Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information: *Ab initio* Investigation of Quantum Size Effects on the Adsorption of CO_2, CO, H_2O, and H_2 on Transition-metal Particles

Paulo C. D. Mendes,[†] Vivianne K. Ocampo-Restrepo,[‡] and Juarez L. F. Da Silva[*,†]

†*São Carlos Institute of Chemistry, University of São Paulo, PO Box* 780, 13560 − 970, *São Carlos, SP, Brazil*
‡*São Carlos Institute of Chemistry, University of São Paulo, PO Box* 780, *13560-970, São Carlos, SP, Brazil*

E-mail: juarez_dasilva@iqsc.usp.br
Phone: +55 (16) 3373 6641. Fax: +55 (16) 3373 9952

I PAW Projectors and Convergence Test for the Simulation Box

The PAW projectors employed in this study are listed in Table S1. Convergence tests for the total energy with respect to the box size is included in Table S2 for the example of CO_2/Cu_{13}.

Table S1: PAW−PBE projectors, number of valence electrons (Z_{val}), electronic configuration for valence electrons and default cutoff energy for the planewave basis set (ENMAX).

Element	PAW–PBE POTCAR	Z_{val}	valence	ENMAX (eV)
Co	Co_GW 31Mar2010	9	$3d^8 4s^1$	323.400
Ni	Ni_GW 31Mar2010	10	$3d^9 4s^1$	357.323
Cu	Cu_GW 19May2006	11	$3d^{10} 4s^1$	417.039
C	C_GW_new 19Mar2012	4	$2s^2 2p^2$	413.992
H	H_GW 21Apr2008	1	$1s^1$	300.000
O	O_GW 19Mar2012	6	$2s^2 2p^4$	434.431

Table S2: Convergence test for the size of the cubic simulation box for PBE and PBE+D3 with a total energy convergence criterion of 10^{-8} eV for the frozen CO_2/Cu_{13} configuration previously optimized with the 20 Å cubic box. The shortest distance between periodic images is shown as d_{im}, E_{tot} is the total electronic energy, ΔE_{tot} is the relative energy with respect to the largest box size and m_{tot} is the total magnetic moment for the unit cell.

		PBE			PBE+D3		
Box (Å)	d_{im} (Å)	E_{tot} (eV)	ΔE_{tot} (meV)	m_{tot} (μ_{B})	E_{tot} (eV)	ΔE_{tot} (meV)	m_{tot} (μ_{B})
9	3.06	−58.622 638 59	−942.66	1.00	−57.199 866 93	−425.87	1.00
10	3.91	−58.093 420 83	−413.44	1.00	−56.952 374 79	−178.37	1.00
11	4.75	−57.857 692 86	−177.71	0.99	−56.842 991 64	−68.99	0.99
12	5.65	−57.752 466 35	−72.49	1.00	−56.792 368 05	−18.37	1.00
13	6.57	−57.723 494 6	−43.52	1.00	−56.788 102 7	−14.10	1.00
14	7.51	−57.693 038 31	−13.06	1.00	−56.769 977 48	4.02	1.00
15	8.47	−57.687 974 92	−8.00	1.00	−56.771 576 07	2.43	1.00
16	9.43	−56.768 848 57	5.15	1.00	−57.681 417 06	−1.44	1.00
17	10.40	−56.770 149 94	3.85	0.99	−57.680 408 4	−0.43	0.99
18	11.38	−56.775 938 39	−1.94	1.00	−57.684 752 46	−4.77	1.00
19	12.36	−56.769 011 14	4.99	1.00	−57.676 893 09	3.09	1.00
20	13.34	−56.779 303 85	−5.30	1.00	−57.686 563 25	−6.59	1.00
21	14.33	−56.768 340 56	5.66	1.00	−57.675 171 64	4.81	1.00
22	15.32	−56.776 949 72	−2.95	1.00	−57.683 481 41	−3.50	1.00
23	16.31	−56.776 707 76	−2.71	1.00	−57.683 026 91	−3.05	1.00
24	17.30	−56.766 751 15	7.25	1.00	−57.672 918 63	7.06	1.00
25	18.29	−56.772 401 24	1.60	0.99	−57.678 458 9	1.52	0.99
26	19.28	−56.774 001 84	0.00	1.00	−57.679 978 1	0.00	1.00

II Bulk and Surface Properties with PBE and PBE+D3

Table S3 shows some bulk properties which characterize and validate our computational model for Co, Ni and Cu. The crystals are fcc (face centered cubic), bcc (body centered cubic) and hcp (hexagonal close-packed). These results are well-converged and detailed discussions were published by other authors, as cited in the main article (Tereshuck, P.; et al. *J. Phys. Chem. C*, 116, 24695-24705, 2012).

Table S3: Bulk (hcp Co, fcc Ni and fcc Cu) properties calculated with PBE and PBE+D3: Lattice parameters, a_0 and c_0, average bond length, d_{av}, effective coordination number, ECN (in number of nearest neighbors), cohesive energy per atom, E_{coh}, magnetic moment per atom, m_{at}, average d-band center per atom for up, ε_d^{up}, and down, ε_d^{dn}, occupied spin states. Clean surface (Co(0001), Ni(111) and Cu(111)) properties calculated from 5 layer, 1×1 slabs using PBE and PBE+D3: work function, Φ and interlayer relaxation between the two layers closer to the vacuum, Δd_{12}.

Property	hcp Co		fcc Ni		fcc Cu	
	PBE	PBE+D3	PBE	PBE+D3	PBE	PBE+D3
a_0 (Å)	2.49	2.47	3.52	3.48	3.63	3.57
c_0 (Å)	4.02	3.99	-	-	-	-
d_{av} (Å)	2.48	2.46	2.49	2.46	2.57	2.52
ECN (NNN)	12.01	12.02	12.02	12.02	12.02	12.02
E_{coh} (eV)	−5.02	−5.37	−4.75	−5.15	−3.52	−4.03
m_{at} (μ_B)	1.58	1.57	0.63	0.62	0.00	0.00
ε_d^{up} (eV)	−2.37	−2.40	−2.18	−2.26	−2.78	−2.94
ε_d^{dn} (eV)	−1.70	−1.78	−1.81	−1.91	−2.78	−2.94
Property	Co(0001)		Ni(111)		Cu(111)	
	PBE	PBE+D3	PBE	PBE+D3	PBE	PBE+D3
Φ (eV)	4.96	4.96	5.05	5.08	4.77	4.83
Δd_{12} (eV)	0.47	−1.83	−1.07	0.00	−0.83	0.64
ε_d^{up} (eV)	−2.28	−2.30	−1.93	−1.96	−2.46	−2.56
ε_d^{dn} (eV)	−1.40	−1.49	−1.49	−1.54	−2.46	−2.56

III Additional Properties for the Clean 13-, 55- and 147-Atom Clusters

Table S4 and Figure S1 show, respectively, some properties and the radial distribution function with respect to the geometric center (r = 0) for the isolated Co, Ni and Cu clusters composed of 13, 55 and 147 atoms.

Table S4: Some properties of Co_n, Ni_n and Cu_n (n = 13, 55, 147) clusters. Binding energy per atom, E_b, total magnetic moment for the unit cell, m_{tot}, effective coordination number, ECN (in number of nearest neighbors, NNN) and average bond length, d_{av}.

Cluster	E_b (eV/atom)	m_{tot} (μ_B)	ECN (NNN)	d_{av} (Å)
Co_{13}	−3.30	27	5.45	2.33
Ni_{13}	−3.18	10	5.67	2.36
Cu_{13}	−2.40	1	5.69	2.45
Co_{55}	−4.14	105	8.37	2.43
Ni_{55}	−3.97	40	8.39	2.43
Cu_{55}	−3.07	3	8.39	2.50
Co_{147}	−4.47	259	9.36	2.44
Ni_{147}	−4.31	100	9.35	2.44
Cu_{147}	−3.33	1	9.38	2.51

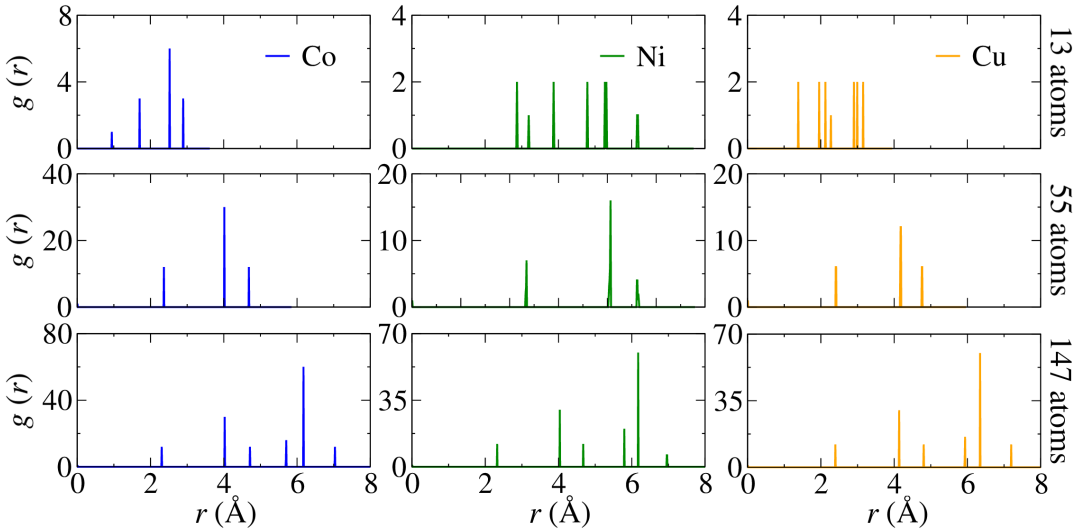

Figure S1: Radial distribution function, $g(r)$, with respect to the geometric center of the clusters (r = 0) for the isolated TM_{13}, TM_{55} and TM_{147} clusters (TM = Co, Ni, Cu).

IV Complete Set of Optimized Adsorption Structures

The complete set of optimized adsorption structures are shown in Figures S2-S11. The configurations are shown in energetic order with respect to the lowest energy configuration of each set. For each configuration, corresponding properties are shown in Section V; the configurations and data can be related through the relative energies.

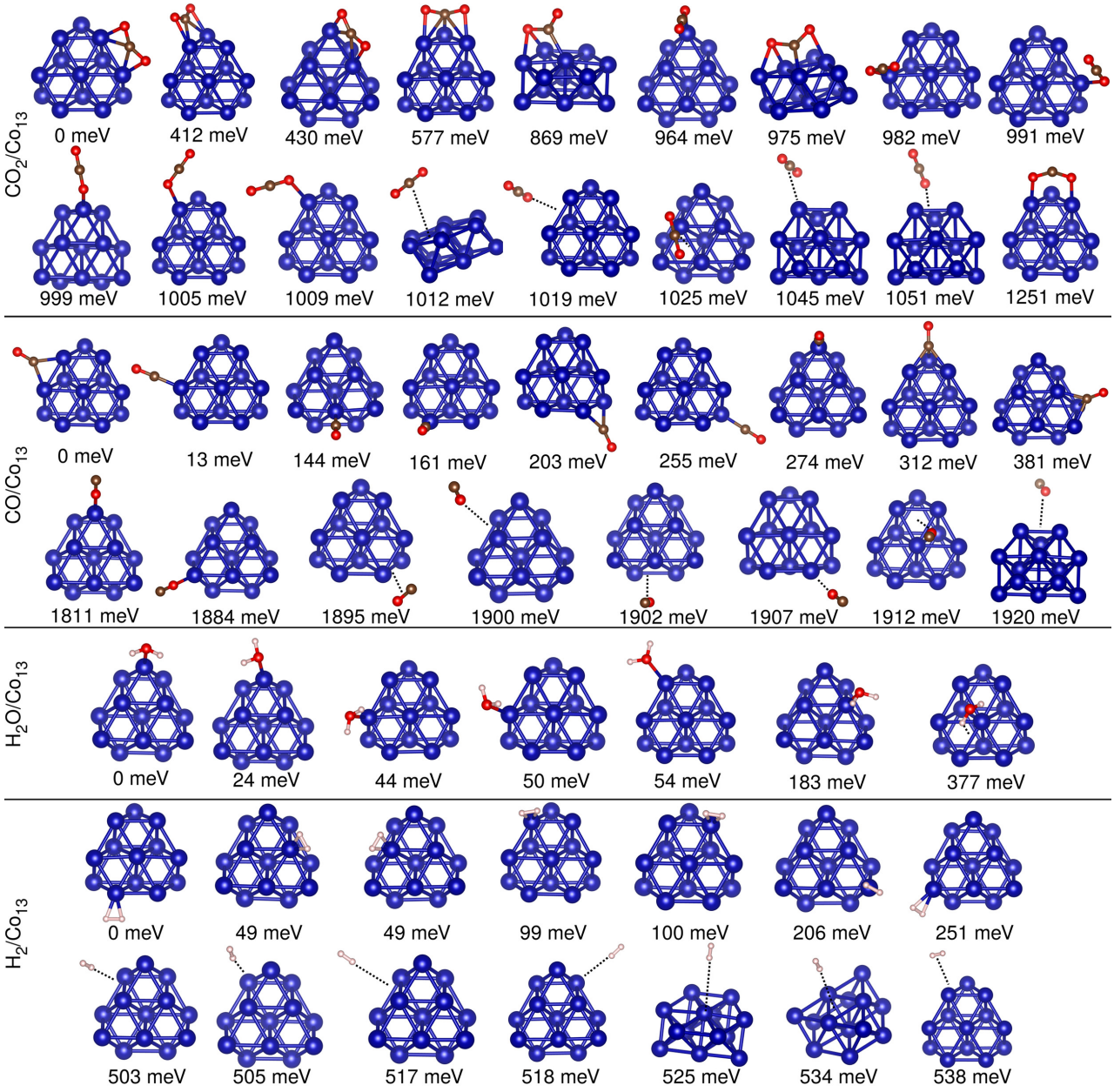

Figure S2: Optimized adsorption configurations for CO_2, CO, H_2O and H_2 on Co_{13} clusters ordered by the energy relative to the lowest energy structure; dotted lines represent long range interaction between the adsorbate the substrate. The degenerate and almost identical configurations were obtained after optimization starting from geometrically unique structures. Corresponding properties available in Tables S5, S6, S7 and S8.

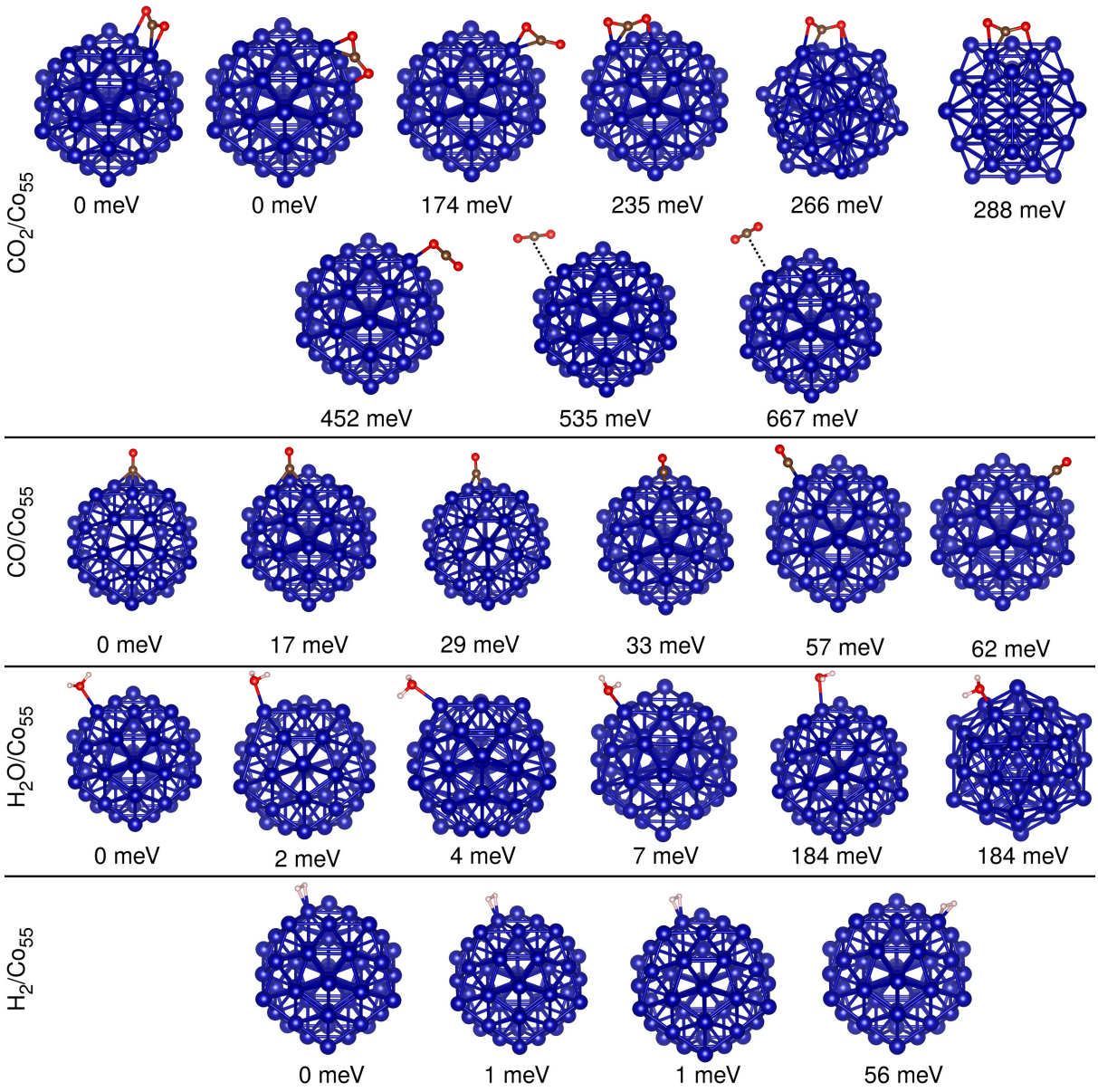

Figure S3: Optimized adsorption configurations for CO_2, CO, H_2O and H_2 on Co_{55} clusters ordered by the energy relative to the lowest energy structure; dotted lines represent long range interaction between the adsorbate the substrate. The degenerate and almost identical configurations were obtained after optimization starting from geometrically unique structures. Corresponding properties available in Tables S5, S6, S7 and S8.

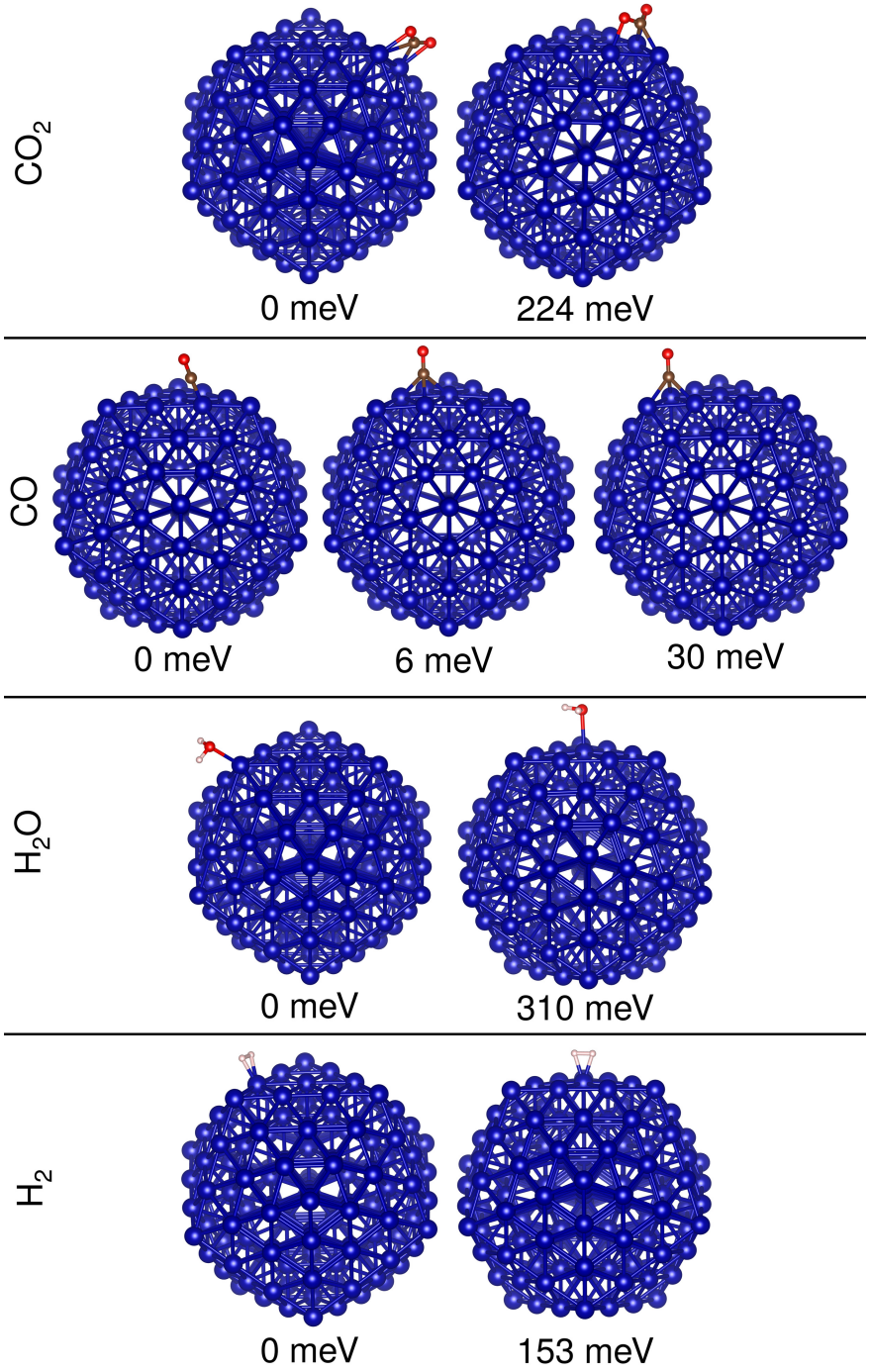

Figure S4: Optimized adsorption configurations for CO_2, CO, H_2O and H_2 on Co_{147} clusters ordered by the energy relative to the lowest energy structure. Corresponding properties available in Tables S5, S6, S7 and S8.

