266193679459	0.7844679863497048	0.6931690703950081	T	T	T
0.1500917956683889	0.5553241213474792	0.7150431616380258	T	T	T
0.0418699681836477	0.5805292721693570	0.7428455202403611	T	T	T
0.2739582057161327	0.5370952740130086	0.7273258026546069	T	T	T

CO_2/Cu(533) E_{ads} = 0.56 eV
1.00000000000000
10.3878408006999994 0.0000000000000000 0.0000000000000000
4.5828709415000004 6.0103788927000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5000000000000000
Cu C O
60 1 2
Selective dynamics
Direct

0.0028167898171247	0.9976489200151235	0.3039441514165659	F	F	F
0.0028168126308827	0.3309822584785778	0.3039441467559953	F	F	F
0.0028166948928572	0.6643157218161591	0.3039441885103784	F	F	F
0.2574744155189990	0.6187501937377888	0.3215671923011243	F	F	F
0.2574743459681059	0.2854169557851023	0.3215672127806215	F	F	F
0.2574743968137767	0.9520835415233222	0.3215672125015629	F	F	F
0.5105906574178505	0.5744865754527027	0.3419001422873720	F	F	F
0.5105905876198378	0.2411532791391480	0.3419001792932548	F	F	F

0.5105906483272449	0.9078198903871950	0.3419001573355089	F	F	F
0.7636894606504967	0.5301109644673829	0.3610473030755728	F	F	F
0.7636894407361865	0.1967776805852210	0.3610473058847674	F	F	F
0.7636894167226558	0.8634443753729286	0.3610473732197121	F	F	F
0.0195132785813925	0.4837611278234846	0.3840689485058775	F	F	F
0.0195133508624821	0.1504277547768567	0.3840689230531780	F	F	F
0.0195133330193613	0.8170944694876141	0.3840689446337322	F	F	F
0.2788346320849726	0.4342671477263238	0.4046315537572127	F	F	F
0.2788346371584254	0.1009338234076012	0.4046315502992286	F	F	F
0.2788346581162955	0.7676004559074485	0.4046315435029300	F	F	F
0.5357270031477697	0.3868634222981058	0.4245696545963042	F	F	F
0.5357269405365486	0.0535301389338798	0.4245696700534936	F	F	F
0.5357269752515279	0.7201967655408623	0.4245696478064147	F	F	F
0.7903599325221791	0.3412600279625764	0.4453948406040951	F	F	F
0.7903598818119377	0.0079267544482065	0.4453948506937095	F	F	F
0.7903598896628807	0.6745933372964998	0.4453948584338505	F	F	F
0.0467456649834661	0.2950415558840748	0.4657802325997104	T	T	T
0.0463492607160342	0.6276572544596217	0.4658327280018979	T	T	T
0.0467801487980940	0.9607983016890967	0.4660165069721957	T	T	T
0.3031496248819956	0.2473045984266381	0.4866895285201928	T	T	T
0.3038682615545690	0.5798912020458602	0.4867208565620199	T	T	T
0.3036092137193511	0.9134862933112630	0.4865513106338802	T	T	T
0.5587069529865930	0.2002052260109301	0.5070199559388594	T	T	T
0.5587898371701150	0.5342818543268736	0.5068945981785691	T	T	T
0.5588020905878102	0.8678592358472871	0.5069918476262349	T	T	T
0.8150421971632619	0.1537577667994529	0.5276431342001157	T	T	T
0.8148627018643111	0.4878143568761322	0.5275986595675013	T	T	T
0.8140272619380295	0.8210328010593221	0.5279184207079454	T	T	T
0.0716087056973938	0.1076824126706827	0.5475122454964682	T	T	T
0.0711578493623037	0.4408429928722871	0.5482964049774943	T	T	T
0.0714606221256553	0.7727360036849447	0.5477031034714089	T	T	T
0.3279842372564732	0.0610232502856057	0.5693351565340278	T	T	T
0.3279507131845970	0.3919220533102490	0.5694389084437810	T	T	T
0.3268418837227407	0.7275591261949326	0.5688387281434918	T	T	T
0.5798829865365991	0.0160263778462057	0.5901520599083364	T	T	T
0.5837738613964282	0.3460512973423421	0.5887068888263453	T	T	T
0.5841313790283040	0.6804006645685372	0.5888448614762810	T	T	T
0.8413806185309846	0.6321832164844560	0.6105669907325468	T	T	T
0.8419674724038536	0.2996572254509655	0.6095524507594177	T	T	T
0.8411201632905040	0.9640279811986230	0.6096040234263764	T	T	T
0.0991183834271706	0.5888648128333042	0.6296546126169007	T	T	T
0.0989499409243052	0.2466333155286260	0.6294412844650735	T	T	T
0.0980518960537630	0.9187127473340713	0.6304334380141019	T	T	T
0.3561915816193667	0.5390366574601247	0.6510427712740925	T	T	T
0.3476092943878039	0.2082738371446838	0.6588105851868701	T	T	T
0.3553834052862130	0.8680696106892055	0.6511068830347027	T	T	T
0.6080978926074055	0.4950252600168206	0.6720997352652107	T	T	T
0.6064121083239418	0.1594798642314258	0.6720491922575585	T	T	T
0.6106142336031094	0.8235959544888478	0.6723249532558225	T	T	T
0.8627530088411710	0.4417294716394176	0.6935378240430287	T	T	T
0.8572785141678213	0.1187348295493682	0.6887461120497286	T	T	T
0.8603252016909313	0.7883315016114262	0.6934854716928562	T	T	T
0.1634058262693072	0.3633847917564641	0.7101208444529346	T	T	T
0.0990065377862361	0.5692737222960390	0.7181063886871178	T	T	T
0.0971694968955195	0.2724031606520245	0.7222290795545742	T	T	T