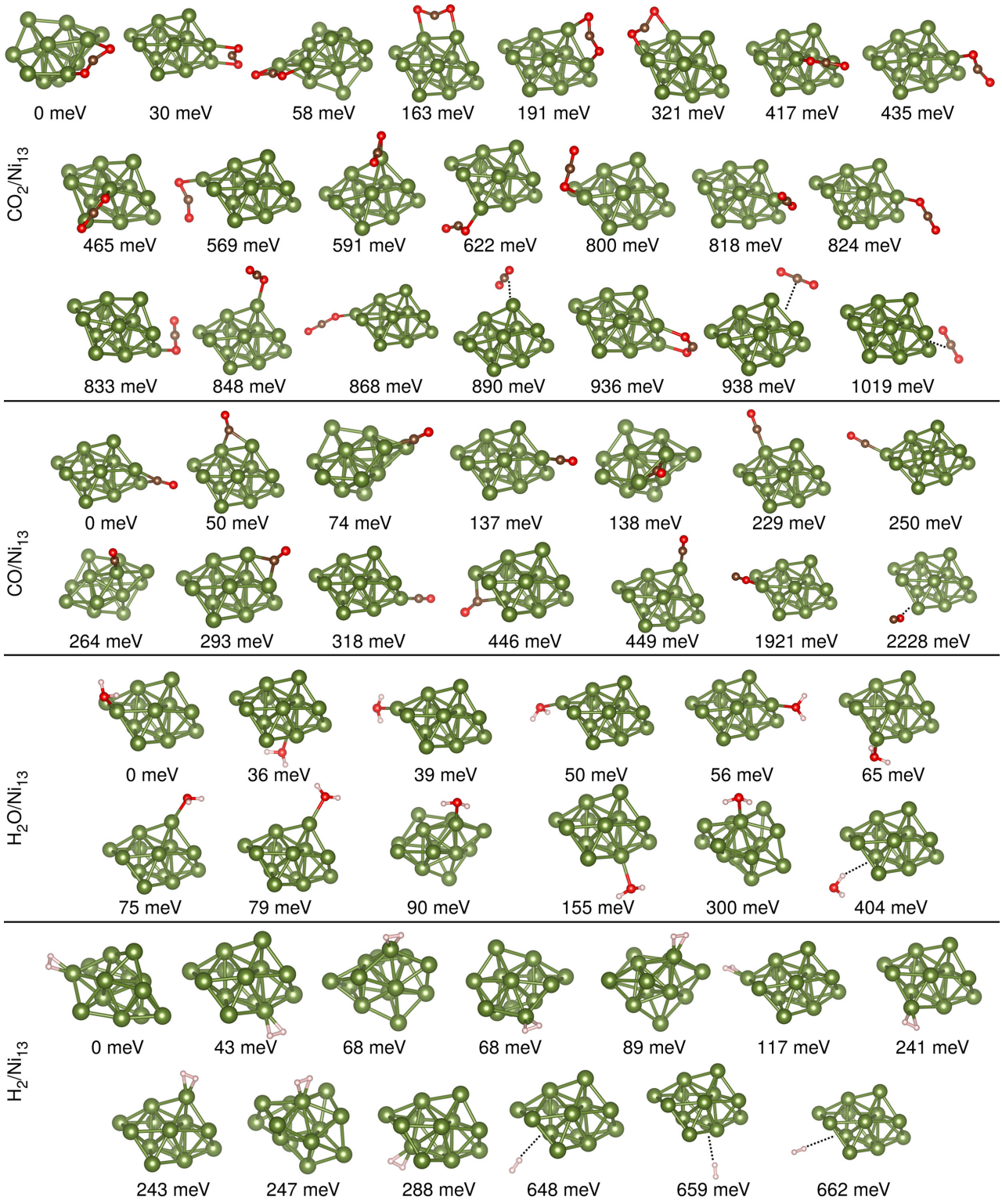

Figure S5: Optimized adsorption configurations for CO_2, CO, H_2O and H_2 on Ni_{13} clusters ordered by the energy relative to the lowest energy structure; dotted lines represent long range interaction between the adsorbate the substrate. The degenerate and almost identical configurations were obtained after optimization starting from geometrically unique structures. Corresponding properties available in Tables S9, S10, S11 and S12.

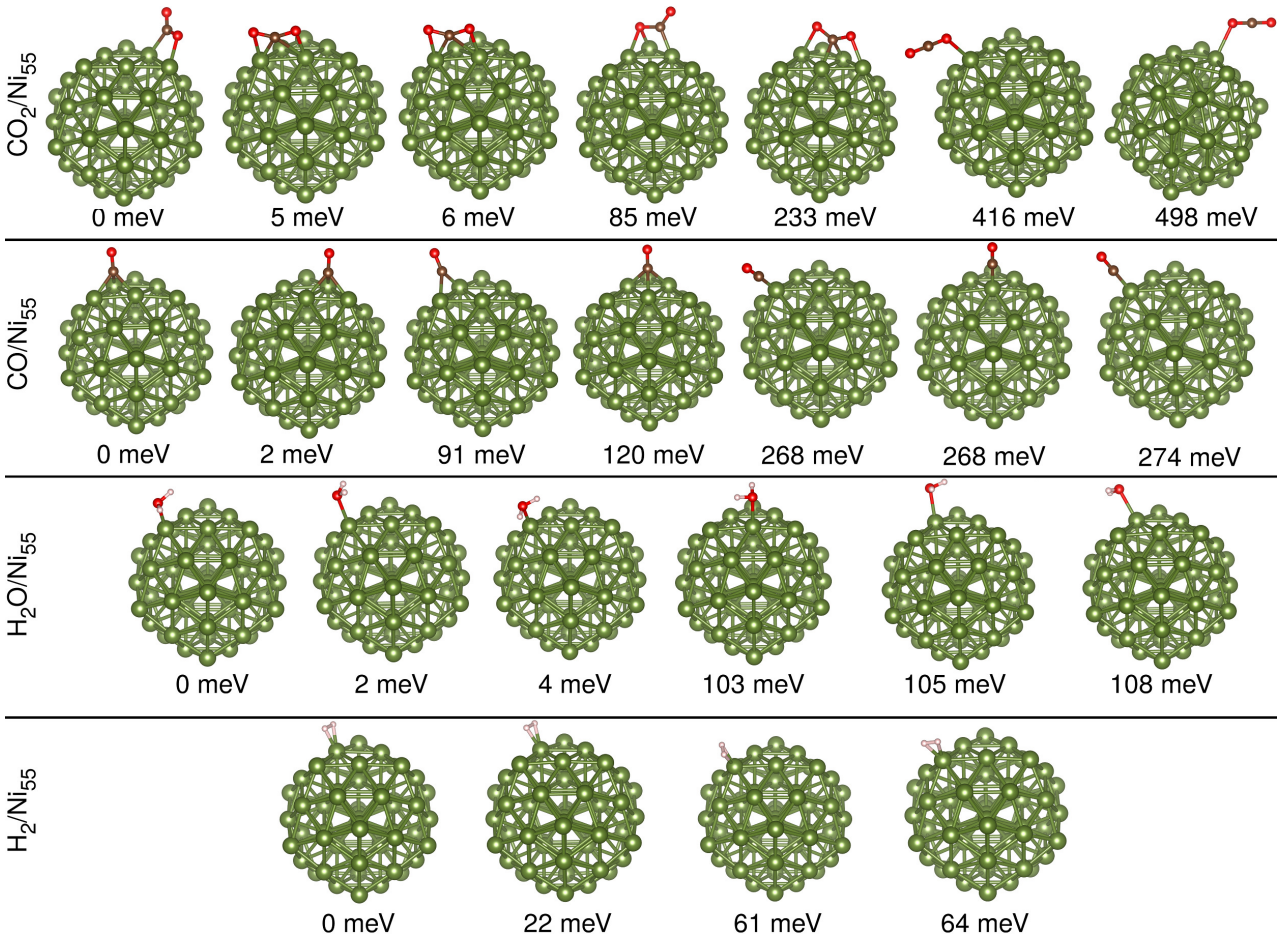

Figure S6: Optimized adsorption configurations for CO_2, CO, H_2O and H_2 on Ni_{55} clusters ordered by the energy relative to the lowest energy structure. The degenerate and almost identical configurations were obtained after optimization starting from geometrically unique structures. Corresponding properties available in Tables S9, S10, S11 and S12.

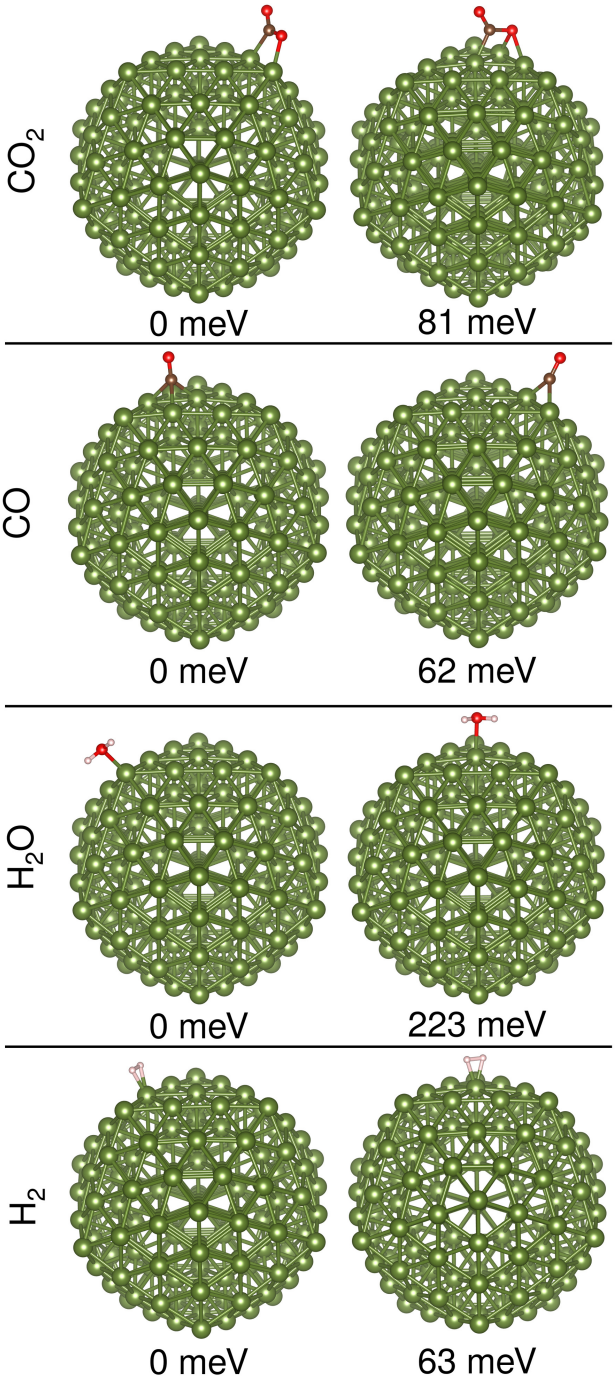

Figure S7: Optimized adsorption configurations for CO_2, CO, H_2O and H_2 on Ni_{147} clusters ordered by the energy relative to the lowest energy structure. Corresponding properties available in Tables S9, S10, S11 and S12.

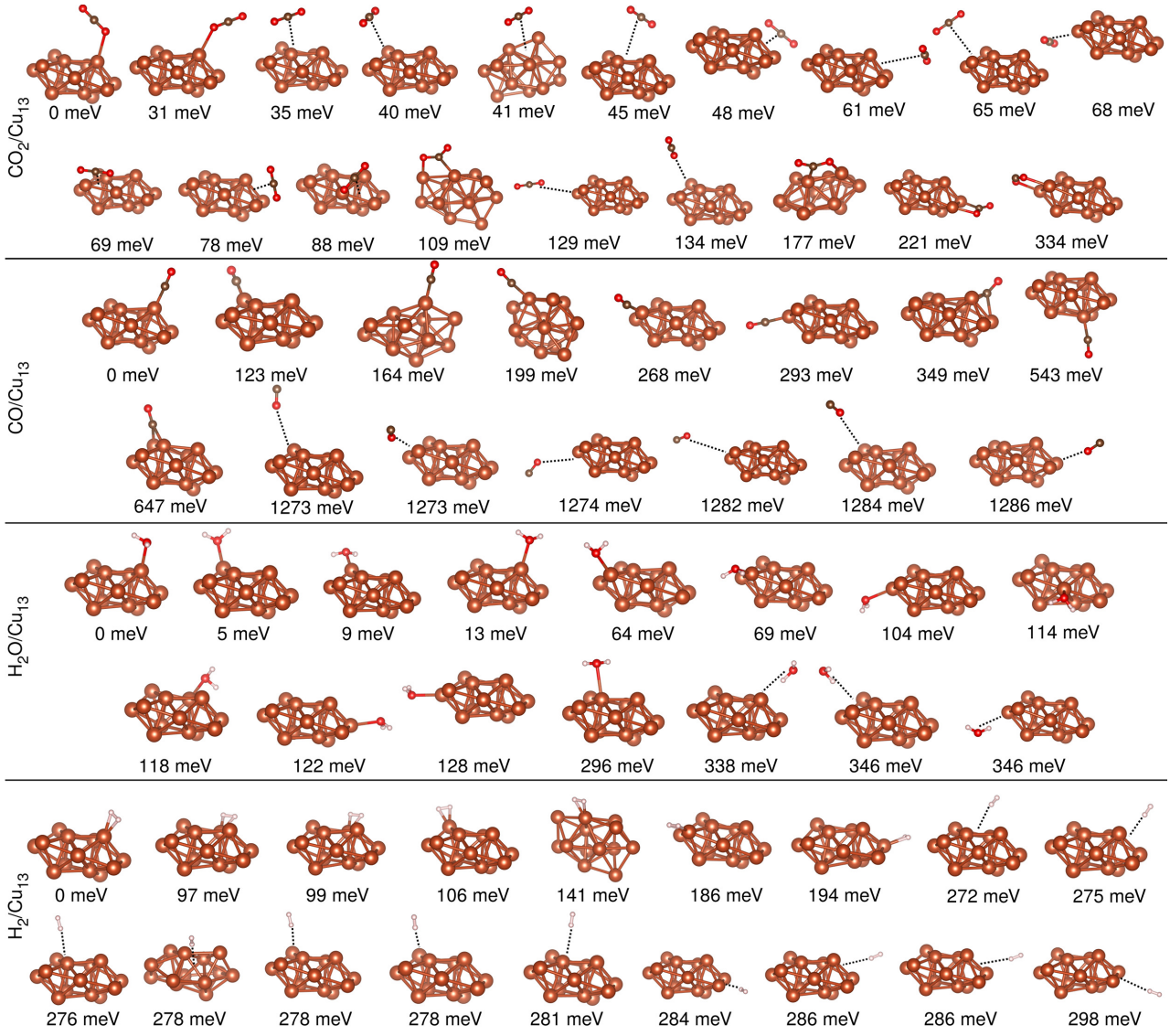

Figure S8: Optimized adsorption configurations for CO_2, CO, H_2O and H_2 on Cu_{13} clusters ordered by the energy relative to the lowest energy structure; dotted lines represent long range interaction between the adsorbate the substrate. The degenerate and almost identical configurations were obtained after optimization starting from geometrically unique structures. Corresponding properties available in Tables S13, S14, S15 and S16.

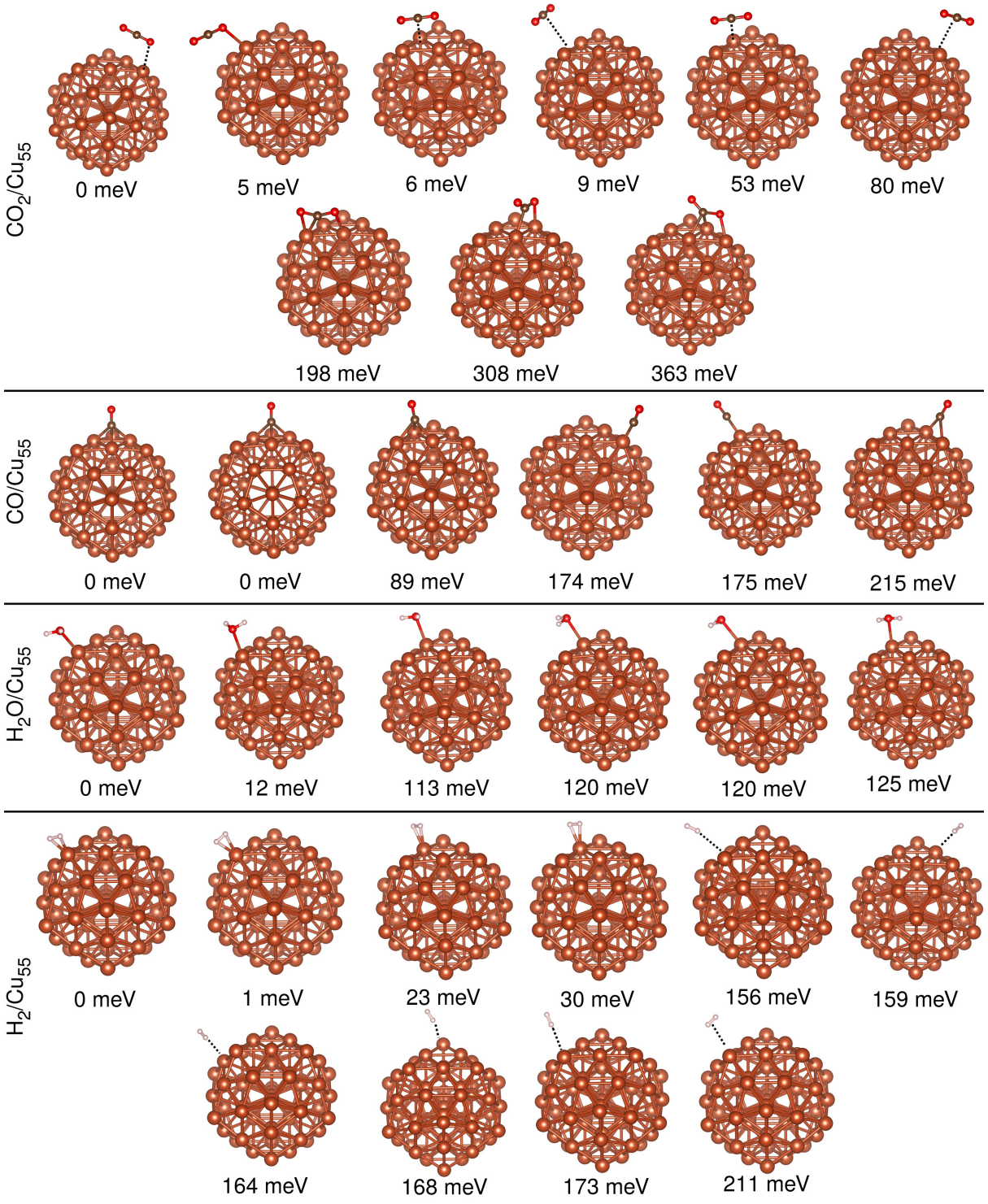

Figure S9: Optimized adsorption configurations for CO_2, CO, H_2O and H_2 on Cu_{55} clusters ordered by the energy relative to the lowest energy structure; dotted lines represent long range interaction between the adsorbate the substrate. The degenerate and almost identical configurations were obtained after optimization starting from geometrically unique structures. Corresponding properties available in Tables S13, S14, S15 and S16.

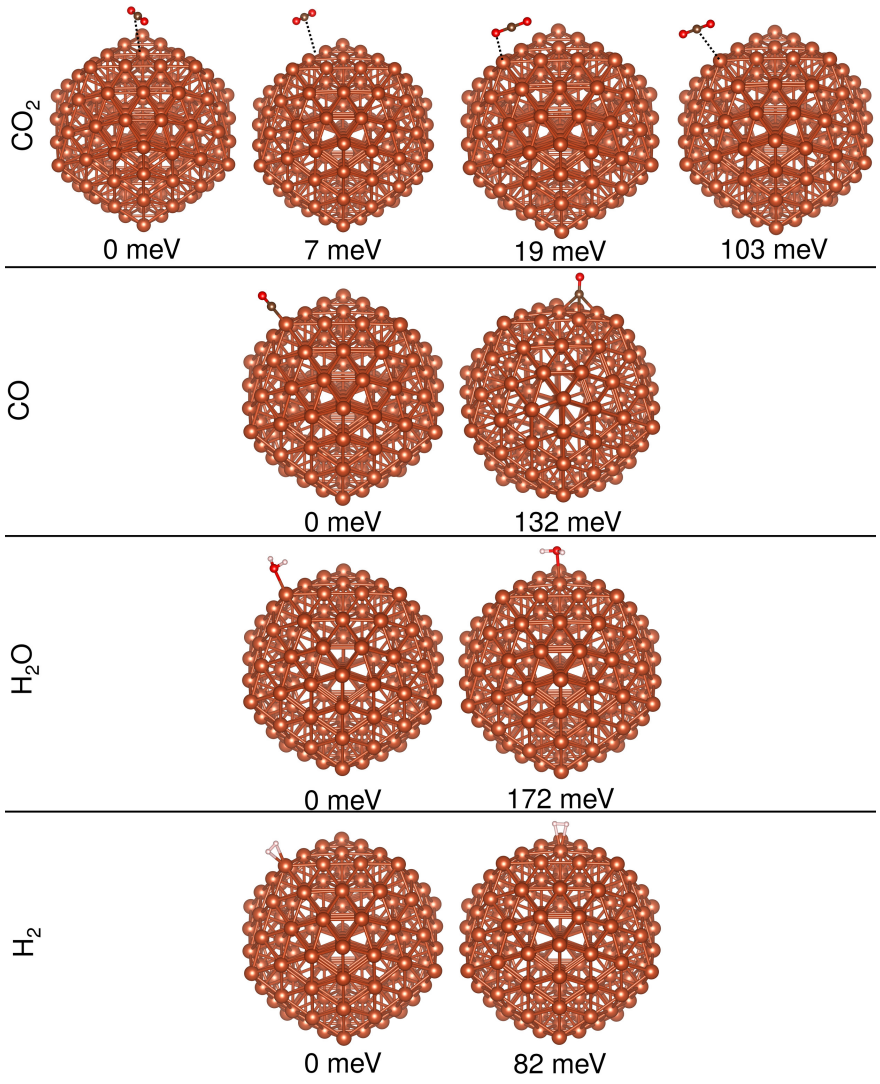

Figure S10: Optimized adsorption configurations for CO_2, CO, H_2O and H_2 on Cu_{147} clusters ordered by the energy relative to the lowest energy structure; dotted lines represent long range interaction between the adsorbate the substrate. Corresponding properties available in Tables S13, S14, S15 and S16.

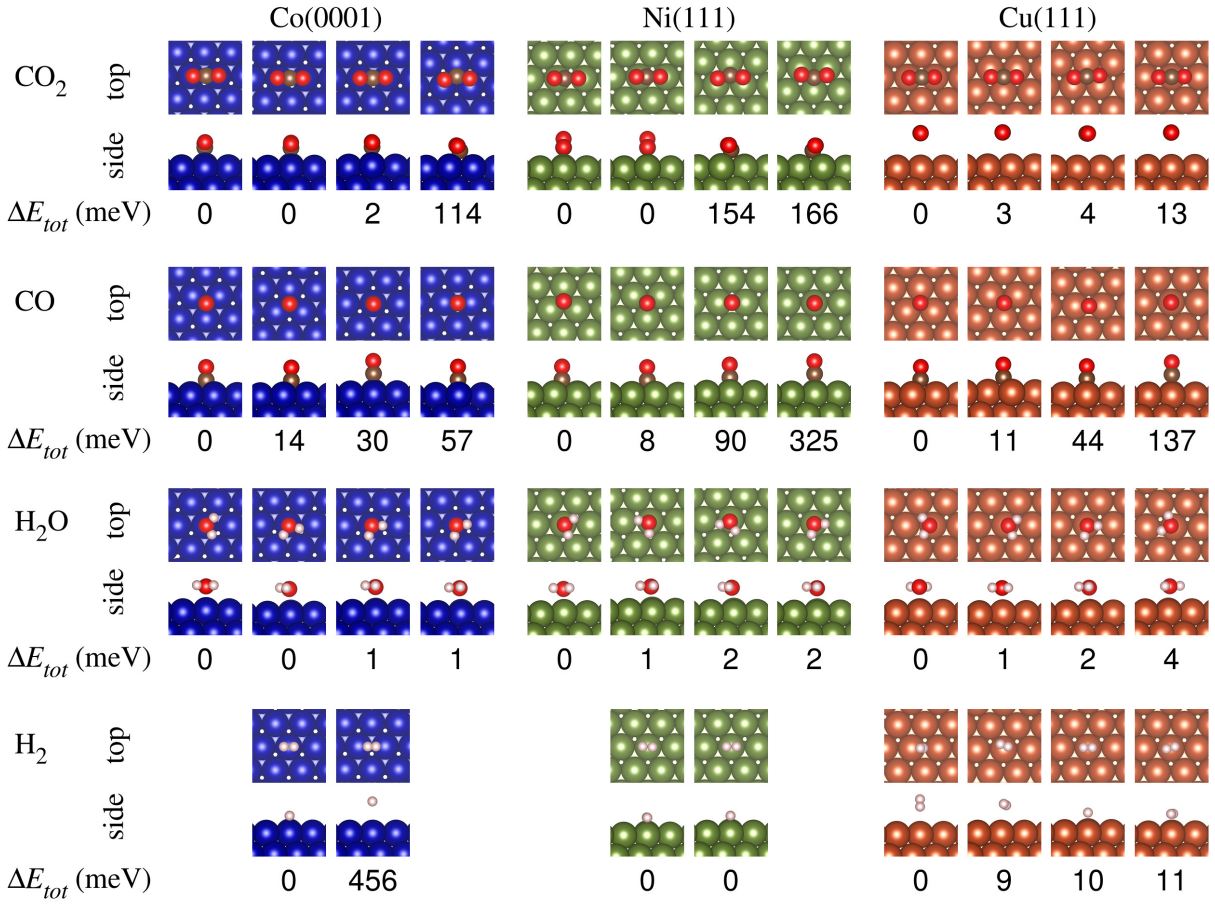

Figure S11: Optimized adsorption configurations for CO_2, CO, H_2O and H_2 adsorbed on Co(0001), Ni(111) and Cu(111) ordered by the energy relative to the lowest energy structure for each composition. The degenerate and almost identical configurations were obtained after optimization starting from geometrically unique structures. Corresponding properties available in Tables S5 – S16.

V Energetic, Electronic and Structural Properties for all Adsorbed Systems

This section shows additional properties for all structures of our study, Tables S5–S16. These results correspond directly to the structures pictured in Section IV; the structures and data can be related through the relative energies.

Table S5: Adsorption properties for all configurations of CO_2 interacting with Co substrates, namely, Co_{13}, Co_{55}, Co_{147} and Co(0001). Total energy relative to the lowest energy configuration for each set (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment for the unit cell (m_{tot}), shortest distances between the C and TM atoms (d_{C-TM}), O atoms and TM (d_{O1-TM} and d_{O2-TM}), and OCO angle (α_{OCO}), percent variations of the average effective coordination number, ΔECN, and average bond length, Δd_{av}, for the clusters and first slab layer with respect to the isolated substrates.

	ΔE_{tot} (meV)	E_{ad} (eV)	m_{tot} (μ_B)	d_{C-TM} (Å)	d_{O1-TM} (Å)	d_{O2-TM} (Å)	α_{OCO} (deg)	ΔECN (%)	Δd_{av} (%)
CO_2/Co_{13}	1251	0.09	27	2.78	2.03	2.03	134.01	0.04	0.26
	1051	−0.11	27	3.34	2.93	4.07	179.51	−0.05	0.00
	1045	−0.12	27	3.52	3.46	3.36	179.11	0.03	0.01
	1025	−0.14	27	3.48	3.23	3.76	179.01	0.04	0.01
	1019	−0.14	27	3.62	4.09	3.40	178.87	0.01	0.03
	1012	−0.15	27	3.60	3.28	3.72	178.80	0.07	0.00
	1009	−0.15	27	3.07	4.03	2.31	179.61	−0.01	0.04
	1005	−0.16	27	3.07	4.01	2.33	179.54	−0.01	0.02
	999	−0.16	27	3.15	4.19	2.23	179.32	0.02	0.03
	991	−0.17	27	3.01	2.33	3.93	179.17	−0.04	0.08
	982	−0.18	27	2.99	3.91	2.32	178.59	−0.04	0.04
	975	−0.19	27	1.92	2.04	2.23	124.31	−1.73	0.39
	964	−0.20	27	2.98	3.93	2.24	179.05	0.05	0.04
	869	−0.29	27	2.02	2.05	2.80	128.09	−0.50	0.27
	577	−0.59	27	1.95	1.99	1.99	126.04	−0.02	0.78
	430	−0.73	27	1.94	2.11	2.03	139.45	−0.19	0.41
	412	−0.75	25	1.88	2.06	2.11	140.49	0.23	0.27
	0	−1.16	25	2.00	2.04	2.04	137.32	0.34	0.15
CO_2/Co_{55}	667	0.01	105	3.45	3.03	3.70	178.90	−0.16	0.13
	535	−0.12	105	3.49	3.96	3.27	179.49	0.00	0.00
	452	−0.20	105	3.02	2.28	3.97	179.30	0.01	0.01
	288	−0.37	105	1.93	2.31	2.08	137.12	−0.12	0.08
	266	−0.39	103	1.91	2.15	2.15	126.03	−0.21	0.05
	235	−0.42	103	1.91	2.15	2.04	139.16	−0.28	0.19
	174	−0.48	103	1.93	1.94	2.99	143.71	0.01	−0.01
	0	−0.65	103	1.93	2.04	2.16	139.11	0.04	0.01
	0	−0.65	103	1.94	2.16	2.04	138.98	0.03	0.01
CO_2/Co_{147}	224	-0.58	255	1.94	2.03	2.02	128.98	−0.05	−0.04
	0	-0.80	257	1.96	2.09	2.00	137.64	−0.03	−0.01
$CO_2/Co(0001)$	114	0.03	76	1.98	2.10	2.09	130.00	−0.26	0.05
	2	−0.08	76	2.08	2.14	2.15	139.27	−0.31	0.01
	0	−0.08	76	2.00	2.14	2.18	139.74	−0.31	0.04
	0	−0.08	76	2.01	2.18	2.13	139.64	−0.31	0.03

Table S6: Adsorption properties for all configurations of CO interacting with Co substrates, namely, Co_{13}, Co_{55}, Co_{147} and Co(0001). Total energy relative to the lowest energy configuration for each set (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment for the unit cell (m_{tot}), shortest distances between the C and TM atoms (d_{C-TM}), and between the O and TM atoms (d_{O-TM}), percent variations of the average effective coordination number, ΔECN, and average bond length, Δd_{av}, for the clusters and first slab layer with respect to the isolated substrates.

	ΔE_{tot} (meV)	E_{ad} (eV)	m_{tot} (μ_B)	d_{C-TM} (Å)	d_{O-TM} (Å)	ΔECN (%)	Δd_{av} (%)
CO/Co_{13}	1920	−0.02	27	5.44	4.42	0.04	0.01
	1912	−0.02	27	5.74	4.69	0.06	0.00
	1907	−0.03	27	5.05	3.93	0.06	0.02
	1902	−0.03	27	4.99	4.03	0.06	0.00
	1900	−0.04	27	5.04	3.93	0.06	0.00
	1895	−0.04	27	4.46	3.99	0.07	0.02
	1884	−0.05	25	3.10	1.94	0.24	0.03
	1811	−0.12	27	3.16	2.02	0.00	0.09
	381	−1.56	27	1.92	2.86	−0.33	0.48
	312	−1.62	25	1.95	2.82	0.09	0.35
	274	−1.66	27	1.76	2.93	0.04	0.39
	255	−1.68	25	1.76	2.92	0.13	0.15
	203	−1.73	25	1.85	2.93	−0.19	0.20
	161	−1.78	27	1.76	2.93	−0.08	0.42
	144	−1.79	27	1.76	2.93	−0.23	0.24
	13	−1.92	25	1.74	2.91	0.12	0.05
	0	−1.94	25	1.90	2.93	−0.11	0.07
CO/Co_{55}	62	−1.79	103	1.75	2.91	−0.02	−0.02
	57	−1.79	103	1.74	2.91	−0.01	−0.02
	33	−1.82	103	1.74	2.91	0.02	−0.01
	29	−1.82	103	1.89	2.90	0.01	0.00
	17	−1.83	103	1.96	2.93	0.00	0.01
	0	−1.85	103	1.96	2.92	−0.05	0.00
CO/Co_{147}	30	−2.02	257	1.93	2.92	0.00	−0.01
	6	−2.04	257	1.96	2.92	−0.01	−0.02
	0	−2.05	257	1.74	2.91	0.01	−0.02
CO/Co(0001)	57	−1.86	75	1.90	2.90	−0.12	0.10
	30	−1.89	75	1.74	2.90	−0.13	0.11
	14	−1.91	75	1.96	2.91	−0.11	0.12
	0	−1.92	74	1.96	2.91	−0.15	0.07

Table S7: Adsorption properties for all configurations of H_2O interacting with Co substrates, namely, Co_{13}, Co_{55}, Co_{147} and Co(0001). Total energy relative to the lowest energy configuration for each set (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment for the unit cell (m_{tot}), shortest distances between the O and TM atoms ($d_{\mathrm{O-TM}}$), H atoms and TM ($d_{\mathrm{H1-TM}}$ and $d_{\mathrm{H2-TM}}$), and HOH angle (α_{HOH}), percent variations of the average effective coordination number, ΔECN, and average bond length, Δd_{av}, for the clusters and first slab layer with respect to the isolated substrates.

	ΔE_{tot} (meV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\mathrm{O-TM}}$ (Å)	$d_{\mathrm{H1-TM}}$ (Å)	$d_{\mathrm{H2-TM}}$ (Å)	α_{HOH} (deg)	ΔECN (%)	Δd_{av} (%)
H_2O/Co_{13}	377	−0.28	27	3.24	2.57	2.89	101.05	0.04	0.01
	183	−0.47	27	2.19	2.56	2.59	104.86	−0.13	0.04
	54	−0.60	27	2.11	2.58	2.57	105.54	0.02	0.07
	50	−0.61	27	2.11	2.54	2.54	104.82	−0.05	0.04
	44	−0.61	27	2.12	2.52	2.59	105.22	−0.06	0.06
	24	−0.63	27	2.10	2.60	2.56	105.45	0.06	0.07
	0	−0.66	27	2.09	2.54	2.56	105.17	0.08	0.06
H_2O/Co_{55}	184	−0.45	105	2.21	2.57	2.58	104.61	−0.02	0.03
	184	−0.45	105	2.22	2.54	2.52	103.96	−0.03	0.02
	7	−0.63	105	2.13	2.68	2.64	106.07	0.01	0.03
	4	−0.63	105	2.14	2.51	2.58	104.69	0.00	0.03
	2	−0.63	105	2.14	2.54	2.56	104.82	0.01	0.03
	0	−0.64	105	2.14	2.58	2.54	104.86	0.01	0.03
H_2O/Co_{147}	310	−0.37	258	2.24	2.54	2.54	103.94	−0.02	−0.02
	0	−0.68	257	2.08	2.52	2.51	104.93	0.02	−0.03
$H_2O/Co(0001)$	1	−0.50	76	2.24	2.58	2.56	104.29	−0.14	0.02
	1	−0.50	76	2.23	2.57	2.57	104.80	−0.13	0.02
	0	−0.50	76	2.23	2.56	2.57	104.30	−0.13	0.02
	0	−0.50	76	2.23	2.57	2.57	104.36	−0.12	0.03

Table S8: Adsorption properties for all configurations of H_2 interacting with Co substrates, namely, Co_{13}, Co_{55}, Co_{147} and Co(0001). Total energy relative to the lowest energy configuration for each set (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment for the unit cell (m_{tot}), shortest distances between the H and TM atoms ($d_{\mathrm{H1-TM}}$ and $d_{\mathrm{H2-TM}}$), percent variation of the average effective coordination number, ΔECN, and average bond length, Δd_{av}, for the clusters and first slab layer with respect to the isolated substrates.

	ΔE_{tot} (meV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\mathrm{H1-TM}}$ (Å)	$d_{\mathrm{H2-TM}}$ (Å)	ΔECN (%)	Δd_{av} (%)
H_2/Co_{13}	538	−0.04	27	3.45	3.27	−0.01	0.00
	534	−0.05	27	4.38	3.68	0.08	0.01
	525	−0.05	27	3.51	4.26	0.08	−0.03
	518	−0.06	27	3.56	2.85	0.03	−0.01
	517	−0.06	27	3.24	3.94	0.08	0.04
	505	−0.07	27	2.69	3.31	0.03	0.00
	503	−0.08	27	2.84	3.53	0.06	0.01
	251	−0.33	25	1.64	1.62	0.26	0.05
	206	−0.37	27	1.64	1.67	0.12	0.21
	100	−0.48	27	1.64	1.64	0.06	0.18
	99	−0.48	27	1.64	1.63	0.08	0.18
	49	−0.53	27	1.63	1.63	−0.08	0.14
	49	−0.53	27	1.63	1.63	−0.04	0.14
	0	−0.58	25	1.58	1.58	0.16	−0.05
H_2/Co_{55}	56	−0.43	103	1.64	1.62	0.04	−0.03
	1	−0.48	105	1.65	1.65	−0.02	0.04
	1	−0.48	105	1.65	1.65	−0.02	0.04
	0	−0.48	105	1.65	1.65	−0.02	0.03
H_2/Co_{147}	153	−0.53	257	1.58	1.58	0.01	−0.03
	0	−0.68	257	1.59	1.59	0.01	−0.02
$H_2/Co(0001)$	456	−0.07	76	3.05	3.05	−0.03	−0.03
	0	−0.53	75	1.58	1.58	−0.09	0.03

Table S9: Adsorption properties for all configurations of CO_2 interacting with Ni substrates, namely, Ni_{13}, Ni_{55}, Ni_{147} and Ni(111). Total energy relative to the lowest energy configuration for each set (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment for the unit cell (m_{tot}), shortest distances between the C and TM atoms (d_{C-TM}), O atoms and TM (d_{O1-TM} and d_{O2-TM}), and OCO angle (α_{OCO}), percent variation of the average effective coordination number, ΔECN, and average bond length, Δd_{av}, for the clusters and first slab layer with respect to the isolated substrates.

	ΔE_{tot} (meV)	E_{ad} (eV)	m_{tot} (μ_B)	d_{C-TM} (Å)	d_{O1-TM} (Å)	d_{O2-TM} (Å)	α_{OCO} (deg)	ΔECN (%)	Δd_{av} (%)
CO_2/Ni_{13}	1019	−0.04	10	4.39	3.99	5.03	179.90	0.13	0.04
	938	−0.12	10	3.73	3.95	3.89	179.10	0.11	0.03
	936	−0.13	10	2.72	1.97	1.96	136.13	0.08	0.14
	890	−0.17	10	3.59	3.39	3.12	178.75	0.27	0.03
	868	−0.19	10	3.10	4.17	2.12	179.58	0.07	0.09
	848	−0.21	10	3.03	2.16	4.04	179.70	0.09	0.11
	833	−0.23	10	2.81	3.75	2.15	177.83	0.11	0.08
	824	−0.24	10	3.06	2.11	4.13	179.53	0.08	0.07
	818	−0.24	10	2.94	2.14	3.94	179.02	0.16	0.08
	800	−0.26	10	2.69	3.61	2.12	175.33	0.14	0.08
	622	−0.44	10	1.92	2.93	1.95	148.67	0.16	0.33
	591	−0.47	10	1.91	1.96	2.92	147.90	0.44	0.38
	569	−0.49	10	1.91	1.93	2.93	148.52	−0.07	0.32
	465	−0.60	10	1.85	2.12	2.11	142.08	−0.21	0.65
	435	−0.63	10	1.91	1.95	2.95	145.60	−0.08	0.20
	417	−0.64	10	1.84	2.11	2.08	141.91	−0.69	0.52
	321	−0.74	10	1.94	1.96	2.14	131.58	−0.40	0.50
	191	−0.87	10	1.85	1.98	2.06	140.54	0.07	0.54
	163	−0.90	10	1.91	2.09	1.99	138.94	0.07	0.43
	58	−1.00	10	1.82	1.99	2.06	141.13	−0.22	0.47
	30	−1.03	8	1.84	1.96	2.07	139.86	−0.04	0.29
	0	−1.06	10	1.98	2.02	2.02	138.82	0.07	0.36
CO_2/Ni_{55}	498	−0.16	40	3.03	3.95	2.36	179.26	−0.02	0.01
	416	−0.25	40	2.98	3.96	2.18	179.30	−0.02	0.01
	233	−0.43	40	1.97	2.15	2.01	131.48	−0.18	0.10
	85	−0.58	40	1.88	2.71	2.00	129.06	−0.06	0.09
	6	−0.66	38	1.87	2.05	2.10	141.77	−0.20	0.05
	5	−0.66	38	1.88	2.04	2.10	141.72	−0.19	0.04
	0	−0.66	40	1.90	2.67	1.89	133.76	−0.01	0.08
CO_2/Ni_{147}	81	−0.44	100	1.89	2.73	2.01	128.53	−0.03	0.03
	0	−0.52	98	1.91	2.61	1.90	135.07	−0.01	0.01
$CO_2/Ni(111)$	166	0.17	31	1.99	2.12	2.09	132.20	−0.31	0.12
	154	0.16	30	1.99	2.12	2.08	132.02	−0.29	0.09
	0	0.00	29	1.97	1.96	2.66	136.71	−0.24	0.15
	0	0.00	29	1.96	1.96	2.66	136.78	−0.24	0.15

Table S10: Adsorption properties for all configurations of CO interacting with Ni substrates, namely, Ni_{13}, Ni_{55}, Ni_{147} and Ni(111). Total energy relative to the lowest energy configuration for each set (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment for the unit cell (m_{tot}), shortest distances between the C and TM atoms (d_{C-TM}), and between the O and TM atoms (d_{O-TM}), percent variation of the average effective coordination number, ΔECN, and average bond length, Δd_{av}, for the clusters and first slab layer with respect to the isolated substrates.

	ΔE_{tot} (meV)	E_{ad} (eV)	m_{tot} (μ_B)	d_{C-TM} (Å)	d_{O-TM} (Å)	ΔECN (%)	Δd_{av} (%)
CO/Ni_{13}	2228	−0.02	10	5.83	4.71	0.03	0.02
	1921	−0.32	10	3.05	1.89	0.19	0.14
	449	−1.80	10	1.74	2.90	0.60	0.38
	446	−1.80	10	1.83	2.81	−1.30	0.40
	318	−1.93	10	1.73	2.90	0.33	0.26
	293	−1.95	10	1.83	2.87	−0.12	0.34
	264	−1.98	10	1.74	2.90	0.44	0.31
	250	−1.99	8	1.72	2.89	0.56	0.14
	229	−2.02	10	1.73	2.90	−0.12	0.27
	138	−2.11	8	1.84	2.85	−0.10	0.29
	137	−2.11	10	1.73	2.89	−0.07	0.22
	74	−2.17	10	1.85	2.87	0.16	0.34
	50	−2.19	10	1.82	2.84	−0.08	0.36
	0	−2.24	8	1.84	2.86	−0.23	0.19
CO/Ni_{55}	274	−1.97	38	1.74	2.90	−0.02	0.00
	268	−1.97	38	1.73	2.89	−0.02	0.01
	268	−1.97	38	1.74	2.89	−0.09	0.00
	120	−2.12	38	1.94	2.90	−0.08	0.03
	91	−2.15	38	1.83	2.86	−0.07	0.02
	2	−2.24	38	1.94	2.90	−0.03	0.03
	0	−2.24	38	1.94	2.90	−0.02	0.01
CO/Ni_{147}	62	−2.01	98	1.84	2.86	−0.02	0.02
	0	−2.08	98	1.90	2.88	−0.03	0.01
CO/Ni(111)	325	−1.76	30	1.73	2.89	−0.14	0.13
	90	−1.99	29	1.87	2.87	−0.16	0.19
	8	−2.07	29	1.94	2.88	−0.20	0.22
	0	−2.08	29	1.94	2.88	−0.19	0.23

Table S11: Adsorption properties for all configurations of H_2O interacting with Ni substrates, namely, Ni_{13}, Ni_{55}, Ni_{147} and Ni(111). Total energy relative to the lowest energy configuration for each set (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment for the unit cell (m_{tot}), shortest distances between the O and TM atoms ($d_{\mathrm{O-TM}}$), H atoms and TM ($d_{\mathrm{H1-TM}}$ and $d_{\mathrm{H2-TM}}$), and HOH angle (α_{HOH}), percent variation of the average effective coordination number, ΔECN, and average bond length, Δd_{av}, for the clusters and first slab layer with respect to the isolated substrates.

	ΔE_{tot} (meV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\mathrm{O-TM}}$ (Å)	$d_{\mathrm{H1-TM}}$ (Å)	$d_{\mathrm{H2-TM}}$ (Å)	α_{HOH} (deg)	ΔECN (%)	Δd_{av} (%)
H_2O/Ni13	404	−0.31	10	3.38	2.51	3.34	102.92	0.19	0.05
	300	−0.41	10	2.15	2.54	2.47	104.73	−0.08	0.22
	155	−0.56	10	2.10	2.51	2.44	104.94	0.10	0.18
	90	−0.62	10	2.06	2.47	2.59	105.55	0.30	0.13
	79	−0.63	10	2.06	2.55	2.54	105.59	0.00	0.09
	75	−0.64	10	2.06	2.52	2.52	105.04	−0.10	0.08
	65	−0.65	10	2.05	2.52	2.52	105.29	0.03	0.09
	56	−0.65	10	2.05	2.48	2.56	105.63	0.22	0.10
	50	−0.66	10	2.07	2.52	2.47	104.98	0.03	0.15
	39	−0.67	10	2.06	2.52	2.49	104.76	−0.05	0.11
	36	−0.68	10	2.06	2.48	2.46	104.85	0.30	0.12
	0	−0.71	10	2.05	2.48	2.45	104.98	−0.03	0.08
H_2O/Ni_{55}	108	−0.60	40	2.10	2.41	2.51	104.51	−0.05	0.02
	105	−0.60	40	2.10	2.45	2.46	104.31	−0.06	0.02
	103	−0.61	40	2.09	2.47	2.50	105.16	−0.04	0.01
	4	−0.70	40	2.05	2.48	2.48	104.73	0.01	0.02
	2	−0.71	40	2.04	2.55	2.47	105.50	0.00	0.01
	0	−0.71	40	2.05	2.48	2.50	105.02	0.02	0.02
H_2O/Ni_{147}	223	−0.53	100	2.13	2.47	2.45	104.34	−0.04	0.00
	0	−0.76	98	2.02	2.54	2.48	105.73	−0.03	−0.01
H_2O/Ni(111)	2	−0.52	31	2.18	2.53	2.53	104.70	−0.10	0.07
	2	−0.52	31	2.18	2.51	2.52	104.23	−0.13	0.07
	1	−0.52	31	2.18	2.51	2.50	104.35	−0.13	0.06
	0	−0.52	31	2.17	2.51	2.50	104.50	−0.11	0.05

Table S12: Adsorption properties for all configurations of H_2 interacting with Ni substrates, namely, Ni_{13}, Ni_{55}, Ni_{147} and Ni(111). Total energy relative to the lowest energy configuration for each set (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment for the unit cell (m_{tot}), shortest distances between the H and TM atoms ($d_{\mathrm{H1-TM}}$ and $d_{\mathrm{H2-TM}}$), percent variation of the average effective coordination number, ΔECN, and average bond length, Δd_{av}, for the clusters and first slab layer with respect to the isolated substrates.