References

1 Calle-Vallejo, F.; Martínez, J. I.; García-Lastra, J. M.; Sautet, P.; Loffreda, D. Fast Prediction of Adsorption Properties for Platinum Nanocatalysts with Generalized Coordination Numbers. *Angew. Chem. Int. Ed.* **2014**, *53*, 8316–8319, DOI: 10.1002/anie.201402958.

2 Calle-Vallejo, F.; Tymoczko, J.; Colic, V.; Vu, Q. H.; Pohl, M. D.; Morgenstern, K.; Loffreda, D.; Sautet, P.; Schuhmann, W.; Bandarenka, A. S. Finding Optimal Surface Sites on Heterogeneous Catalysts by Counting Nearest Neighbors. *Science* **2015**, *350*, 185–189, DOI: 10.1126/science.aab3501.

3 Gazzarrini, E.; Rossi, K.; Baletto, F. Born to be Different: The Formation Process of Cu Nanoparticles Tunes the Size Trend of the Activity for CO_2 to CH_4 Conversion. *Nanoscale* **2021**, *13*, 5857–5867, DOI: 10.1039/D0NR07889A.

4 Verga, L. G.; Mendes, P. C. D.; Ocampo-Restrepo, V. K.; Da Silva, J. L. F. The Role of Site Coordination on the CO_2 Electroreduction Pathway on Stepped and Defective Copper Surfaces. *Catal. Sci. Technol.* **2021**, *11*, 2770–2781, DOI: 10.1039/D0CY02337J.

5 Nørskov, J. K.; Rossmeisl, J.; Logadottir, A.; Lindqvist, L.; Kitchin, J. R.; Bligaard, T.; Jónsson, H. Origin of the Overpotential for Oxygen Reduction at a Fuel-Cell Cathode. *J. Phys. Chem. B* **2004**, *108*, 17886–17892, DOI: 10.1021/jp047349j.