	ΔE_{tot} (meV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\mathrm{H1-TM}}$ (Å)	$d_{\mathrm{H2-TM}}$ (Å)	ΔECN (%)	Δd_{av} (%)
H_2/Ni_{13}	662	−0.09	10	3.15	2.48	0.05	0.01
	659	−0.10	10	3.34	2.62	0.20	0.04
	648	−0.11	10	2.53	3.28	−0.01	−0.01
	288	−0.47	10	1.58	1.58	−2.35	0.05
	247	−0.51	10	1.60	1.60	−0.54	0.25
	243	−0.51	10	1.61	1.61	0.45	0.20
	241	−0.51	10	1.61	1.60	0.31	0.19
	117	−0.64	10	1.58	1.58	0.45	0.19
	89	−0.67	10	1.60	1.59	0.44	0.19
	68	−0.69	10	1.58	1.58	0.35	0.18
	68	−0.69	10	1.58	1.59	0.35	0.18
	43	−0.71	10	1.58	1.58	0.16	0.20
	0	−0.75	10	1.58	1.58	0.20	0.16
H_2/Ni_{55}	64	−0.63	40	1.60	1.61	−0.05	0.02
	61	−0.63	40	1.60	1.61	−0.05	0.02
	22	−0.67	40	1.57	1.57	−0.04	0.02
	0	−0.69	38	1.57	1.57	−0.05	−0.02
H_2/Ni_{147}	63	−0.55	100	1.58	1.58	−0.03	0.02
	0	−0.61	100	1.58	1.57	0.00	0.01
H_2/Ni(111)	0	−0.48	30	1.58	1.58	−0.09	0.09
	0	−0.48	30	1.58	1.57	−0.12	0.07

Table S13: Adsorption properties for all configurations of CO_2 interacting with Cu substrates, namely, Cu_{13}, Cu_{55}, Cu_{147} and Cu(111). Total energy relative to the lowest energy configuration for each set (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment for the unit cell (m_{tot}), shortest distances between the C and TM atoms (d_{C-TM}), O atoms and TM (d_{O1-TM} and d_{O2-TM}), and OCO angle (α_{OCO}), percent variation of the average effective coordination number, ΔECN, and average bond length, Δd_{av}, for the clusters and first slab layer with respect to the isolated substrates.

	ΔE_{tot} (meV)	E_{ad} (eV)	m_{tot} (μ_B)	d_{C-TM} (Å)	d_{O1-TM} (Å)	d_{O2-TM} (Å)	α_{OCO} (deg)	ΔECN (%)	Δd_{av} (%)
CO_2/Cu_{13}	334	0.16	1	2.82	2.10	2.12	146.92	−1.05	0.04
	221	0.04	1	2.05	2.07	2.49	141.14	−0.06	0.22
	177	0.00	1	2.04	2.65	1.97	136.31	−0.46	0.22
	134	−0.04	1	4.58	3.58	5.64	179.92	−0.10	0.04
	129	−0.05	1	4.40	3.40	5.47	179.95	−0.07	0.01
	109	−0.07	1	2.03	1.97	2.65	136.43	−0.08	0.24
	88	−0.09	1	3.64	4.08	3.56	179.55	−0.02	0.01
	78	−0.10	1	3.44	2.81	4.30	179.77	−0.09	−0.02
	69	−0.11	1	3.69	3.49	3.59	179.59	−0.04	0.03
	68	−0.11	1	3.46	2.99	4.21	179.75	−0.08	0.03
	65	−0.11	1	3.69	3.73	3.59	179.43	−0.08	−0.02
	61	−0.12	1	3.52	3.23	3.87	179.45	0.07	0.02
	48	−0.13	1	3.40	3.93	2.94	179.41	0.00	0.07
	45	−0.13	1	3.51	4.01	3.19	179.31	−0.05	0.01
	41	−0.14	1	3.42	4.05	2.87	179.91	−0.08	0.00
	40	−0.14	1	3.51	3.66	3.14	179.57	0.11	0.01
	35	−0.14	1	3.69	3.25	3.69	179.47	0.09	0.00
	31	−0.15	1	3.21	2.40	4.19	179.79	0.35	0.05
	0	−0.18	1	3.08	2.39	4.00	179.78	0.33	0.03
CO_2/Cu_{55}	363	0.20	1	2.17	2.85	2.00	133.52	−0.12	0.03
	308	0.15	1	2.10	2.10	2.58	140.07	−0.10	0.03
	198	0.04	1	2.06	2.34	2.18	145.43	−0.06	0.02
	80	−0.08	3	3.25	3.28	3.63	179.75	0.02	−0.01
	53	−0.10	3	3.33	3.18	3.03	179.26	0.02	−0.01
	9	−0.15	3	3.49	3.17	3.36	179.27	0.02	−0.01
	6	−0.15	3	3.33	3.18	3.03	179.26	0.02	−0.01
	5	−0.15	3	3.19	4.13	2.44	179.81	0.02	0.00
	0	−0.16	3	3.15	2.65	3.57	179.41	0.02	0.00
CO_2/Cu_{147}	103	−0.08	1	3.09	3.27	3.34	179.55	−1.70	−1.05
	19	−0.16	1	3.13	3.55	2.63	179.87	−0.01	0.02
	7	−0.17	1	3.30	3.07	3.04	179.51	−1.67	−1.04
	0	−0.18	1	3.34	3.52	3.37	179.35	0.00	0.02
$CO_2/Cu(111)$	13	−0.22	0	3.31	3.51	3.52	179.80	−0.04	−0.03
	4	−0.23	0	3.50	3.40	3.34	179.82	−0.04	−0.03
	3	−0.23	0	3.54	3.34	3.35	179.63	−0.04	−0.04
	0	−0.24	0	3.50	3.29	3.29	179.60	−0.03	−0.02

Table S14: Adsorption properties for all configurations of CO interacting with Cu substrates, namely, Cu_{13}, Cu_{55}, Cu_{147} and Cu(111). Total energy relative to the lowest energy configuration for each set (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment for the unit cell (m_{tot}), shortest distances between the C and TM atoms (d_{C-TM}), and between the O and TM atoms (d_{O-TM}), percent variation of the average effective coordination number, ΔECN, and average bond length, Δd_{av}, for the clusters and first slab layer with respect to the isolated substrates.

	ΔE_{tot} (meV)	E_{ad} (eV)	m_{tot} (μ_B)	d_{C-TM} (Å)	d_{O-TM} (Å)	ΔECN (%)	Δd_{av} (%)
CO/Cu_{13}	1286	−0.02	1	5.32	4.27	−0.05	−0.01
	1284	−0.02	1	5.13	4.08	−0.06	−0.02
	1282	−0.02	1	4.97	4.17	−0.02	0.00
	1274	−0.03	1	4.72	3.78	−0.05	0.02
	1273	−0.03	1	4.69	3.67	−0.03	−0.02
	1273	−0.03	1	4.70	3.70	−0.01	0.01
	647	−0.66	1	1.92	2.95	−4.06	0.10
	543	−0.76	1	1.84	2.99	−5.47	−0.11
	349	−0.96	1	1.97	2.96	−2.21	0.26
	293	−1.01	1	1.83	2.98	−0.16	0.31
	268	−1.04	1	1.83	2.97	−0.09	0.24
	199	−1.11	1	1.82	2.97	0.21	0.20
	164	−1.14	1	1.82	2.97	4.37	−0.24
	123	−1.18	1	1.82	2.96	0.18	0.18
	0	−1.31	1	1.81	2.96	0.56	0.22
CO/Cu_{55}	215	−1.10	1	1.87	2.91	−0.05	0.03
	175	−1.14	1	1.83	2.98	−0.03	0.02
	174	−1.14	3	1.83	2.98	0.04	0.03
	89	−1.22	1	2.00	2.93	−0.06	0.06
	0	−1.31	1	2.04	2.97	−0.01	0.06
	0	−1.31	1	2.04	2.97	−0.01	0.06
CO/Cu_{147}	132	−0.89	1	2.06	3.01	−0.01	0.04
	0	−1.02	1	1.84	2.99	−0.01	0.03
CO/Cu(111)	137	−1.00	0	1.85	3.00	−0.14	0.01
	44	−1.10	0	1.97	2.96	−0.18	0.10
	11	−1.13	0	2.03	2.97	−0.22	0.14
	0	−1.14	0	2.03	2.97	−0.20	0.13

Table S15: Adsorption properties for all configurations of H_2O interacting with Cu substrates, namely, Cu_{13}, Cu_{55}, Cu_{147} and Cu(111). Total energy relative to the lowest energy configuration for each set (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment for the unit cell (m_{tot}), shortest distances between the O and TM atoms ($d_{\mathrm{O-TM}}$), H atoms and TM ($d_{\mathrm{H1-TM}}$ and $d_{\mathrm{H2-TM}}$), and HOH angle (α_{HOH}), percent variation of the average effective coordination number, ΔECN, and average bond length, Δd_{av}, for the clusters and first slab layer with respect to the isolated substrates.

	ΔE_{tot} (meV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\mathrm{O-TM}}$ (Å)	$d_{\mathrm{H1-TM}}$ (Å)	$d_{\mathrm{H2-TM}}$ (Å)	α_{HOH} (deg)	ΔECN (%)	Δd_{av} (%)
H_2O/Cu_{13}	346	−0.20	1	3.42	3.68	2.61	103.74	0.03	0.02
	346	−0.20	1	3.29	2.51	3.39	102.58	−0.02	0.05
	338	−0.21	1	3.51	2.66	3.52	103.67	−0.08	0.04
	296	−0.26	1	2.45	2.72	2.62	104.04	−1.01	−0.01
	128	−0.42	1	2.15	2.67	2.62	105.52	0.04	0.10
	122	−0.43	1	2.15	2.68	2.66	105.65	−0.06	0.12
	118	−0.43	1	2.20	2.60	2.56	104.47	−0.05	0.14
	114	−0.44	1	2.13	2.60	2.63	105.96	0.23	0.16
	104	−0.45	1	2.15	2.63	2.62	105.35	−0.14	0.13
	69	−0.48	1	2.12	2.61	2.65	105.65	−0.23	0.08
	64	−0.49	1	2.12	2.62	2.62	105.50	−0.14	0.09
	13	−0.54	1	2.13	2.52	2.60	105.01	0.56	0.13
	9	−0.54	1	2.10	2.63	2.61	105.57	0.12	0.06
	5	−0.55	1	2.10	2.60	2.61	105.49	0.15	0.10
	0	−0.55	1	2.13	2.60	2.52	104.95	0.55	0.14
H_2O/Cu_{55}	125	−0.40	1	2.22	2.61	2.51	104.11	−0.05	0.01
	120	−0.40	1	2.23	2.54	2.54	103.80	−0.09	0.00
	120	−0.40	1	2.23	2.46	2.67	104.33	−0.05	0.01
	113	−0.41	1	2.21	2.61	2.57	104.85	−0.04	0.01
	12	−0.51	3	2.18	2.53	2.59	104.23	0.02	0.00
	0	−0.52	3	2.13	2.67	2.62	105.58	0.02	0.01
H_2O/Cu_{147}	172	−0.36	1	2.32	2.62	2.58	104.14	−0.01	0.03
	0	−0.53	1	2.13	2.59	2.61	105.16	−0.01	0.02
$H_2O/Cu(111)$	4	−0.43	0	2.33	2.65	2.64	104.46	−0.10	0.00
	2	−0.43	0	2.33	2.65	2.64	104.46	−0.09	−0.03
	1	−0.43	0	2.36	2.66	2.66	103.92	−0.11	0.00
	0	−0.43	0	2.35	2.64	2.64	103.82	−0.11	−0.01

Table S16: Adsorption properties for all configurations of H_2 interacting with Cu substrates, namely, Cu_{13}, Cu_{55}, Cu_{147} and Cu(111). Total energy relative to the lowest energy configuration for each set (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment for the unit cell (m_{tot}), shortest distances between the H and TM atoms ($d_{\mathrm{H1-TM}}$ and $d_{\mathrm{H2-TM}}$), percent variation of the average effective coordination number, ΔECN, and average bond length, Δd_{av}, for the clusters and first slab layer with respect to the isolated substrates.

	ΔE_{tot} (meV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\mathrm{H1-TM}}$ (Å)	$d_{\mathrm{H2-TM}}$ (Å)	ΔECN (%)	Δd_{av} (%)
H_2/Cu_{13}	298	−0.06	1	3.04	3.75	−0.02	0.02
	286	−0.07	1	3.05	2.33	0.01	0.02
	286	−0.07	1	3.24	2.56	−0.03	0.00
	284	−0.08	1	2.82	2.13	−0.09	0.04
	281	−0.08	1	3.55	2.81	−0.07	0.02
	278	−0.08	1	3.47	2.81	−0.12	0.00
	278	−0.08	1	3.57	2.88	−0.10	0.02
	278	−0.08	1	2.65	3.35	−0.03	−0.02
	276	−0.08	1	3.40	2.65	−0.15	−0.01
	275	−0.08	1	2.81	3.48	0.02	0.01
	272	−0.09	1	2.99	2.36	0.03	0.06
	194	−0.17	1	1.79	1.79	−0.04	0.12
	186	−0.17	1	1.77	1.78	−0.13	0.13
	141	−0.22	1	1.73	1.73	0.29	0.20
	106	−0.25	1	1.74	1.74	0.16	0.13
	99	−0.26	1	1.74	1.74	0.15	0.12
	97	−0.26	1	1.75	1.75	−0.01	0.14
	0	−0.36	1	1.72	1.71	0.55	0.10
H_2/Cu_{55}	211	−0.04	1	3.10	3.08	−0.07	−0.01
	173	−0.08	1	2.86	3.51	0.02	0.00
	168	−0.08	3	2.65	3.23	0.02	−0.01
	164	−0.09	3	2.93	2.39	0.03	0.00
	159	−0.09	3	2.42	2.96	0.02	−0.01
	156	−0.10	3	3.17	2.57	0.03	0.00
	30	−0.22	1	1.75	1.76	−0.04	0.01
	23	−0.23	1	1.75	1.76	−0.02	0.01
	1	−0.25	3	1.77	1.78	0.03	0.00
	0	−0.25	3	1.77	1.78	0.03	0.01
H_2/Cu_{147}	82	−0.10	1	1.91	1.92	−0.01	0.03
	0	−0.19	1	1.82	1.82	−0.01	0.02
$H_2/Cu(111)$	11	−0.11	0	1.85	1.86	−0.12	−0.03
	10	−0.11	0	1.85	1.85	−0.10	0.00
	9	−0.11	0	2.68	2.79	−0.03	−0.01
	0	−0.12	0	3.41	2.84	−0.03	−0.02

VI Electron Density Difference for the Lowest Energy Adsorption Structures

In the main article we show the electron density difference isosurfaces for the lowest energy adsorption structures in the region around the molecules and the nearest TM neighbors. Here, Figures S12-S15 present the same isosurfaces, but showing the whole clusters and the two surface layers closer to the molecules.

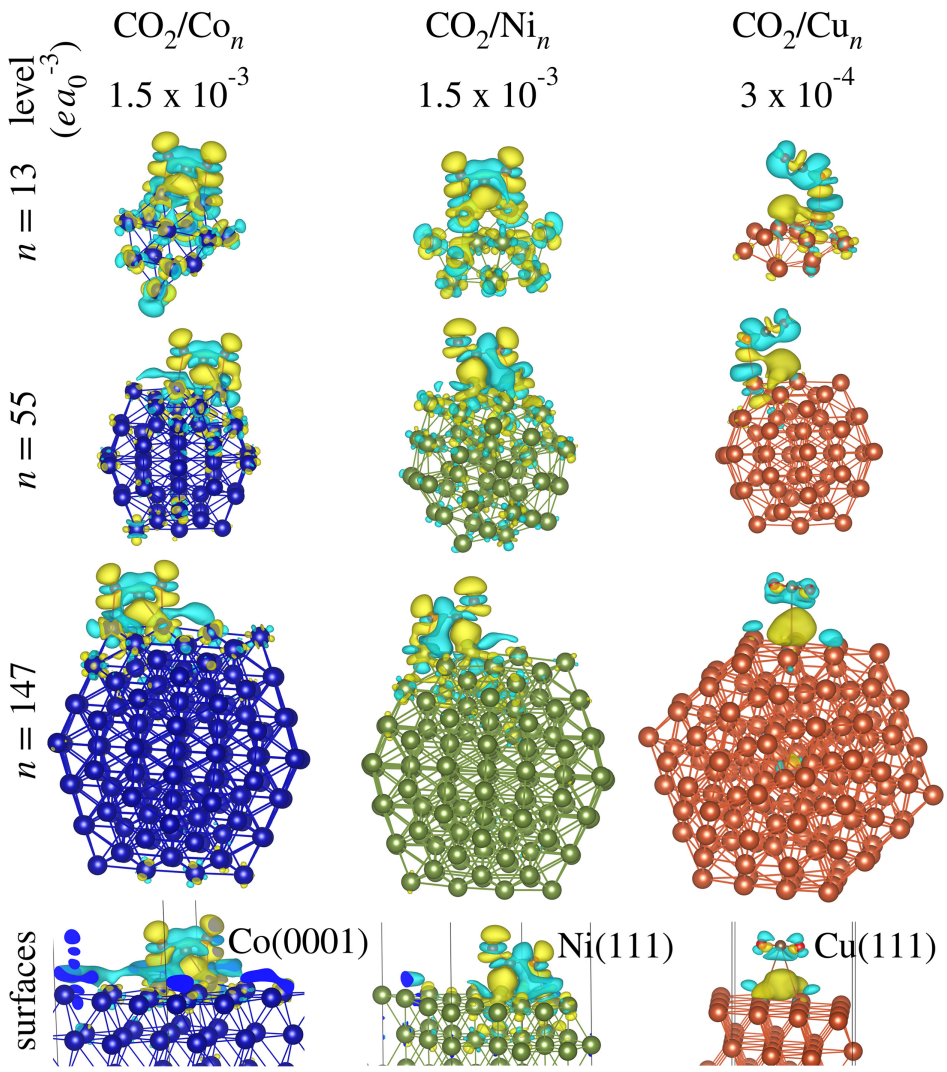

Figure S12: Electron density difference isosurfaces ($1.5 \times 10^{-3}\, e\, {a_0}^{-3}$ for Co and Ni and $3 \times 10^{-4}\, e\, {a_0}^{-3}$ for Cu systems) for the lowest energy configurations of CO_2, adsorbed on Co_n, Co(0001), Ni_n, Ni(111), Cu_n and Cu(111), n = {13, 55, 147}. Yellow and blue regions represent electron density accumulation and depletion, respectively.

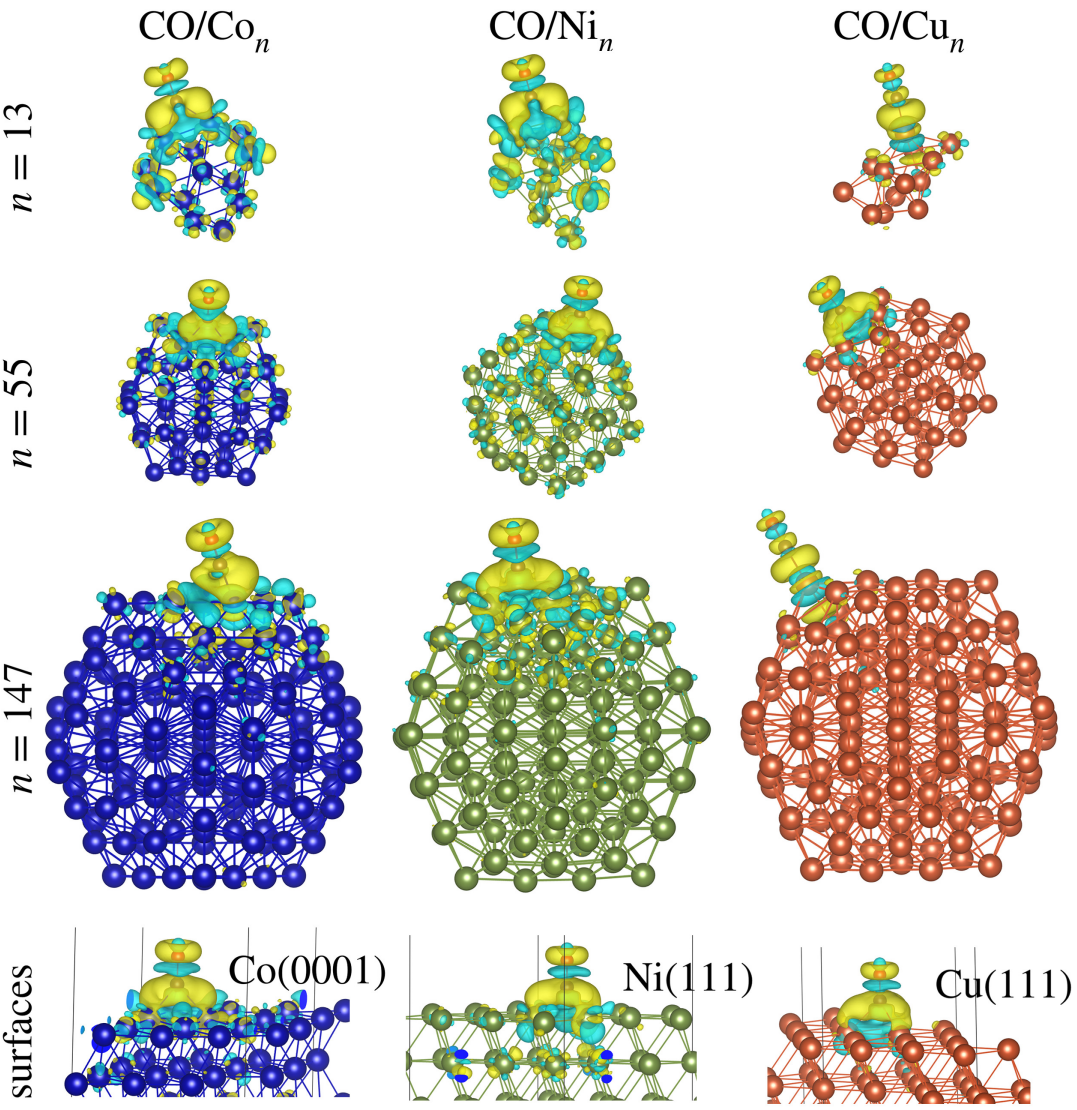

Figure S13: Electron density difference isosurfaces ($1.5 \times 10^{-3}\, e\, {a_0}^{-3}$) for the lowest energy configurations of CO, adsorbed on Co_n, Co(0001), Ni_n, Ni(111), Cu_n and Cu(111), n = {13, 55, 147}. Yellow and blue regions represent electron density accumulation and depletion, respectively.

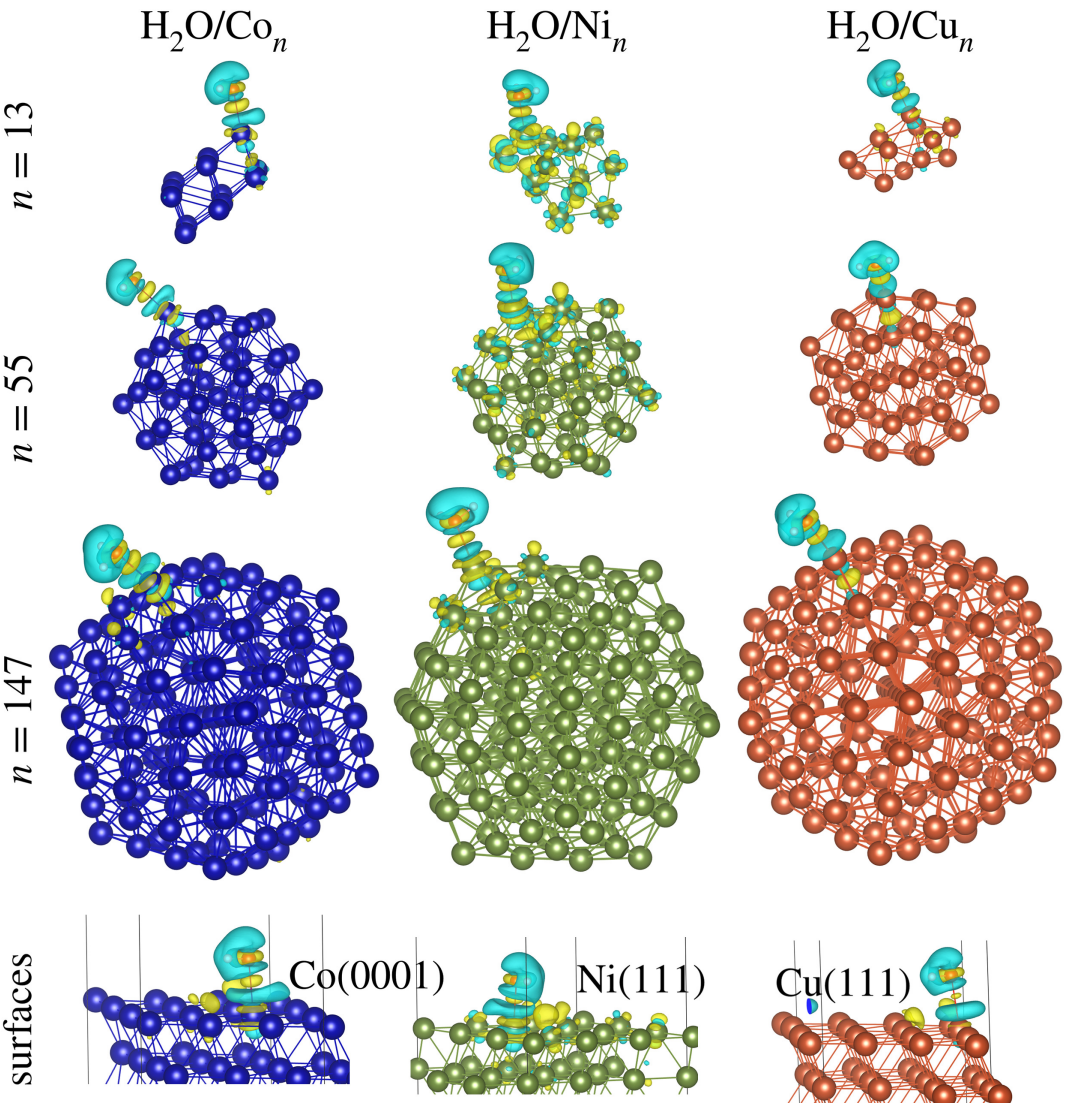

Figure S14: Electron density difference isosurfaces ($1.5 \times 10^{-3}\, e\, {a_0}^{-3}$) for the lowest energy configurations of H_2O, adsorbed on Co_n, Co(0001), Ni_n, Ni(111), Cu_n and Cu(111), n = {13, 55, 147}. Yellow and blue regions represent electron density accumulation and depletion, respectively.

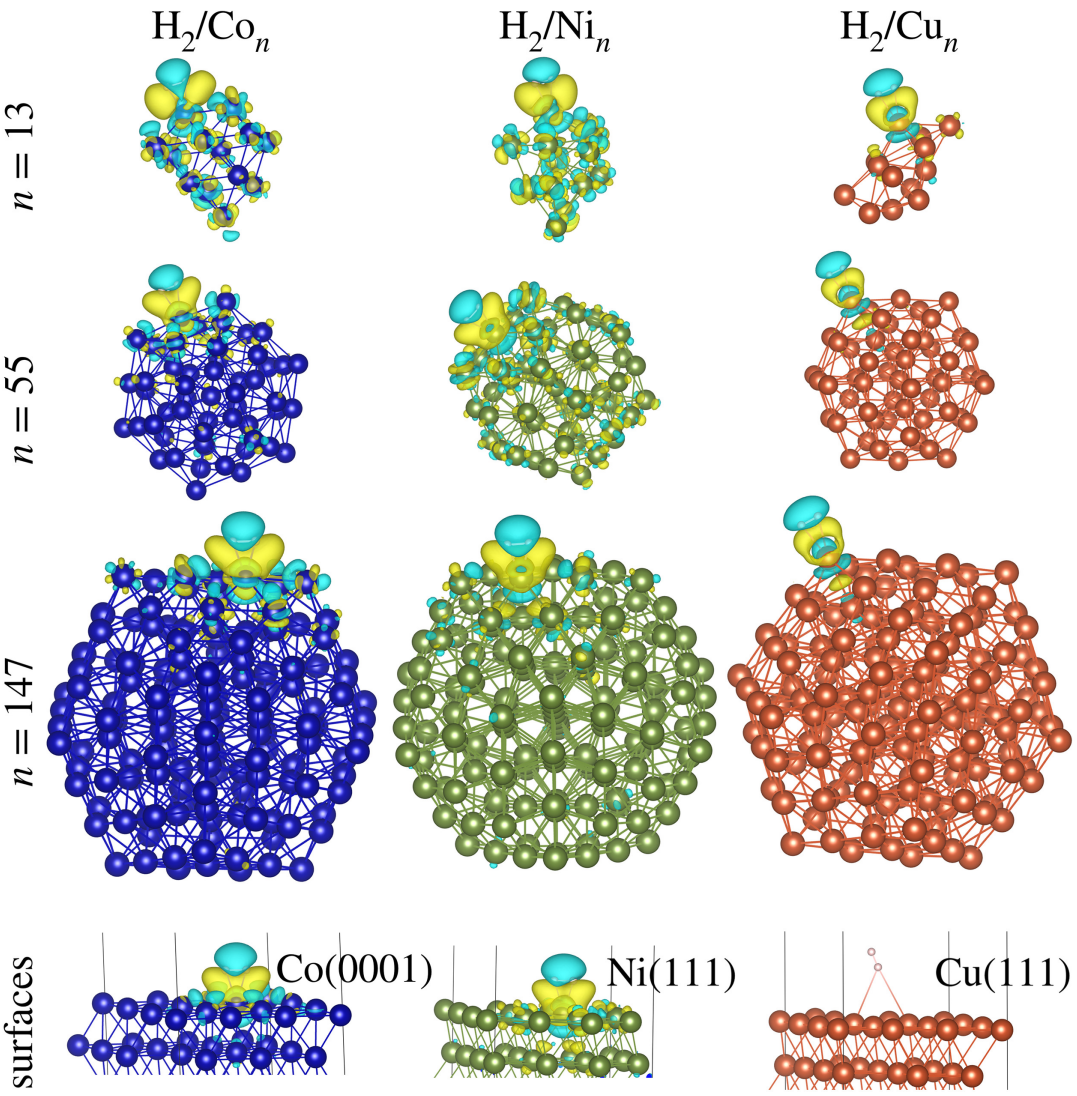

Figure S15: Electron density difference isosurfaces ($1.5 \times 10^{-3}\, e\, a_0{}^{-3}$) for the lowest energy configurations of H_2, adsorbed on Co_n, Co(0001), Ni_n, Ni(111), Cu_n and Cu(111), n = {13, 55, 147}. Yellow and blue regions represent electron density accumulation and depletion, respectively.

VII Density of States for the Lowest Energy Adsorption Structures

Figures S17-S19 show the local density of states (LDOS, $s + p + d + f$) for the lowest energy adsorption configurations of CO_2, CO, H_2O and H_2 interacting with each substrate studied, namely, Co_n, Co(0001), Ni_n, Ni(111), Cu_n and Cu(111), n = {13, 55, 147}. The analysis of the center of the *d*-states shown in the main article considered the *d*-states for the clean substrates. The profiles shown here are complementary and the LDOS of the clean substrates were omitted, because they are very similar to the profile for the adsorbed systems.

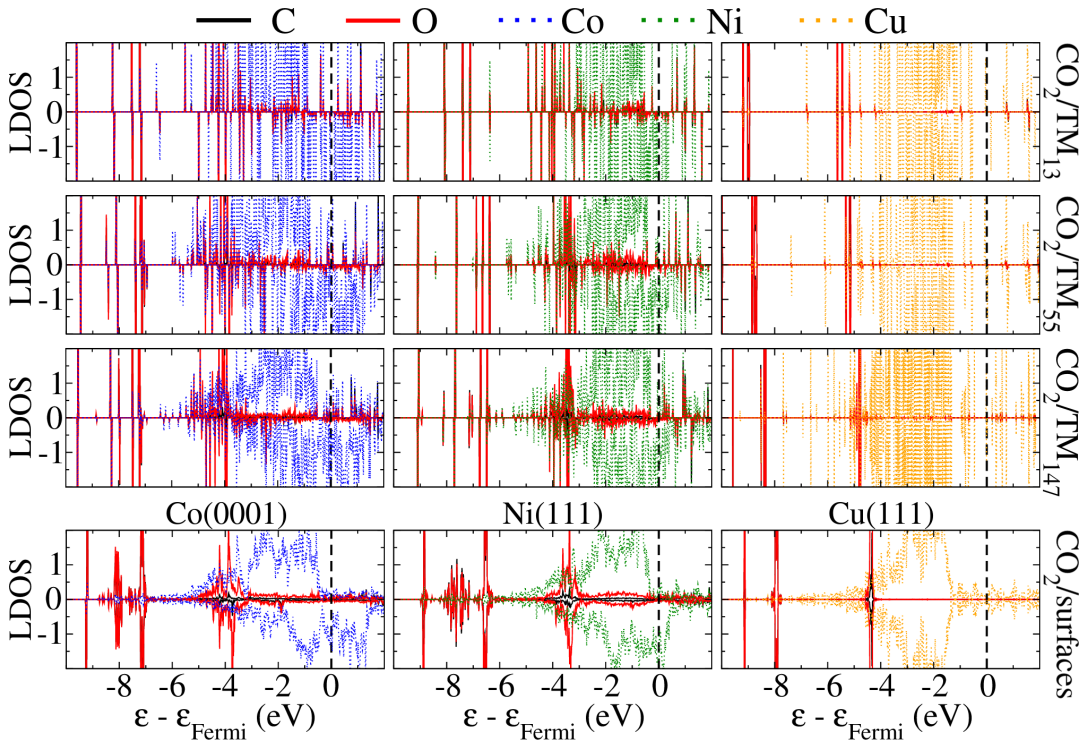

Figure S16: Total local density of states per atom including *s*-, *p*-, *d*- and *f*-states for the lowest energy configurations of CO_2, adsorbed on Co_n, Co(0001), Ni_n, Ni(111), Cu_n and Cu(111), n = {13, 55, 147}. The represented transition metal atoms correspond to the adsorption sites for the clusters and to the first layer for the periodic surfaces.

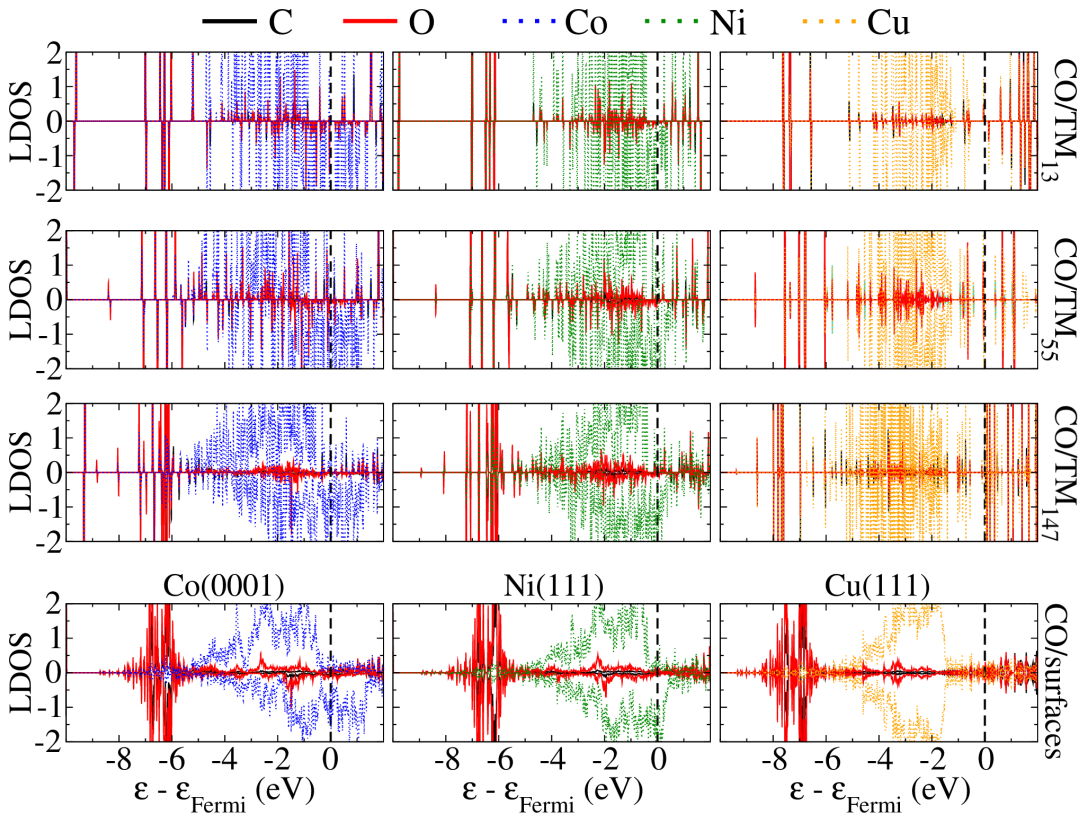

Figure S17: Total local density of states per atom including *s*-, *p*-, *d*- and *f*-states for the lowest energy configurations of CO, adsorbed on Co_n, Co(0001), Ni_n, Ni(111), Cu_n and Cu(111), n = {13, 55, 147}. The represented transition metal atoms correspond to the adsorption sites for the clusters and to the first layer for the periodic surfaces.

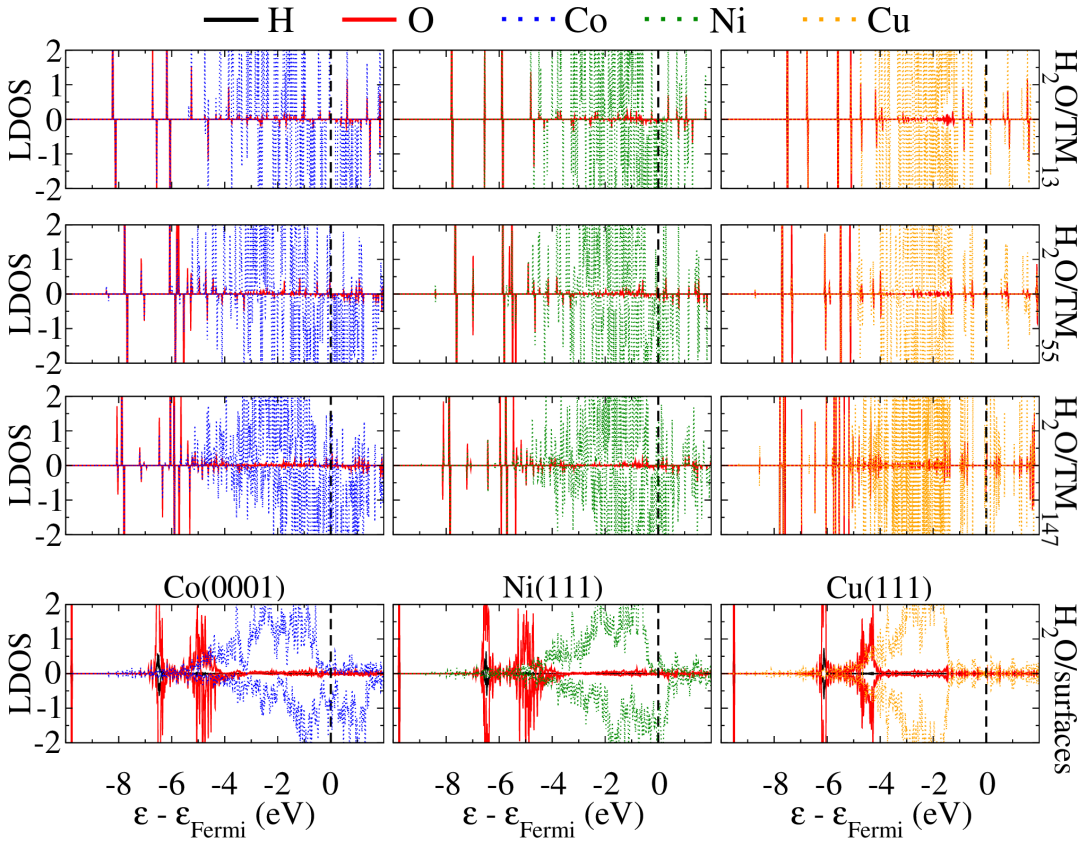

Figure S18: Total local density of states per atom including *s*-, *p*-, *d*- and *f*-states for the lowest energy configurations of H_2O, adsorbed on Co_n, Co(0001), Ni_n, Ni(111), Cu_n and Cu(111), n = {13, 55, 147}. The represented transition metal atoms correspond to the adsorption sites for the clusters and to the first layer for the periodic surfaces.

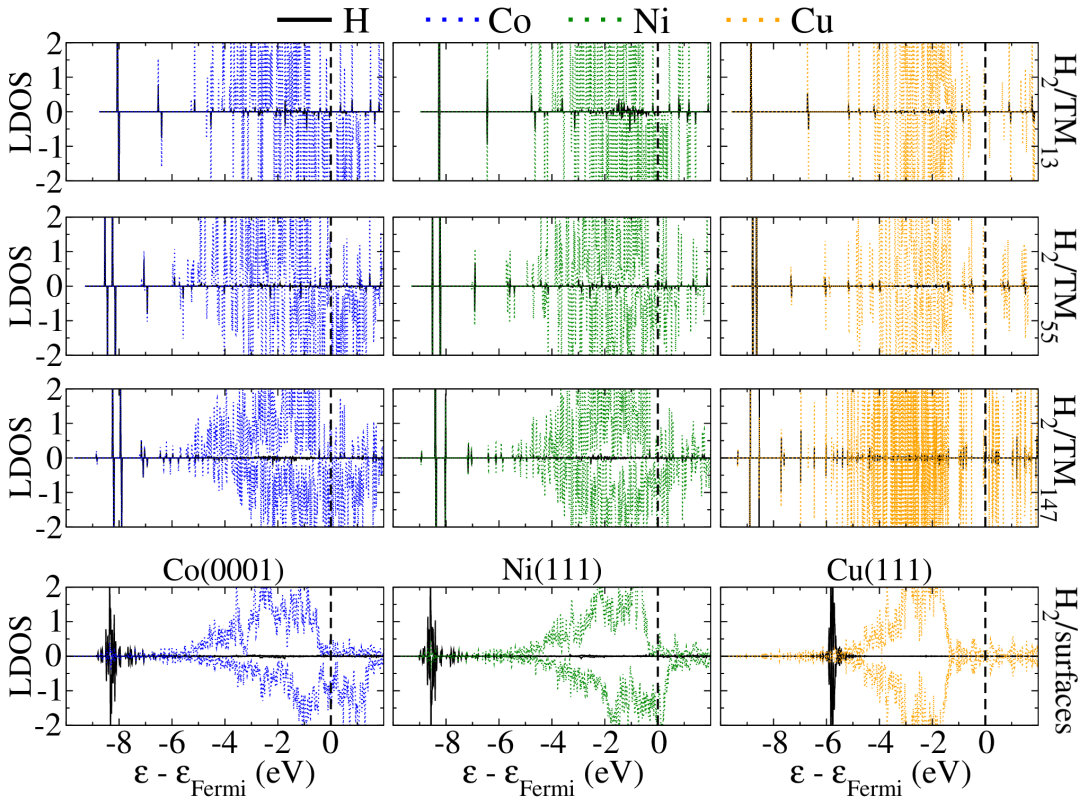

Figure S19: Total local density of states per atom including *s*-, *p*-, *d*- and *f*-states for the lowest energy configurations of H_2, adsorbed on Co_n, Co(0001), Ni_n, Ni(111), Cu_n and Cu(111), n = {13, 55, 147}. The represented transition metal atoms correspond to the adsorption sites for the clusters and to the first layer for the periodic surfaces.

VIII Additional Energetic Properties for the Lowest Energy Adsorption Structures

Table S17 shows some energetic properties calculated for the lowest energy adsorption configurations. As explained in the main article, the adsorption energy, E_{ad}, was calculated with respect to the isolated and relaxed substrate and molecules, while the interaction energy was calculated with respect to the isolated systems frozen in the atomic positions after the geometric perturbations due to adsorption using the adsorption simulation box, with $\Delta E_{tot}^{\mathrm{Mol}}$ and $\Delta E_{tot}^{\mathrm{sub}}$ corresponding to the deformation energies for the molecules and substrates, respectively.

Table S17: Adsorption energy, E_{ad}, with respect to the relaxed isolated systems, interaction energy, E_{int}, with respect to isolated systems frozen in the respective adsorption configurations and energy difference for the molecule and substrate due to adsorption, respectively $\Delta E_{tot}^{\mathbf{Mol}}$ and $\Delta E_{tot}^{\mathbf{sub}}$, for the lowest energy structures of CO_2, CO, H_2O and H_2 interacting with Co_n, Ni_n, Cu_n (n = 13, 55, 147) and Co(0001), Ni(111) and Cu(111).