6 Peterson, A. A.; Abild-Pedersen, F.; Studt, F.; Rossmeisl, J.; Nørskov, J. K. How copper catalyzes the electroreduction of carbon dioxide into hydrocarbon fuels. *Energy Environ. Sci.* **2010**, *3*, 1311–1315, DOI: 10.1039/C0EE00071J.

7 Larsen, A. H.; Mortensen, J. J.; Blomqvist, J.; Castelli, I. E.; Christensen, R.; Dułak, M.; Friis, J.; Groves, M. N.; Hammer, B.; Hargus, C.; Hermes, E. D.; Jennings, P. C.; Jensen, P. B.; Kermode, J.; Kitchin, J. R.; Kolsbjerg, E. L.; Kubal, J.; Kaasbjerg, K.; Lysgaard, S.; Maronsson, J. B.; Maxson, T.; Olsen, T.; Pastewka, L.; Peterson, A.; Rostgaard, C.; Schiøtz, J.; Sch utt, O.; Strange, M.; Thygesen, K. S.; Vegge, T.; Vilhelmsen, L.; Walter, M.;

Zeng, Z.; ; Jacobsen, K. W. The atomic simulation environment—a Python library for working with atoms. *Journal of Physics: Condensed Matter* **2017**, *29*, 273002, DOI: 10.1088/1361-648x/aa680e.

8 Rendón-Calle, A.; Builes, S.; Calle-Vallejo, F. Substantial improvement of electrocatalytic predictions by systematic assessment of solvent effects on adsorption energies. *Appl. Catal., B* **2020**, *276*, 119147, DOI: 10.1016/j.apcatb.2020.119147.

9 Schouten, K. J. P.; Kwon, Y.; van der Ham, C. J. M.; Qin, Z.; Koper, M. T. M. A new mechanism for the selectivity to C1 and C2 species in the electrochemical reduction of carbon dioxide on copper electrodes. *Chem. Sci.* **2011**, *2*, 1902–1909, DOI: 10.1039/C1SC00277E.

10 Durand, W. J.; Peterson, A. A.; Studt, F.; Abild-Pedersen, F.; Nørskov, J. K. Structure effects on the energetics of the electrochemical reduction of CO_2 by copper surfaces. *Surf. Sci.* **2011**, *605*, 1354–1359, DOI: 10.1016/j.susc.2011.04.028.

11 Schouten, K. J. P.; Qin, Z.; Pérez Gallent, E.; Koper, M. T. M. Two Pathways for the Formation of Ethylene in CO Reduction on Single-Crystal Copper Electrodes. *J. Am. Chem. Soc.* **2012**, *134*, 9864–9867, DOI: 10.1021/ja302668n.

12 Calle-Vallejo, F.; Koper, M. T. M. Theoretical Considerations on the Electroreduction of CO to C2 Species on Cu(100) Electrodes. *Angew. Chem. Int. Ed.* **2013**, *52*, 7282–7285, DOI: 10.1002/anie.201301470.

13 Nie, X.; Esopi, M. R.; Janik, M. J.; Asthagiri, A. Selectivity of CO_2 Reduction on Copper Electrodes: The Role of the Kinetics of Elementary Steps. *Angew. Chem. Int. Ed.* **2013**, *52*, 2459–2462, DOI: 10.1002/anie.201208320.

14 Nie, X.; Luo, W.; Janik, M. J.; Asthagiri, A. Reaction mechanisms of CO_2 electrochemical reduction on Cu(111) determined with density functional theory. *J. Catal.* **2014**, *312*, 108–122, DOI: 10.1016/j.jcat.2014.01.013.

15 Zhao, Z.; Chen, Z.; Zhang, X.; Lu, G. Generalized Surface Coordination Number as an Activity Descriptor for CO_2 Reduction on Cu Surfaces. *J. Phys. Chem. C* **2016**, *120*, 28125–28130, DOI: 10.1021/acs.jpcc.6b10155.

16 Liu, S.; Huang, S. Structure engineering of Cu-based nanoparticles for electrochemical reduction of CO_2. *Journal of Catalysis* **2019**, *375*, 234–241, DOI: 10.1016/j.jcat.2019.05.035.