Structure	E_{ad} (eV)	E_{int} (eV)	$\Delta E_{tot}^{\mathrm{Mol}}$ (eV)	$\Delta E_{tot}^{\mathrm{sub}}$ (eV)	Structure	E_{ad} (eV)	E_{int} (eV)	$\Delta E_{tot}^{\mathrm{Mol}}$ (eV)	$\Delta E_{tot}^{\mathrm{sub}}$ (eV)
CO_2/Co_{13}	−1.16	−2.87	1.67	0.04	H_2O/Co_{13}	−0.66	−0.67	0.00	0.01
CO_2/Co_{55}	−0.65	−2.23	1.51	0.07	H_2O/Co_{55}	−0.64	−0.66	0.00	0.01
CO_2/Co_{147}	−0.80	−2.50	1.61	0.09	H_2O/Co_{147}	−0.68	−0.70	0.00	0.01
$CO_2/Co(0001)$	−0.08	−1.59	1.40	0.11	$H_2O/Co(0001)$	−0.50	−0.54	−0.01	0.04
CO_2/Ni_{13}	−1.06	−2.70	1.55	0.08	H_2O/Ni_{13}	−0.71	−0.73	0.00	0.02
CO_2/Ni_{55}	−0.66	−2.66	1.93	0.06	H_2O/Ni_{55}	−0.71	−0.73	0.00	0.01
CO_2/Ni_{147}	−0.52	−2.39	1.79	0.08	H_2O/Ni_{147}	−0.76	−0.77	0.00	0.01
$CO_2/Ni(111)$	0.00	−1.70	1.62	0.08	$H_2O/Ni(111)$	−0.52	−0.56	−0.01	0.05
CO_2/Cu_{13}	−0.18	−0.18	0.00	0.00	H_2O/Cu_{13}	−0.55	−0.57	0.00	0.02
CO_2/Cu_{55}	−0.16	−0.16	0.00	0.00	H_2O/Cu_{55}	−0.52	−0.53	0.00	0.01
CO_2/Cu_{147}	−0.18	−0.18	0.00	−0.01	H_2O/Cu_{147}	−0.53	−0.53	0.00	0.00
$CO_2/Cu(111)$	−0.24	−0.24	0.00	0.00	$H_2O/Cu(111)$	−0.43	−0.44	−0.01	0.02
CO/Co_{13}	−1.94	−2.13	0.11	0.08	H_2/Co_{13}	−0.58	−1.06	0.44	0.04
CO/Co_{55}	−1.85	−2.12	0.21	0.06	H_2/Co_{55}	−0.48	−0.72	0.21	0.03
CO/Co_{147}	−2.05	−2.13	0.05	0.03	H_2/Co_{147}	−0.68	−1.05	0.34	0.02
$CO/Co(0001)$	−1.92	−2.10	0.15	0.04	$H_2/Co(0001)$	−0.53	−0.93	0.37	0.03
CO/Ni_{13}	−2.24	−2.42	0.11	0.06	H_2/Ni_{13}	−0.75	−0.99	0.20	0.03
CO/Ni_{55}	−2.24	−2.46	0.16	0.06	H_2/Ni_{55}	−0.69	−1.00	0.28	0.03
CO/Ni_{147}	−2.08	−2.31	0.16	0.07	H_2/Ni_{147}	−0.61	−0.90	0.25	0.03
$CO/Ni(111)$	−2.08	−2.26	0.13	0.05	$H_2/Ni(111)$	−0.48	−0.79	0.26	0.04
CO/Cu_{13}	−1.31	−1.37	0.01	0.06	H_2/Cu_{13}	−0.36	−0.43	0.05	0.02
CO/Cu_{55}	−1.31	−1.49	0.11	0.07	H_2/Cu_{55}	−0.25	−0.30	0.03	0.02
CO/Cu_{147}	−1.02	−1.05	0.01	0.02	H_2/Cu_{147}	−0.19	−0.21	0.02	0.00
$CO/Cu(111)$	−1.14	−1.25	0.08	0.03	$H_2/Cu(111)$	−0.12	−0.12	0.00	0.00

IX Geometric Properties for the Lowest Energy Adsorption Structures

Table S18 shows, for the lowest energy adsorption configurations, the OCO and HOH angles, in degrees, and the shortest distances, in Å, from the molecule to the nearest substrate atom. Moreover, the percent variations in the molecular bond lengths and angles, with respect to the gas-phase molecules, are shown in Table S19.

Table S18: Shortest distances, in Å, from C, O and H atoms to the nearest substrate atom (d_{C-TM}, d_{O-TM} and d_{H-TM}) and molecular angles (α_{OCO} and α_{HOH}), in degrees, for the lowest energy structures of CO_2, CO, H_2O and H_2 adsorbed on Co_n, Ni_n, Cu_n (n = 13, 55, 147) and on Co(0001), Ni(111) and Cu(111).

Structure	d_{C-TM} (Å)	d_{O1-TM} (Å)	d_{O2-TM} (Å)	α_{OCO} (deg)	Structure	d_{O-TM} (Å)	d_{H1-TM} (Å)	d_{H2-TM} (Å)	α_{HOH} (deg)
CO_2/Co_{13}	2.00	2.04	2.04	137.32	H_2O/Co_{13}	2.09	2.54	2.56	105.17
CO_2/Co_{55}	1.94	2.16	2.04	138.98	H_2O/Co_{55}	2.14	2.58	2.54	104.86
CO_2/Co_{147}	1.96	2.09	2.00	137.64	H_2O/Co_{147}	2.08	2.52	2.51	104.93
CO_2/Co(0001)	2.01	2.18	2.13	139.64	H_2O/Co(0001)	2.23	2.57	2.57	104.36
CO_2/Ni_{13}	1.98	2.02	2.02	138.82	H_2O/Ni_{13}	2.05	2.48	2.45	104.98
CO_2/Ni_{55}	1.90	2.67	1.89	133.76	H_2O/Ni_{55}	2.05	2.48	2.50	105.02
CO_2/Ni_{147}	1.91	2.61	1.90	135.07	H_2O/Ni_{147}	2.02	2.54	2.48	105.73
CO_2/Ni(111)	1.96	1.96	2.66	136.78	H_2O/Ni(111)	2.17	2.51	2.50	104.50
CO_2/Cu_{13}	3.08	2.39	4.00	179.78	H_2O/Cu_{13}	2.13	2.60	2.52	104.95
CO_2/Cu_{55}	3.15	2.65	3.57	179.41	H_2O/Cu_{55}	2.13	2.67	2.62	105.58
CO_2/Cu_{147}	3.34	3.52	3.37	179.35	H_2O/Cu_{147}	2.13	2.59	2.61	105.16
CO_2/Cu(111)	3.50	3.29	3.29	179.60	H_2O/Cu(111)	2.35	2.64	2.64	103.81
CO/Co_{13}	1.90	2.93	-	-	H_2/Co_{13}	-	1.58	1.58	-
CO/Co_{55}	1.96	2.92	-	-	H_2/Co_{55}	-	1.65	1.65	-
CO/Co_{147}	1.74	2.91	-	-	H_2/Co_{147}	-	1.59	1.59	-
CO/Co(0001)	1.96	2.91	-	-	H_2/Co(0001)	-	1.58	1.58	-
CO/Ni_{13}	1.84	2.86	-	-	H_2/Ni_{13}	-	1.58	1.58	-
CO/Ni_{55}	1.94	2.90	-	-	H_2/Ni_{55}	-	1.57	1.57	-
CO/Ni_{147}	1.90	2.88	-	-	H_2/Ni_{147}	-	1.58	1.57	-
CO/Ni(111)	1.94	2.88	-	-	H_2/Ni(111)	-	1.58	1.57	-
CO/Cu_{13}	1.81	2.96	-	-	H_2/Cu_{13}	-	1.72	1.71	-
CO/Cu_{55}	2.04	2.97	-	-	H_2/Cu_{55}	-	1.77	1.78	-
CO/Cu_{147}	1.84	2.99	-	-	H_2/Cu_{147}	-	1.82	1.82	-
CO/Cu(111)	2.03	2.97	-	-	H_2/Cu(111)	-	3.41	2.84	-

Table S19: Percent variations of molecular bond lengths (ΔO-C, ΔH-H and ΔH-O) and angles (ΔOCO and ΔHOH), with respect to the gas-phase molecule, for the lowest energy structures of CO_2, CO, H_2O and H_2 interacting with Co_n, Ni_n, Cu_n (n = 13, 55, 147) and Co(0001), Ni(111) and Cu(111).

Structure	ΔO1-C (%)	ΔO2-C (%)	ΔOCO (%)	Structure	ΔH1-H2 (%)	ΔH1-O (%)	ΔH2-O (%)	ΔHOH (%)
CO_2/Co_{13}	7.12	7.11	−23.70	H_2O/Co_{13}	-	0.58	0.61	1.00
CO_2/Co_{55}	5.79	7.04	−22.78	H_2O/Co_{55}	-	0.54	0.66	0.71
CO_2/Co_{147}	6.07	7.26	−23.53	H_2O/Co_{147}	-	0.69	0.66	0.77
CO_2/Co(0001)	5.51	5.81	−22.42	H_2O/Co(0001)	-	0.86	0.84	0.65
CO_2/Ni_{13}	6.81	6.79	−22.87	H_2O/Ni_{13}	-	0.53	0.63	0.82
CO_2/Ni_{55}	3.44	10.28	−25.69	H_2O/Ni_{55}	-	0.68	0.58	0.87
CO_2/Ni_{147}	3.59	9.42	−24.96	H_2O/Ni_{147}	-	0.42	0.49	1.55
CO_2/Ni(111)	8.51	3.19	−24.01	H_2O/Ni(111)	-	0.97	0.94	0.37
CO_2/Cu_{13}	0.59	−0.39	−0.12	H_2O/Cu_{13}	-	0.41	0.50	0.79
CO_2/Cu_{55}	0.42	−0.25	−0.32	H_2O/Cu_{55}	-	0.30	0.35	1.40
CO_2/Cu_{147}	0.07	0.05	−0.35	H_2O/Cu_{147}	-	0.42	0.41	1.00
CO_2/Cu(111)	0.04	0.05	−0.21	H_2O/Cu(111)	-	0.74	0.74	−0.29
CO/Co_{13}	4.13	-	-	H_2/Co_{13}	25.67	-	-	-
CO/Co_{55}	5.75	-	-	H_2/Co_{55}	16.90	-	-	-
CO/Co_{147}	2.82	-	-	H_2/Co_{147}	22.21	-	-	-
CO/Co(0001)	4.76	-	-	H_2/Co(0001)	23.17	-	-	-
CO/Ni_{13}	4.14	-	-	H_2/Ni_{13}	16.49	-	-	-
CO/Ni_{55}	4.96	-	-	H_2/Ni_{55}	19.68	-	-	-
CO/Ni_{147}	4.98	-	-	H_2/Ni_{147}	18.39	-	-	-
CO/Ni(111)	4.41	-	-	H_2/Ni(111)	19.06	-	-	-
CO/Cu_{13}	1.17	-	-	H_2/Cu_{13}	7.73	-	-	-
CO/Cu_{55}	4.13	-	-	H_2/Cu_{55}	6.13	-	-	-
CO/Cu_{147}	0.89	-	-	H_2/Cu_{147}	4.91	-	-	-
CO/Cu(111)	3.40	-	-	H_2/Cu(111)	0.74	-	-	-

X Additional Results from Bader Charge Analysis

Table S20 shows results for the effective Bader charge analysis for the lowest energy adsorption configurations in comparison to the respective gas-phase molecules. For C, O and H atoms, we show the average charges ($\overline{Q}$), while for the adsorbed molecules, the atomic charges were summed (Q^{Mol}), corresponding to the charge transferred between adsorbate and substrate.

Table S20: Average effective Bader charges, ($\overline{Q}$, in e) for each atom of the molecules ($\overline{Q}^{\mathbf{C}}$, $\overline{Q}^{\mathbf{O}}$, $\overline{Q}^{\mathbf{H}}$), total effective charge of the adsorbed molecule ($Q^{\mathbf{Mol}}$) and of the transition metal atom closer to the molecule ($Q^{\mathbf{TM}}$) corresponding to the lowest energy structures of CO_2, CO, H_2O and H_2 adsorbed on Co_n, Ni_n, Cu_n (n = 13, 55, 147) particles and on Co(0001), Ni(111) and Cu(111) surfaces.

CO_2/substrate	$\overline{Q}^{\mathrm{C}}$	$\overline{Q}^{\mathrm{O}}$	Q^{TM}	Q^{Mol}	Structure	$\overline{Q}^{\mathrm{O}}$	$\overline{Q}^{\mathrm{H}}$	Q^{TM}	Q^{Mol}
CO_2 gas	2.17	−1.09	-	0.00	H_2O gas	−1.18	0.59	-	0.00
CO_2/Co_{13}	1.39	−1.06	0.29	−0.74	H_2O/Co_{13}	−1.21	0.63	0.11	0.04
CO_2/Co_{55}	1.46	−1.07	0.27	−0.68	H_2O/Co_{55}	−1.22	0.64	0.08	0.04
CO_2/Co_{147}	1.44	−1.06	0.23	−0.68	H_2O/Co_{147}	−1.21	0.63	0.09	0.05
CO_2/Co(0001)	1.51	−1.06	0.11	−0.61	H_2O/Co(0001)	−1.22	0.61	0.12	0.01
CO_2/Ni_{13}	1.45	−1.05	0.24	−0.64	H_2O/Ni_{13}	−1.21	0.63	0.13	0.06
CO_2/Ni_{55}	1.53	−1.04	0.22	−0.56	H_2O/Ni_{55}	−1.22	0.64	0.08	0.06
CO_2/Ni_{147}	1.55	−1.04	0.19	−0.54	H_2O/Ni_{147}	−1.19	0.63	0.05	0.07
CO_2/Ni(111)	1.59	−1.04	0.21	−0.48	H_2O/Ni(111)	−1.18	0.60	0.13	0.03
CO_2/Cu_{13}	2.18	−1.10	0.13	−0.02	H_2O/Cu_{13}	−1.20	0.62	0.18	0.05
CO_2/Cu_{55}	2.17	−1.10	0.01	−0.04	H_2O/Cu_{55}	−1.20	0.62	0.08	0.04
CO_2/Cu_{147}	2.16	−1.11	−0.07	−0.05	H_2O/Cu_{147}	−1.21	0.63	0.10	0.04
CO_2/Cu(111)	2.16	−1.10	−0.01	−0.05	H_2O/Cu(111)	−1.20	0.61	0.11	0.01
CO gas	1.14	−1.14	-	0.00	H_2 gas	-	0.00	-	0.00
CO/Co_{13}	0.65	−1.07	0.17	−0.43	H_2/Co_{13}	-	−0.06	0.04	−0.13
CO/Co_{55}	0.50	−1.06	0.16	−0.56	H_2/Co_{55}	-	−0.04	0.04	−0.09
CO/Co_{147}	0.78	−1.11	0.05	−0.33	H_2/Co_{147}	-	−0.05	−0.02	−0.10
CO/Co(0001)	0.56	−1.02	0.07	−0.45	H_2/Co(0001)	-	−0.03	−0.01	−0.06
CO/Ni_{13}	0.70	−1.06	0.15	−0.36	H_2/Ni_{13}	-	−0.03	0.03	−0.06
CO/Ni_{55}	0.61	−1.03	0.13	−0.43	H_2/Ni_{55}	-	−0.02	0.05	−0.04
CO/Ni_{147}	0.60	−1.02	0.12	−0.42	H_2/Ni_{147}	-	−0.02	0.02	−0.04
CO/Ni(111)	0.66	−1.01	0.08	−0.36	H_2/Ni(111)	-	0.00	−0.01	−0.01
CO/Cu_{13}	0.95	−1.09	0.22	−0.14	H_2/Cu_{13}	-	0.00	0.13	0.00
CO/Cu_{55}	0.63	−1.05	0.13	−0.42	H_2/Cu_{55}	-	0.00	0.03	0.01
CO/Cu_{147}	0.97	−1.08	0.14	−0.11	H_2/Cu_{147}	-	0.01	0.04	0.01
CO/Cu(111)	0.67	−1.01	0.10	−0.35	H_2/Cu(111)	-	−0.01	−0.01	−0.02

XI Adsorption Properties for the Lowest Energy Configurations

In the main article, we compared several adsorption properties using the same scale for each property to identify the systems that were most susceptible to size effects. Here, in Figure S20, we show the same adsorption properties, each on its own scale, to convey the fine details of each case.

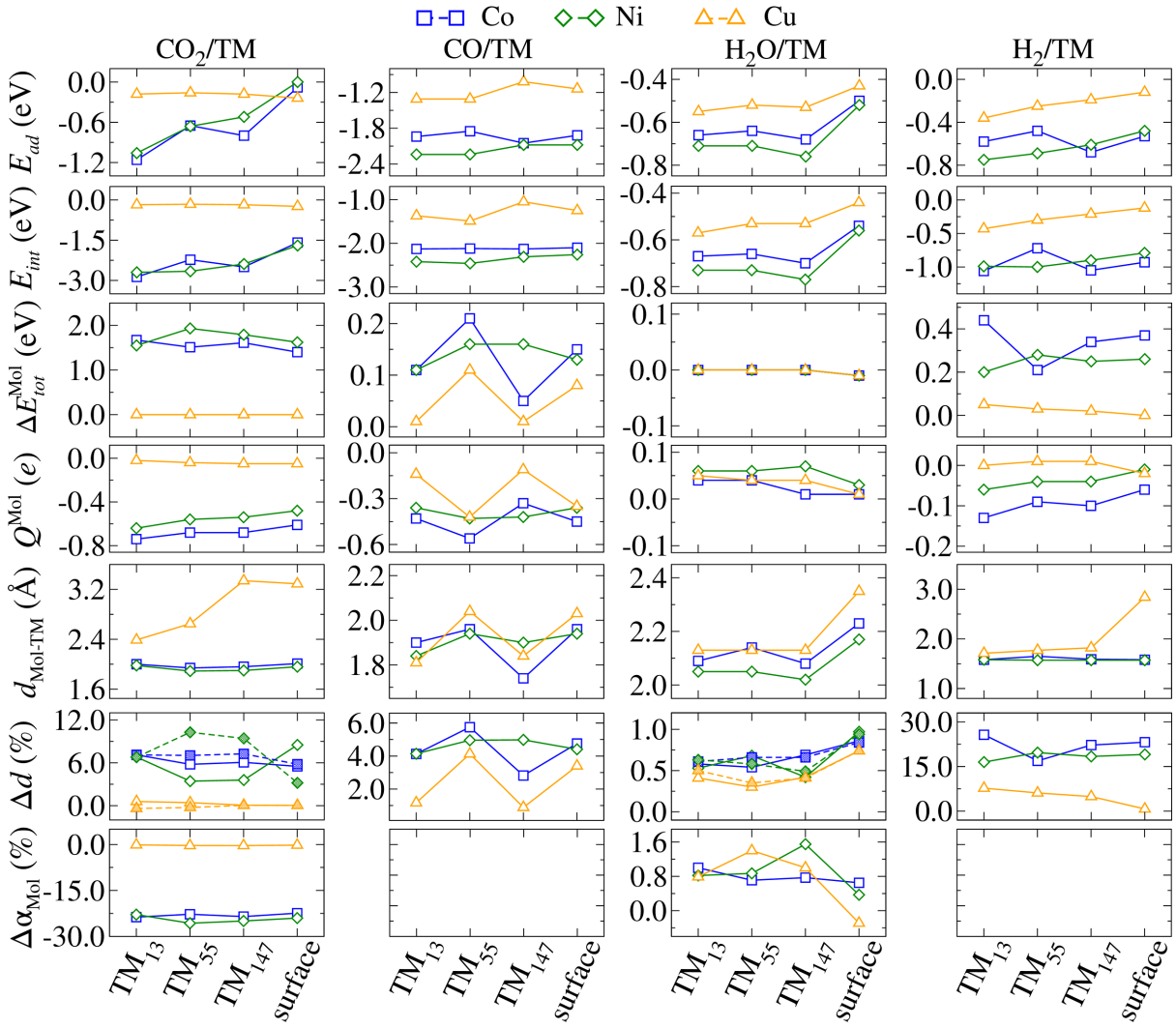

Figure S20: Adsorption properties as a function of substrate size for the lowest energy adsorption configurations for CO_2, CO, H_2O and H_2 interacting with Co, Ni and Cu substrates. The lines connect the data to guide the reader. From the top: adsorption energy, E_{ad}, interaction energy, E_{int}, energy difference between the adsorbed and gas-phase molecules, $\Delta E_{tot}^{\mathrm{Mol}}$, total effective charge of the adsorbed molecule, Q^{Mol}, shortest distance between an atom of the adsorbate and a TM, $d_{\mathrm{Mol\text{-}TM}}$, percent variation of the bond lengths of the molecules due to adsorption (open and shaded symbols distinguish more than one of the same type of bond (C−O or H−O), respectively), Δd, and percent variation of the OCO and HOH angles, $\Delta\alpha_{\mathrm{Mol}}$.

XII Cartesian Atomic Coordinates and POSCAR files for the Lowest Energy Adsorption Structures

In this section we provide coordinates for the most stable adsorption structures. Cartesian atomic coordinates are provided for the systems containing the molecules adsorbed on the clusters, while the POSCAR files are provided for systems containing the molecules adsorbed on the surfaces.

A 13-atom Substrates

CO_2/Co_{13}

C 0.5228802406082346 2.5365915953702807 1.5174546302557346
O 1.2250595862240645 2.3247060120549730 2.5371338263280663
O -0.1160826141692971 3.4963939014794754 1.0194241362780687
Co -0.2589404040191389 1.8881482536692393 -0.2253118579659841
Co -1.1198966989697643 -2.7130775483768765 0.6493649258281309
Co -0.7172084697068292 -0.4128134664645169 0.3010263832092264
Co 0.8141066101384277 -2.0734749100284411 -0.4532139679243485
Co 1.2279160489389975 0.2207454490883796 -0.9039461384636027
Co -2.4300701547777770 -1.5526102634826524 -0.8559869393477371
Co -1.9872792200430032 0.7991687217533714 -1.3206200820093628
Co 0.7276611511997012 -1.6050538656697635 1.7915444493413801
Co 1.1496949363455580 0.6383078270255813 1.3939490740986216
Co -0.5633726662562387 -0.8545637500935224 -2.0332914949473846
Co -0.1173502248429335 1.3958677511258164 -2.4501761737638006
Co -0.9244516763052067 -3.1076974854881634 -1.5936565869002450
Co 2.5673335556352050 -0.9806382219631795 0.6263058159832369

CO/Co_{13}

C -3.0849902456277984 0.0064983498555227 -0.6872044377648664
O -4.2176347624865880 0.0097139601875551 -1.0365227178609089
Co 0.1080624870246364 2.3978659326429876 0.8257251885272657
Co 0.0926767367796603 -2.3942132454641309 0.8354186386894261
Co 0.1016562796692514 0.0023322045900909 0.9429072077250359
Co 1.6609735957538700 -1.2183827995042418 -0.3550162920103802
Co 1.6688486812742380 1.2073106821298996 -0.3602848491724061
Co -1.6425449504133578 -1.1421971777113538 -0.2388693785445824
Co -1.6358373754754236 1.1518836623226048 -0.2449567695231466
Co 1.9003021416452075 -1.1821985316129269 1.9336658816903978
Co 1.9084394104269902 1.1780406091392626 1.9287369854559515
Co -0.0653619923041245 -0.0028622486007646 -1.4567730017171427
Co -0.0787852505121319 2.4000808640293756 -1.3911760622919374
Co -0.0927281480935190 -2.4045408002608339 -1.3818041867681259
Co 3.3769233923390889 -0.0093314617430462 0.6861537935654197

H_2O/Co_{13}

O 1.3862118004712956 1.6579041028071624 -3.1278379173936437
H 1.3135206820361691 0.8079829992151095 -3.6033429012992673
H 2.2989214065331409 1.6789436262390718 -2.7800641739628289
Co -0.4959205272498334 2.2080479789369121 0.5876471980276209
Co -1.5869011738662862 -2.2900890179207392 1.7524573998462123
Co -1.1045257762050762 -0.0015913872058363 1.2582487139942122
Co 0.5187547579691355 -1.7504142873785449 1.0170450945795872
Co 1.0659191329978392 0.5187185265640644 0.4426367939693819
Co -2.5509104226216128 -1.2997508604406798 -0.1277828117088654
Co -1.9812066817502247 1.0102920256900678 -0.7185263850701818
Co -0.0221579454381192 -1.0262362097100579 3.1260295086625152
Co 0.5133001571047947 1.1741753018527386 2.5651082068759190
Co -0.4793936503672102 -0.7284500873203930 -0.9157850285119152
Co 0.1028859051029697 1.4909689840543845 -1.4833093914803408
Co -1.0000672547195697 -2.9445398175841899 -0.3226903907013013
Co 2.0215695900025876 -0.5059618777990698 2.3301660841728951

H_2/Co_{13}

H -2.3317166664699038 2.0062514321411591 -1.7094341792190932
H -2.7098866854085855 1.1525012739685023 -1.5604933774760661
Co 0.0424447076629824 2.1926116201788655 0.8809191286228839
Co -0.5992203672907943 -2.5470210442143886 0.6461093769021091
Co -0.2924207325090339 -0.2059536534186915 0.8994314990955803
Co 1.4124432498590360 -1.6144852150605773 0.0660045103753708
Co 1.7305345870878146 0.8087228016012379 0.1951027104423436
Co -1.7050194093428968 -1.0953686998674719 -0.8106205854795996
Co -1.3880059422053643 1.2480050173294430 -0.7009197738841828
Co 0.9216451051215395 -1.6018612367240406 2.3098442879803298
Co 1.2160715057419640 0.7257918554429784 2.4412070936957568
Co 0.2765270524110791 -0.1512577907775839 -1.4444087795248923
Co 0.6212487054912301 2.1876085603775826 -1.2975721192569396
Co -0.0506067849158305 -2.4909097516814276 -1.5401614906762835
Co 2.8559616747667644 -0.6146351692955879 1.6249916984026829

CO_2/Ni_{13}

C -1.4257416768808440 -2.3982110370863201 -0.9186601505347268
O -0.6637768957914403 -3.1345105129214450 -1.5865455383519487
O -2.6148022770101678 -2.3813853742195694 -0.5262481836537701
Ni 0.2880592592574971 2.8366561474262038 -1.1996688595315061
Ni 0.2158016132983398 0.5254730316238816 -1.1810689913571435
Ni 0.4117250302094255 -1.7120423424736591 -0.6382673663087600
Ni 2.2988566425823063 1.6166698895822069 -1.3106542493315840
Ni 2.0773460806303214 -0.2694545289793031 0.2935493688324798
Ni -1.2252040121328178 1.7047123895186540 0.2572577488133377
Ni -1.7672116617488853 -0.5715582221031572 -0.2366955507612899
Ni 1.1168090760454852 1.8807564355312318 0.7192367377713184

Ni -0.3331073814158259 1.6904609584503656 2.5764924771469211
Ni -2.1857635154494206 0.4811501413984249 1.9469733653478374
Ni 1.7318791810781142 0.5639514560849452 2.5011118018957368
Ni -0.0562269194846265 -0.2577167508976790 1.2848543311364937
Ni 2.1313574568125384 -0.5749516809347814 -1.9816669411133956

CO/Ni_{13}

C -2.2106242378621417 0.4592726301602504 2.5963424977826426
O -2.9564280179237974 0.8291086661068884 3.4402604782019335
Ni 0.2401667741210115 2.2831247720949315 -1.6447879080551406
Ni 0.2500117651119751 -0.0226588640781552 -1.9131499709160658
Ni 0.5999393854018734 -2.2444677164207811 -1.4843076064612835
Ni 2.2726618394097686 1.0925992356044392 -1.8464547538910356
Ni 2.2304861338974318 -0.8119017894033173 -0.4372182570232550
Ni -1.1833386417591705 0.9387119587629303 -0.3522215309512974
Ni -1.5935225278485030 -1.3042608608699788 -1.1670468163769485
Ni 1.0919691765545883 1.2064392741326071 0.2262190924832022
Ni -0.4798108196736736 0.6387324793172059 2.0058437797731514
Ni -2.2265777320445741 -0.5847038260042799 1.0678215022299111
Ni 1.7438695157402619 -0.3258182202901280 1.7942351329235720
Ni 0.0334920363424909 -1.0706603114529354 0.4545307828295211
Ni 2.1877053505324584 -1.0835174276596768 -2.7400664225489075

H_2O/Ni_{13}

O -0.4155436529275734 2.1148477615747314 2.9461930441293149
H -1.1541416761845578 2.6619213424671768 2.6175663429795337
H 0.3915480685928787 2.5552135813871009 2.6153580870856064
Ni 0.3268181999914223 1.7674872332894929 -1.8864245020632042
Ni -0.0453643312947115 -0.5118084612853726 -2.0781158670686439
Ni -0.1869844845169886 -2.7500332693614586 -1.5929441454853288
Ni 2.1259876185709734 0.2129425677211502 -2.0964607606449004
Ni 1.6873593341228457 -1.6421844591482617 -0.6282752748452625
Ni -1.2932360299337895 0.7558881521640191 -0.5016096451727536
Ni -2.0831776067194987 -1.3823319891665766 -1.2180355542177601
Ni 1.0415011353984185 0.5879983335801551 -0.0354195608170782
Ni -0.4868309762051380 0.4233375782143975 1.7935908845607029
Ni -2.5324744513922406 -0.4789936449282786 0.9939052863585784
Ni 1.4545367472874662 -0.9945484697347220 1.6042091308961437
Ni -0.4636901427243410 -1.3926896089514675 0.3843864838618805
Ni 1.6336922479348339 -1.9270466478220862 -2.9179239495568288

H_2/Ni_{13}

H 0.0195020141552253 1.9430082493200942 3.0292398939628202
H -0.8448388972637629 2.0417371846740942 2.9221471486644930
Ni 0.1799372300259809 1.8816902991625319 -1.9548755130104194
Ni -0.2018023115522246 -0.4093523561073429 -1.8537945551422457

Ni -0.1831104522754286 -2.5983378227636775 -1.2010285429427396
Ni 1.9832615595804375 0.3499513574151960 -2.1411662781997425
Ni 1.7092711229283435 -1.3467114992952975 -0.4354328086734487
Ni -1.3330612490786027 1.0240435880176060 -0.3609951665642868
Ni -2.1468948452991397 -1.2116850972888580 -0.7880081197632620
Ni 1.0287343529303776 0.9247300342755462 -0.0456687789506542
Ni -0.4006424137893079 0.9190014811278626 1.9002684780888330
Ni -2.4725999915651817 -0.1463018439530881 1.2638198700298049
Ni 1.5715330879951332 -0.4467729043422217 1.7099424455984087
Ni -0.3850008898641651 -1.0533086609975282 0.6388479220396555
Ni 1.4757116830723154 -1.8716920092449172 -2.6832959951372164

CO_2/Cu_{13}

C -1.5297255415713815 3.0837888325858747 -1.4127929916977513
O -0.7317515917127801 2.6182237463895679 -2.1461948060218905
O -2.3213414798627960 3.5473935726654187 -0.6898874919593203
Cu 0.0087701792741504 -3.3153242475857421 -0.9160913904956038
Cu -2.2651019240428392 -1.1087677240585589 1.4959765883504070
Cu 0.5762297361109616 -1.5457525030046424 -2.5343801343188321
Cu 0.9349480593129313 1.3834520529443142 2.6077021635960929
Cu 1.5767567742492630 -0.8487128728428315 2.0623417350200324
Cu -0.5555452011963533 -0.5719974770887502 3.1699140472578975
Cu 2.5074069750640873 -0.0418401221331164 -1.8762056965427922
Cu 0.2586674815811576 0.5766708280185997 -1.3977800738757031
Cu 1.9575499311718416 0.9090710324854359 0.3730283040103808
Cu 1.3519268216402494 -1.3970530212941055 -0.2819818197958404
Cu -0.3686506692870504 0.2842814574201549 0.9398157311316100
Cu -0.2192106103762379 -2.2986698676836776 1.3392963808164546
Cu -1.1809289403552024 -1.2747636868179411 -0.7327605454751398

CO/Cu_{13}

C 0.1109251119584219 1.9695040314421490 -2.7196284371933306
O -0.1053094420247948 2.8201179819163285 -3.4651017494978449
Cu -0.7468540489005316 -3.0629109037600228 -0.2841182455668687
Cu -2.7228935316228764 -0.0209544922115840 1.3450243656513974
Cu 0.2847514835210195 -1.7681562349643904 -2.1387626231251984
Cu 0.7898795618840347 1.9627537036487324 2.4282559398944841
Cu 1.0106306066721069 -0.4198823471447150 2.3639934720573796
Cu -1.1045290197739057 0.4702950641483433 3.1123810521941708
Cu 2.4199900811455555 -0.5634141836027347 -1.5167209714698002
Cu 0.3436984731363822 0.6260563494717424 -1.5227426041488077
Cu 1.8885321857278334 0.9050064341748048 0.4402049010131728
Cu 0.8540574879969619 -1.2957568556223293 0.1199072749214583
Cu -0.5379783062647637 0.8295310291043294 0.8058481864810065
Cu -0.9818608476921621 -1.6184613603241544 1.6890104598892910
Cu -1.5030397957632815 -0.8337282162764987 -0.6575510211005107

H_2O/Cu_{13}

O 2.2857701673945421 -0.7682684296439859 2.2643361057761364
H 2.9659209673799367 -0.0698153055695785 2.2738223125996933
H 2.5749102979344043 -1.3917974899332488 1.5716198074652095
Cu -1.0551310387858714 -2.4474873723357176 -1.6037251217860975
Cu -3.3431626092352831 0.0632073140286568 0.4829748685452824
Cu -0.2257150011766063 -0.8444391667751929 -3.2603652199904225
Cu -0.0253124076905153 2.3557393835166680 1.7296239529025521
Cu 0.5133244463184050 0.0463815611945925 1.4206554926629318
Cu -1.7174808622425786 0.5552716306661851 2.2720929666174356
Cu 1.7567654311500858 0.5259348052542265 -2.5229830240238620
Cu -0.4753152945907180 1.3368604658348879 -2.2510578245528050
Cu 1.1231798960200179 1.6646162845690291 -0.3861229743872734
Cu 0.3893961491926723 -0.6295349305317968 -0.9486981932401877
Cu -1.2562522543512900 1.2108705864287803 0.0343283194773409
Cu -1.3866702892682647 -1.2795269793440125 0.5657868141805062
Cu -2.1242275980489369 -0.3280123573594931 -1.6422882822464429

H_2/Cu_{13}

H 0.9317094432023127 1.9118777834671019 -2.6488465383575202
H 0.2316652129880410 2.1884876043296964 -2.3480708465948510
Cu -1.0564614886926220 -2.8444133767462731 -0.6426606057510654
Cu -2.8229652980318569 0.2481797233036786 1.1071379837190918
Cu 0.2464189519276889 -1.5592520105851571 -2.3074793012524966
Cu 0.7993649080161909 1.7800152741181186 2.5542933501071783
Cu 0.7698576972440092 -0.5949876833001988 2.3177465494329761
Cu -1.2893669232296938 0.4665274257064023 2.9994549528143901
Cu 2.4411569101059456 -0.6191149123480533 -1.4669419609528935
Cu 0.4820453372146067 0.7370042560429813 -1.4697901864800391
Cu 1.9266921001640420 0.7404629928220352 0.5723593684917626
Cu 0.6974664350311639 -1.3107882458832987 0.0145662962696901
Cu -0.5283559799887776 0.9147787780254180 0.7677703619286956
Cu -1.2763281472490000 -1.5254458054435838 1.4274293402486613
Cu -1.5528991587020506 -0.5333318035088674 -0.8769687636235791

B 55-atom Substrates

CO_2/Co_{55}

C -2.1079227288784361 4.9207731429028660 -1.5073685809188826
O -1.6982394609097291 5.0075957745165587 -2.6750328307774249
O -2.7714870308103916 5.5967301214350096 -0.6837889384901239
Co 0.1166490053937191 -0.2795010492857896 0.0910743782064127
Co 0.1551460132545535 0.9456080358672850 2.1023153522204026
Co 0.1783241223122397 0.9820840501233857 -1.9184639006270034
Co 0.0507854578269243 -1.5287100283324209 2.0937663975047096

Co 0.0835589521424452 -1.5066913291488027 -1.9214908315483641
Co 1.4507827397380701 1.6664759368467357 0.1050430193688665
Co -1.0217370923596536 1.7634354486398887 0.0635182658892934
Co 1.2713836962436771 -2.3323282108636696 0.0914812382779275
Co -1.2043685736943672 -2.2353677981472773 0.0763378239077759
Co 2.1114690165558532 -0.3693096531993396 1.3494023639475794
Co 2.1275767350901282 -0.3572277873442308 -1.1372685936899731
Co -1.8954216222292164 -0.2081029465272814 1.3154594557804067
Co -1.8757051237201017 -0.2032179326844498 -1.1706908867234114
Co -3.8442244510066752 -0.1172625919336069 -2.4071313255173021
Co 0.1888863604924994 2.1609553973306910 4.0858149269560124
Co 0.2793671760501427 2.1644759505633662 -3.9166327051821299
Co -0.0167331489444482 -2.7561657616364981 4.0675377390598966
Co 0.0428635571736924 -2.7231088691156438 -3.9008841989157657
Co 2.7570814290777439 3.5911287977402191 0.1260769450914123
Co -2.1694181397820831 3.8073259341674932 0.0780873150297447
Co 2.4054247187750457 -4.3516824033565769 0.1010300821403087
Co -2.5088802166015829 -4.1583623052623526 0.0583703762193341
Co 4.0774909909889328 -0.4533571174876540 2.5861946516491114
Co 4.1150878970040745 -0.4327388654146127 -2.3388543598870362
Co -3.8828994256105998 -0.1265938673147395 2.5215183423833718
Co 0.3216210355616303 3.7151629686845453 0.1183132799770772
Co -0.0518297329981312 -4.2931819255909254 0.0788383466881830
Co -3.8889235934594302 -0.1134055204414547 0.0562621239470020
Co 4.1296041859799857 -0.4517006276526676 0.1234417285986728
Co 0.1506532066350810 -0.2675998560375678 -3.9237514918861791
Co 0.0861456351147832 -0.2959804542381123 4.1059007622143850
Co 1.2089704062336133 -3.5878838126987973 2.0958314732237584
Co -1.2685086336029223 -3.4893546924610095 2.0771570955497842
Co 1.2364628396087083 -3.5660317101387280 -1.9216617673788365
Co -1.2376372818755232 -3.4718708840392241 -1.9357818974100238
Co 3.2880366486674775 -2.4129950777191023 -1.1351946015131584
Co 3.2701003479729498 -2.4242950832799868 1.3529668523762364
Co -3.2009721619424689 -2.1559236152593608 -1.1835431230797326
Co -3.2198005349573608 -2.1565823304496021 1.3038095998802663
Co 1.5119856016480302 2.9158178029601602 -1.8987599599711060
Co 1.4749275791821845 2.9023166101665465 2.1169332567374100
Co -0.9801677548709544 3.0949385840306407 -1.9873187374221561
Co -1.0106661321893720 2.9978018153913677 2.1059099594835455
Co -1.8064956998177339 1.0543227897694991 -3.1698053737497061
Co 2.1994110166584488 0.8829471384018127 -3.1386615121934982
Co -1.9150807542461443 -1.4299811938219713 -3.1815914550271867
Co 2.1010590476996600 -1.5967581167591216 -3.1501267772149038
Co -3.0457218562569945 1.8539108050742108 1.3241559494087880
Co -3.0370395351996557 1.8316131886509248 -1.1727533450831362
Co -1.9664975018493238 -1.4509223633332369 3.3169799466670162
Co 2.0496687993878684 -1.6217568296649298 3.3509311127991412
Co 2.1447161434631457 0.8613813746799038 3.3635097569837864
Co -1.8659635913581845 1.0364941730019805 3.3234423836785441

Co 3.4632715428201286 1.5925161651864388 -1.1187544224141874
Co 3.4438298744180540 1.5801406045092150 1.3678993147750664

CO/Co_{55}

C -4.6076543967397328 -1.7974374589063038 -0.0054215693815394
O -5.7273501283501203 -2.2391698550804100 -0.0124496527230331
Co 0.1745871198013119 0.0689261663334256 0.0003808296405343
Co 0.1945670998388690 1.3110077482732037 1.9966657656464206
Co 0.1944452970621323 1.3111141069512462 -1.9958117005299760
Co 0.1767488553067361 -1.1703797221004979 2.0076261891225062
Co 0.1769044780359396 -1.1705157173622835 -2.0065259351549560
Co 1.4235347734056634 2.0825308478206899 0.0004815769539248
Co -1.0652879179451100 2.0753013067957391 0.0007633507533522
Co 1.4308838917724467 -1.9183308912266808 0.0002748248576998
Co -1.0740582750286112 -1.9385246464525967 0.0003676828070271
Co 2.1921253120512434 0.0734612833873850 1.2417337981201935
Co 2.1925323129886869 0.0737607249951021 -1.2411413488407086
Co -1.8417846770205386 0.0601757498204284 1.2354795661420148
Co -1.8414899238144666 0.0612965831929880 -1.2352667805246944
Co -3.7717190850460218 0.1063152290029966 -2.5074704618362658
Co 0.1952474028824681 2.5376924003093722 3.9810393020631976
Co 0.1949890594739342 2.5382323666947424 -3.9798743139149648
Co 0.2023609737753770 -2.3812523381463722 3.9811392926612124
Co 0.2020562380933956 -2.3814329204316325 -3.9798931882589601
Co 2.6526267170216151 4.0555484421422916 0.0008134673429787
Co -2.2638162645557167 4.0557948971709772 0.0013274694846408
Co 2.6599838257667163 -3.9014260354893922 0.0002492617402105
Co -2.2160793556451304 -3.9500529974121950 0.0003536933964163
Co 4.1736505937131536 0.0805076233250851 2.4566710217431540
Co 4.1738935544774565 0.0815444112320970 -2.4568382150485775
Co -3.7724026395048855 0.1052535704187235 2.5070570976954292
Co 0.1804024791521620 4.0888724033511687 0.0007893154468585
Co 0.1855763684616200 -3.9381967629492141 0.0010358109143746
Co -3.8760786879535414 0.0466754877355889 -0.0003039945986707
Co 4.2047507495695093 0.0752695452701896 0.0004525265083768
Co 0.2001173619260736 0.0761640135703580 -4.0100575969708423
Co 0.2001838475030588 0.0763278090059482 4.0112042874362386
Co 1.4402043843709373 -3.1634805372157415 2.0083805087805091
Co -1.0462475584642774 -3.1834480661662243 2.0054081704176987
Co 1.4402279625636625 -3.1640044111633161 -2.0072757678884630
Co -1.0447697102492428 -3.1845215674815273 -2.0041014353290825
Co 3.4404358686834153 -1.9302266658030580 -1.2416314611714911
Co 3.4400726294028741 -1.9306882286067524 1.2415274792369990
Co -3.0968002164340933 -1.9585981306892355 -1.2490714739594435
Co -3.1002757348915648 -1.9588229501619836 1.2453086707591059
Co 1.4284393581324411 3.3254812938672513 -2.0064546144988862
Co 1.4284855223568884 3.3255201635256020 2.0076426789438648
Co -1.0443105724897366 3.3229237231168325 -2.0011652401642790

Co -1.0441410657163079 3.3227723776306171 2.0030963412696350
Co -1.8239585150849054 1.3103966947765724 -3.2425147289325187
Co 2.1973634899395513 1.3167717032882493 -3.2481717067598517
Co -1.8194583301124039 -1.1598090204798541 -3.2554400239274770
Co 2.1916880999459374 -1.1676588999566391 -3.2487629547896395
Co -3.0637120364437025 2.0769155548015705 1.2481856731244036
Co -3.0636551891649657 2.0775989420512486 -1.2473682630195357
Co -1.8204360017158352 -1.1609282936969463 3.2552969850916806
Co 2.1917655210282296 -1.1675221742763531 3.2497196365531105
Co 2.1975638431274018 1.3166351029371042 3.2489124819905464
Co -1.8240354672047097 1.3093433361097440 3.2427145348900757
Co 3.4357637294405783 2.0852889018789362 -1.2416832037463812
Co 3.4353430285041333 2.0850077804717406 1.2425963404358378

H_2O/Co_{55}

O -0.4807207730966358 -2.7069530257612278 5.8283983330168683
H 0.0598763926857840 -2.0795993764092882 6.3454396674204308
H -1.4038020801366367 -2.4189750990201895 5.9707463401602938
Co 0.0338219239731024 0.1276707713142289 -0.3250431775085350
Co -0.0127074120484864 1.4471019890488608 1.6293580536109560
Co 0.1127039733411924 1.2970479610588990 -2.3788216482514177
Co -0.0457515714960610 -1.0425620285624488 1.7274990568588313
Co 0.0796394896750208 -1.1833549800392025 -2.2921666478479259
Co 1.3020503782418680 2.1215989693021906 -0.3617621071239432
Co -1.1800223790744342 2.1526132319940410 -0.4394968846807714
Co 1.2487960749982792 -1.8913488292769027 -0.2255640708422004
Co -1.2353059235290065 -1.8604137533038034 -0.3016470526339776
Co 2.0033439050357829 0.1533397025273589 0.9703192517404853
Co 2.0797904966894212 0.0592681414067924 -1.5071557488747653
Co -2.0134437873103672 0.2040309316317162 0.8431479990818620
Co -1.9354532032930067 0.1085832753183709 -1.6334655971485970
Co -3.8708268999549200 0.0945592518620087 -2.9160684682901992
Co -0.0566483497932206 2.7304434666299469 3.5648118552955661
Co 0.1890181618588159 2.4486486222723616 -4.3924312930272409
Co -0.1285572191131443 -2.2063276497199653 3.7793416562947439
Co 0.1227772249290101 -2.4683680314557468 -4.2261913845911634
Co 2.5472527724779783 4.0811901219676754 -0.3968394597685800
Co -2.3723366650877713 4.1417190773778607 -0.5500350754380960
Co 2.4415524502546995 -3.8807071216406146 -0.1137652811197052
Co -2.4809476636153205 -3.8202490103443343 -0.2661584387886204
Co 3.9370598851757586 0.1678019850799680 2.2561481038055184
Co 4.0904480904359524 -0.0025277205308553 -2.6670346772997475
Co -4.0224350125023625 0.2653820219353374 2.0074337825489530
Co 0.0888392372294241 4.1459130963799158 -0.4727223737546580
Co -0.0201905005119247 -3.8823988745295899 -0.1885167630976636
Co -3.9834263303021475 0.1809222735985281 -0.4566525110781559
Co 4.0504127631715514 0.0834408103083571 -0.2048923316583107
Co 0.1571313437871707 -0.0126395567160015 -4.3427504195179765

Co -0.0926529262221622 0.2869660420017775 3.6780368354448476
Co 1.1672218939800427 -3.0578387806961254 1.8283197870655288
Co -1.3115516728090606 -3.0271037983227758 1.7536973485385667
Co 1.2948469808246990 -3.2057234268055530 -2.1856573808839275
Co -1.1910802174250801 -3.1743395910983279 -2.2625179564000812
Co 3.2958044630874297 -1.9622397590910456 -1.4003803149523817
Co 3.2150421758046761 -1.8710295146661389 1.0819199243550452
Co -3.2058130429273741 -1.8817166486504349 -1.6032378956164521
Co -3.2798230608302807 -1.7928548515955811 0.8789816474501180
Co 1.3782937572438352 3.2922627239175255 -2.4126500749553892
Co 1.2558256463477804 3.4371770618676947 1.6013413799952179
Co -1.1011857894778161 3.3219377560792052 -2.4908296550125031
Co -1.2263606441832811 3.4682764404267625 1.5231677252477911
Co -1.8574332545327619 1.2805504124928637 -3.6828290230558136
Co 2.1585647917522959 1.2303183086601226 -3.5568809080014963
Co -1.8919185223597168 -1.2022706680333035 -3.5980447108224465
Co 2.1264244940214803 -1.2511908945536641 -3.4722740746293392
Co -3.2274818652199415 2.2249235491029435 0.7365735538361560
Co -3.1511012646792125 2.1329757272426950 -1.7443679017016360
Co -2.0974657629855074 -0.9610202320536836 2.8913973269321103
Co 1.9206224011874433 -1.0168254040682128 3.0238699358579613
Co 1.9575700475522235 1.4618765894092600 2.9366887826808594
Co -2.0594519616912179 1.5126748950396534 2.8125087482189244
Co 3.3489392000281284 2.0550167615935773 -1.5406438212614466
Co 3.2722253404180108 2.1443466580965160 0.9403480341775361