17 Jo, D. Y.; Ham, H. C.; Lee, K.-Y. Facet-dependent electrocatalysis in the HCOOH synthesis from CO_2 reduction on Cu catalyst: a density functional theory study. *Appl. Surf. Sci.* **2020**, *527*, 146857, DOI: 10.1016/j.apsusc.2020.146857.

18 Tang, M. T.; Peng, H.; Lamoureux, P. S.; Bajdich, M.; Abild-Pedersen, F. From electricity to fuels: Descriptors for C1 selectivity in electrochemical CO_2 reduction. *Appl. Catal., B* **2020**, *279*, 119384, DOI: 10.1016/j.apcatb.2020.119384.

19 Liu, X.; Sun, L.; Deng, W.-Q. Theoretical Investigation of CO_2 Adsorption and Dissociation on Low Index Surfaces of Transition Metals. *J. Phys. Chem. C* **2018**, *122*, 8306–8314, DOI: 10.1021/acs.jpcc.7b12660.

20 Wang, G.-C.; Jiang, L.; Morikawa, Y.; Nakamura, J.; Cai, Z.-S.; Pan, Y.-M.; Zhao, X.-Z. Cluster and periodic DFT calculations of adsorption and activation of CO_2 on the Cu(hkl) surfaces. *Surf. Sci.* **2004**, *570*, 205–217, DOI: https://doi.org/10.1016/j.susc.2004.08.001.

21 Ocampo-Restrepo, V. K.; Zibordi-Besse, L.; Da Silva, J. L. F. Ab initio investigation of the atomistic descriptors in the activation of small molecules on 3d transition-metal 13-atom clusters: The example of H_2, CO, H_2O, and CO_2. *J. Chem. Phys.* **2019**, *151*, 214301, DOI: 10.1063/1.5125769.

22 Mendes, P. C. D.; Ocampo-Restrepo, V. K.; Da Silva, J. L. F. *Ab Initio* Investigation of Quantum Size Effects on the Adsorption of CO_2, CO, H_2O and H_2 on Transition-metal Particles. *Phys. Chem. Chem. Phys.* **2020**, *22*, 8998–9008, DOI: 10.1039/d0cp00880j.

23 Peterson, A. A.; Nørskov, J. K. Activity Descriptors for CO_2 Electroreduction to Methane on Transition-metal Catalysts. *J. Phys. Chem. Lett.* **2012**, *3*, 251–258, DOI: 10.1021/jz201461p.

24 De Souza, D. G.; Cezar, H. M.; Rondina, G. G.; de Oliveira, M. F.; Da Silva, J. L. F. A Basin-Hopping Monte Carlo Investigation of the Structural and Energetic Properties of 55- and 561-atom Bimetallic Nanoclusters: The Examples of the ZrCu, ZrAl, and CuAl Systems. *J. Phys.: Condens. Matter* **2016**, *28*, 175302, DOI: 10.1088/0953-8984/28/17/175302.

25 Daw, M. S.; Baskes, M. I. Semiempirical, Quantum Mechanical Calculation of Hydrogen Embrittlement in Metals. *Phys. Rev. Lett.* **1983**, *50*, 1285–1288, DOI: 10.1103/physrevlett.50.1285.

26 Daw, M. S.; Foiles, S. M.; Baskes, M. I. The Embedded-Atom Method: A Review of Theory and Applications. *Mater. Sci. Rep.* **1993**, *9*, 251–310, DOI: 10.1016/0920-2307(93)90001-u.

27 Reske, R.; Mistry, H.; Behafarid, F.; Roldan Cuenya, B.; Strasser, P. Particle Size Effects in the Catalytic Electroreduction of CO_2 on Cu Nanoparticles. *J. Am. Chem. Soc.* **2014**, *136*, 6978–6986, DOI: 10.1021/ja500328k.