H_2/Co_{55}

H -0.0445238887498992 -0.4822670698256210 5.4899749098920303
H -0.0742933096990358 0.3945313796088180 5.4810461260785566
Co 0.0019555106421380 0.0011920530314714 -0.2054291756826696
Co -0.0246349765202635 1.2052475383024328 1.8247800124843796
Co 0.0252787583978008 1.2690279381456280 -2.1988338782862806
Co -0.0207882458783895 -1.2631980553602775 1.7898809007466956
Co 0.0294948538098697 -1.2042512607563476 -2.2377745487152101
Co 1.2374501671944274 2.0155684396833307 -0.1539398261894418
Co -1.2387079113737343 2.0121026633382026 -0.1840253334022852
Co 1.2422688313547268 -2.0095691387296766 -0.2139074822297305
Co -1.2320704172666674 -2.0132914494573781 -0.2447956552485324
Co 1.9926237421925781 -0.0148516864992637 1.0664737919672460
Co 2.0299686691387486 0.0228791339652196 -1.4165601695518848
Co -2.0190616975672393 -0.0209806196046894 1.0163728934702052
Co -1.9953855647750436 0.0170471566152087 -1.4662187458815648
Co -3.9532984797963300 0.0329291459701907 -2.7109435700332245
Co -0.0513232832333016 2.4149350723518763 3.8059034920358501
Co 0.0475248037020465 2.5263598360949828 -4.1512357469980117
Co -0.0431282790737696 -2.5255872069487144 3.7345537213910842
Co 0.0555312662651281 -2.4004404187419848 -4.2276359795586673
Co 2.4591388079932428 3.9896037469461891 -0.1062307642286389

Co -2.4671632642176693 3.9829824264591216 -0.1677772762478192
Co 2.4703061080428159 -3.9804438908000628 -0.2276520123555310
Co -2.4539892337503879 -3.9876602911882517 -0.2890543436788346
Co 3.9533374539975474 -0.0315927407248658 2.3134722332672881
Co 4.0186834483030944 0.0446335030836532 -2.6127823793485110
Co -4.0106577471441165 -0.0425784389247038 2.2150955992503985
Co -0.0038278213539086 4.0236627849228386 -0.1364389689727708
Co 0.0080244107799929 -4.0208355654934786 -0.2587457996873972
Co -4.0176093895374576 -0.0045144245609404 -0.2495812664722614
Co 4.0215921537130930 0.0057338296523336 -0.1512365021793574
Co 0.0531816111407940 0.0642313193400535 -4.2272983850689156
Co -0.0491678522584581 -0.0567770125138892 3.8980347476573662
Co 1.2189719249718187 -3.2782175085085119 1.7774778513770439
Co -1.2548102204262006 -3.2818912988620212 1.7468204229587736
Co 1.2730766374034428 -3.2133004318043819 -2.2425483642713973
Co -1.2092775638025512 -3.2161325834500016 -2.2733237613020982
Co 3.2651769615952633 -1.9860542268163284 -1.4286904210372195
Co 3.2366542141663870 -2.0227811804637423 1.0541630696711550
Co -3.2247485084408134 -1.9935949274320379 -1.5078148003024763
Co -3.2565310243824777 -2.0322846127003906 0.9736236560202525
Co 1.2634869644311915 3.2806284792240765 -2.1425253855098854
Co 1.2097980731170388 3.2236747347936880 1.8745618801190347
Co -1.2194669387508223 3.2777176655071165 -2.1729046770725744
Co -1.2649575335596739 3.2205601833042472 1.8438759732635164
Co -1.9677459508987132 1.2868095526691847 -3.4588774982892172
Co 2.0492100340731763 1.2921683636794628 -3.4090818556967735
Co -1.9630306212291273 -1.1892677093847375 -3.4979531177011483
Co 2.0528655205983024 -1.1841696047541450 -3.4486047271915607
Co -3.2638222062727458 1.9866592890944983 1.0354778634119957
Co -3.2321132654269240 2.0251767957727482 -1.4452725029775768
Co -2.0451612189787589 -1.2944980679634088 3.0004381161130511
Co 1.9733013624115345 -1.2897146187107704 3.0507313725752452
Co 1.9700934641263181 1.2007074510682545 3.0866794092514418
Co -2.0504803077961493 1.1942102199404963 3.0373019690008509
Co 3.2611078670411282 2.0344691815777969 -1.3657552914029087
Co 3.2316731015569808 1.9952961568375001 1.1147102007689125

CO_2/Ni_{55}

C -2.1928249944497558 4.5320216392004911 2.4686069266867090
O -2.1380077832828057 4.9136129802898019 3.6186332810327309
O -2.8169693161218925 4.9505789010153354 1.4162152082129995
Ni 0.1311818578643957 -0.2604089291007395 -0.1304222852850327
Ni 0.1679784512828486 0.8898196946008147 1.8920732154630748
Ni 0.0856757296764618 1.0255492634706316 -2.0889960433272856
Ni 0.1892714611016299 -1.5657409448092052 1.8104074895097726
Ni 0.1153549312230308 -1.4364585943264048 -2.1616199988840901
Ni 1.3454328617691178 1.7376963498899090 -0.0938386576324448
Ni -1.1089342703154368 1.7066405458888536 -0.0703865112561632

Ni 1.3890372905197448 -2.2456428292106470 -0.2122192840941345
Ni -1.0705739924668221 -2.2708667034387395 -0.1799729077513898
Ni 2.1445487670192445 -0.2902445630500950 1.0593767992343608
Ni 2.1004005037749445 -0.2077794801884832 -1.3996284019609297
Ni -1.8305643365652844 -0.3236766782400671 1.1240618638221023
Ni -1.8648158267689849 -0.2476680675490122 -1.3459378077694284
Ni -3.8329906823702147 -0.2384150995085551 -2.4960076844779993
Ni 0.1507919596697604 2.0695470234649171 3.8659956540288603
Ni 0.0461307781714899 2.2750164564159907 -3.9872615389952593
Ni 0.2094716445089288 -2.7920126765130240 3.7122615757876289
Ni 0.1029616680389107 -2.5824943906964268 -4.1255572261528881
Ni 2.5162211163502310 3.7030222176755752 -0.0599909839489960
Ni -2.3839258671828141 3.7142490206812950 0.0517134464041012
Ni 2.6021882772733060 -4.1630434745354821 -0.3023158942554173
Ni -2.2578296105168603 -4.2116400936225222 -0.2075263682366870
Ni 4.0818563186323651 -0.2784305661587916 2.2262929223961243
Ni 4.0191972291286344 -0.1417042095814872 -2.6171306252589872
Ni -3.7852035910001689 -0.3830666378916852 2.3556678843761452
Ni 0.1005609913919136 3.7737304866838195 -0.0468627071008538
Ni 0.1771370325078503 -4.3245257955385883 -0.2437743984022513
Ni -3.9099728192242598 -0.3137416852060331 -0.0807556568022516
Ni 4.1821203426929472 -0.2018218931294702 -0.1965726419428839
Ni 0.0615697782725077 -0.1519486859861843 -4.1884375045518354
Ni 0.1906214806822843 -0.3719687481337557 3.9152809455133406
Ni 1.4590655205843335 -3.5998837774288734 1.7726337613778962
Ni -1.0606560353404224 -3.6188493318755928 1.8152739124202220
Ni 1.3894716444045494 -3.4811098183484126 -2.2773857243677913
Ni -1.1232455474776195 -3.4998469913904837 -2.2418323339866353
Ni 3.4204663007575848 -2.2153043520027489 -1.4955187220320698
Ni 3.4533370798121616 -2.3016536340941456 1.0146194123999872
Ni -3.1421458471256409 -2.2936791796695966 -1.3938115573330538
Ni -3.1044154774206651 -2.3565838998858379 1.1079050047590506
Ni 1.3104274125852484 3.0946714996763331 -2.0936818061572389
Ni 1.3609692618168459 2.9720127131544434 1.9591715359903203
Ni -1.2075598976911861 3.0545005108948189 -2.0302307707315039
Ni -1.1670961325171527 2.9964249751259655 2.0299281655447841
Ni -1.9636821806960603 1.0658133246357229 -3.3589316878253621
Ni 2.0987165902956026 1.1117941461596288 -3.4075139286607445
Ni -1.9269204341560231 -1.4480203695771661 -3.4238041839810842
Ni 2.1183322490300287 -1.3916413999464130 -3.4881242956188876
Ni -3.1500266636392098 1.6462039113183538 1.2042191407836904
Ni -3.1610244195448107 1.7739724253304685 -1.2854499808902382
Ni -1.8351349794573228 -1.6256869933495135 3.1322597507382279
Ni 2.2235290533108425 -1.5876915747028424 3.0841185350717755
Ni 2.1842976984938529 0.9263968050398311 3.1533881783992719
Ni -1.8531323603858691 0.8667173472877591 3.1905362833584698
Ni 3.3616662539442026 1.8452638063690376 -1.3852812603624569
Ni 3.3976635291294790 1.7779960244172319 1.1361404867226303

CO/Ni_{55}

C -1.0837632282268879 1.2349801583413929 -4.8718138366255817
O -1.4517003920243554 1.3314576929144217 -6.0043476345907196
Ni 0.0484997655044674 -0.0413432585991336 0.1953714474691937
Ni 0.0472599779920483 1.1898855844236911 2.1841795155301256
Ni 0.0495614713878600 1.1758036684801316 -1.7826675987478988
Ni 0.0458578485049796 -1.2690193173484647 2.1842308868650302
Ni 0.0386321519354104 -1.2845078102706073 -1.7841441542861598
Ni 1.2745832362378735 1.9453399746068851 0.1861605421953379
Ni -1.1938491024093683 1.9359182265226267 0.1940853628727840
Ni 1.2768454551362929 -2.0391879879058528 0.2012620607159981
Ni -1.1829487386887991 -2.0394397123899544 0.2076168969911279
Ni 2.0372052279695279 -0.0411058998690353 1.4267295782643121
Ni 2.0334852881991945 -0.0629902253659627 -1.0344570442504786
Ni -1.9468533608290275 -0.0434682060220102 1.4271760167139453
Ni -1.9407307440662001 -0.0574927522148181 -1.0318898964855991
Ni -3.8786459728347360 -0.0601738149667377 -2.2233947957127143
Ni 0.0518199078888488 2.3938920485220732 4.1216053033941522
Ni 0.0394360752596085 2.3661053236688776 -3.7485155526642528
Ni 0.0406283748417184 -2.4622695409919939 4.1128614561684476
Ni 0.0407711305864311 -2.4880554935586177 -3.7142068246502138
Ni 2.4853296093286499 3.8889716186692342 0.2065909758804080
Ni -2.3861169818669024 3.8762025900507537 0.1938262940113570
Ni 2.4813436487837857 -3.9642906765350125 0.1999366561991197
Ni -2.3720452672767598 -3.9671002136788505 0.2208871249471410
Ni 3.9759517698454938 -0.0342877580863361 2.6297169514600216
Ni 3.9741080655456393 -0.0609371568224033 -2.2250306234048485
Ni -3.8798276487691350 -0.0253465881159787 2.6190633118803937
Ni 0.0494522554903329 3.9930222694081681 0.1856766316833417
Ni 0.0564363922486565 -4.1042967403145090 0.2235846673749509
Ni -4.0060279340303833 -0.0287832644152024 0.1926786015616070
Ni 4.1046301775425400 -0.0512596516182311 0.2084843159953023
Ni 0.0025188518663024 -0.0508136983424128 -3.9132429434403599
Ni 0.0487508947346408 -0.0397865502372013 4.2547647717708310
Ni 1.3155110439436202 -3.3245670586837117 2.2313652879446186
Ni -1.2078619923918716 -3.3275044785358951 2.2395799253852933
Ni 1.3110914779180813 -3.3202246685986165 -1.8291712723245110
Ni -1.2053764638343920 -3.3362434876760516 -1.8156007940120897
Ni 3.3378201864482233 -2.0733909799532975 -1.0496079185450058
Ni 3.3304747599302229 -2.0661476126296718 1.4636157552731277
Ni -3.2348774939065144 -2.0782766474282970 -1.0426567123987356
Ni -3.2325912585640855 -2.0672973356031998 1.4731550105034072
Ni 1.3082149957008360 3.2435524720194930 -1.8387708899017543
Ni 1.3008336464913834 3.2334444253894246 2.2198105644342427
Ni -1.1950739472066561 3.2345098810565429 -1.8234544556839647
Ni -1.2075027818160020 3.2358104275972814 2.2292035145502185
Ni -1.9893926932148598 1.1834006267426369 -3.1571365058748166
Ni 2.0832384572790428 1.2069559595268236 -3.0686604295695399

Ni -2.0009128815858239 -1.3452085022378475 -3.0667651251123562
Ni 2.0471839900251192 -1.2821250347068076 -3.0981632210105738
Ni -3.2351577400820792 1.9946850804024627 1.4487009158379758
Ni -3.2142123218240206 1.9748263236011643 -1.0972111052355831
Ni -1.9890414604247360 -1.2788272212466676 3.4866222486807357
Ni 2.0708593875062751 -1.2910256287406041 3.4853083290484737
Ni 2.0665450470273963 1.1943189510741519 3.4895624232317068
Ni -1.9756693274386490 1.2179556844647681 3.4803604930347389
Ni 3.3125196850303942 1.9735683173382854 -1.0539956344955774
Ni 3.3227794791813463 1.9821876688887055 1.4511311311538631

H_2O/Ni_{55}

O 3.8154873911836722 -4.9701550487183654 -0.5723182884496597
H 4.6215323670144279 -4.4305894489354269 -0.6942618965018686
H 3.5836197942511365 -5.2846942201045959 -1.4673166509800248
Ni -0.2186132681114158 0.2732208730870209 0.0479981650013666
Ni -0.2492221891693159 1.4697348618116675 2.0550202645020583
Ni -0.2858225570000547 1.5316523592739775 -1.9242279415330774
Ni -0.1804798780078302 -0.9939975500394294 2.0210773285102044
Ni -0.2206237596599664 -0.9259278975900562 -1.9552169272876916
Ni 0.9402413977730560 2.2990361198540894 0.0705524489255115
Ni -1.5161828902962149 2.2269794817778017 0.0834495238656593
Ni 1.0594412538607816 -1.7035576146011739 0.0148393374006398
Ni -1.3918406923309339 -1.7586620046410819 0.0317748821351434
Ni 1.7623175029357292 0.3060144159036293 1.2663434437397991
Ni 1.7353728490386058 0.3592575999060887 -1.2001166971536410
Ni -2.1979868553127306 0.1893936192894156 1.2891577348574557
Ni -2.2206111928330294 0.2184617658702314 -1.1573575870078519
Ni -4.1565465326313618 0.1872859001102429 -2.3360914681114613
Ni -0.2472416723708785 2.6319324616194848 4.0150512275619317
Ni -0.3148583864684321 2.7420476704486632 -3.8396058595281115
Ni -0.1071276819637489 -2.2140496626172910 3.9418708479007112
Ni -0.1829336754923051 -2.0999651920546132 -3.9145141755253752
Ni 2.0968706802223531 4.2632958189283050 0.0855635597374252
Ni -2.7577404820754463 4.1224691032393004 0.1290723266213952
Ni 2.3670686172771256 -3.6202517588545122 -0.0489199902660792
Ni -2.5209972219336132 -3.7241539888847734 0.0151779301987761
Ni 3.7450647406498021 0.3491824821839351 2.4517190202556307
Ni 3.7075662846949413 0.4102911615315147 -2.4124761560583821
Ni -4.1104280916279894 0.1224798672269384 2.5059467790834411
Ni -0.3374734305276578 4.3283260322018284 0.0986782616883245
Ni -0.0926065802819954 -3.7923980745072274 -0.0083643026455219
Ni -4.2723120023730692 0.1348316590838014 0.0867382904448531
Ni 3.8094992242891670 0.3872420990302769 0.0207457666349170
Ni -0.2455356492591571 0.3244646205542225 -4.0095236999027071
Ni -0.1773519244612293 0.2060558401038825 4.1072665940986637
Ni 1.1434076746384567 -3.0049984636416589 2.0068035505594652
Ni -1.3503600028719613 -3.0954476714782695 2.0483288983792911

Ni 1.0923530805335713 -2.9375244785748000 -2.0304330877086034
Ni -1.3910344628115763 -3.0332775868794259 -2.0139926982277307
Ni 3.0837021299610159 -1.6177205991073764 -1.2578568033687927
Ni 3.1152548848854198 -1.6688040148529586 1.2480395458582041
Ni -3.4524883691193584 -1.8457417184201339 -1.2079507878906708
Ni -3.4195202253455053 -1.8861019723282348 1.3180634349480786
Ni 0.9288481492618285 3.6132394277932223 -1.9453128923173169
Ni 0.9615285653147557 3.5579058440225704 2.1163631338744473
Ni -1.5725680402583742 3.5616817321129091 -1.9207658926290709
Ni -1.5344808285644811 3.4898192163677999 2.1347952688380500
Ni -2.3047467895238150 1.5108510154045147 -3.2026166053081546
Ni 1.7565104845572892 1.6274634087440067 -3.2251177214487683
Ni -2.2408607765792561 -0.9963850235228575 -3.2357096514581745
Ni 1.8080759951705601 -0.8710352422307484 -3.2583294647036602
Ni -3.5390923408885753 2.1870970087479247 1.3666895611567109
Ni -3.5590005012831316 2.2249858121227684 -1.1566199135837736
Ni -2.1800560186145614 -1.1027256486979935 3.3360117387361452
Ni 1.8714619888953219 -0.9766758555025552 3.2892956039684313
Ni 1.8016681012888018 1.5270149547737857 3.3211003781110060
Ni -2.2421086773501822 1.4009094462023954 3.3769731626843331
Ni 2.9829985940128378 2.4060909479293957 -1.2082726142516269
Ni 3.0009618956884929 2.3641261095279402 1.3027817635697307

H_2/Ni_{55}

H -4.4826945213549019 2.4702682140208729 -1.8638744489550323
H -4.1975957088769906 3.1725582918296773 -1.3776772566056148
Ni 0.1520195250478884 -0.0986946836660896 0.0560382285086592
Ni 0.1817358599486913 1.1143332867415023 2.0613607494258299
Ni 0.1709990914525219 1.1485804240593316 -1.9202654187842008
Ni 0.1231164649570717 -1.3440227240814098 2.0364387026738351
Ni 0.1170330658719791 -1.3078909299542816 -1.9501540968571924
Ni 1.4164362208705765 1.8734893585633157 0.0715099976952940
Ni -1.0493580424444984 1.8988886054071830 0.0725280357097434
Ni 1.3237759537007630 -2.1088307456594473 0.0173078842118124
Ni -1.1195136651849125 -2.0666673998867280 0.0392765793640486
Ni 2.1327702078649819 -0.1261141846592180 1.2778477297504640
Ni 2.1294081134156446 -0.1112055437515451 -1.1923225906516031
Ni -1.8281011294885490 -0.0786426954029196 1.2967446448175022
Ni -1.8389093762352671 -0.0320580213758333 -1.1570964830563066
Ni -3.7702245014350382 -0.0256599022998398 -2.3546375115193601
Ni 0.2230075958577089 2.2772996747490799 4.0096017583147052
Ni 0.1926838838228859 2.3593604181834116 -3.8399680516089352
Ni 0.1358440544602808 -2.5747286296002487 3.9675764419435740
Ni 0.1046018670371760 -2.4916822888645567 -3.8866430958165048
Ni 2.6585729278210639 3.7724291551659865 0.0897712291186850
Ni -2.1815844939926938 3.8693233570711429 0.1220984072113298
Ni 2.5114250011651738 -4.0698657584854896 0.0088242598980633
Ni -2.3298253279398695 -3.9875705466811042 0.0312580361994761

Ni 4.0910463592785877 -0.1963417451483873 2.4701189822982559
Ni 4.0821291251128891 -0.1510759283081899 -2.3855315792783069
Ni -3.7497458407488837 -0.0644150756353335 2.5038090271888138
Ni 0.2400402764943439 3.9540256583879376 0.1185382388479724
Ni 0.0811800099761319 -4.1618127029689429 0.0105710819913903
Ni -3.8879492924724977 -0.0697483446150500 0.0794867695884594
Ni 4.1926509993106329 -0.1581177535620215 0.0422139215885454
Ni 0.1523698045416117 -0.0730293849120507 -4.0023975026714327
Ni 0.1757978993699465 -0.1510056308970533 4.1241440644881733
Ni 1.3419787943093380 -3.4154508497741256 2.0341895710475488
Ni -1.1445730924567195 -3.3887415097835092 2.0676878663583511
Ni 1.3378663113502958 -3.3906268708975462 -2.0106579140822647
Ni -1.1517688504071608 -3.3646480679560953 -1.9999972508450079
Ni 3.3727693124149267 -2.1681191392205550 -1.2337543673247406
Ni 3.3721087155427281 -2.1783892310485644 1.2653626722800719
Ni -3.1524691028179159 -2.0723777084046917 -1.2128376997543886
Ni -3.1485581808849528 -2.1017220365335954 1.3096115111105164
Ni 1.4782921407908702 3.1779418610282817 -1.9379914181687012
Ni 1.5003912229662213 3.1380473130069388 2.1301320978816229
Ni -1.0103255161169558 3.2301415722660916 -1.9171948410892621
Ni -1.0086782981915428 3.1854366256156470 2.1286188672931252
Ni -1.8416653070460995 1.1909653996423972 -3.2136858968883284
Ni 2.2016030750607611 1.1448528706965335 -3.2189863258814220
Ni -1.9041437830176058 -1.3054186826483574 -3.2215129896843959
Ni 2.1584938515241037 -1.3596197904057927 -3.2483047107458876
Ni -3.0567599088491972 1.9717200139495901 1.3749133366178441
Ni -3.1447083407308218 2.0310864925058536 -1.1796439953321527
Ni -1.8742016666105283 -1.3594845299218665 3.3397350946632254
Ni 2.1610662539179835 -1.4063401090436694 3.3119539532060061
Ni 2.2227913071322112 1.0900507103191597 3.3475924551805778
Ni -1.8223733621874527 1.1493368369130095 3.3748213050219982
Ni 3.4803949744530716 1.8780022334452917 -1.1924855745971721
Ni 3.4793270426499885 1.8619807724858732 1.3259375187026943

CO_2/Cu_{55}

C 1.9852446101811758 0.6183149641650194 -6.6492300548249830
O 0.8546508872662110 0.3476977238615477 -6.8366442031116836
O 3.1101920323444068 0.8868591680712399 -6.4748758978081664
Cu -0.1080019321691519 -0.0346146011123380 0.3610078726169930
Cu -0.1016054263541384 -0.0405238762891011 2.7664803540423288
Cu -0.0985575477992736 -0.0456377206515461 5.1189038998712757
Cu 1.6890991710364163 -1.3135352003699490 3.9109805366440891
Cu 1.6439324334852907 -1.2955824561792184 1.4347149241038117
Cu 1.6375163081427668 1.2324980103979808 1.4406087557040053
Cu -0.7784717778783913 2.0081100089125070 1.4423553630679411
Cu -2.2627605467793201 -0.0406507785563481 1.4419903561949279
Cu -0.7702817427047904 -2.0848144090520786 1.4320920495369649
Cu 0.5630084866482864 -2.0765341358023508 -0.7162510488228220

Cu 2.0479315541650034 -0.0280332531493639 -0.7122299671830339
Cu 0.5560587093010431 2.0153414027694350 -0.7058610614655358
Cu -1.8596082013651913 1.2294933420963010 -0.7064536323015131
Cu -1.8548915319646704 -1.2986210784392673 -0.7124014774913476
Cu -0.1193994248046440 -0.0288215165531285 -2.0479087572821624
Cu 3.3549877609007446 -2.5315282620817565 2.4841910657666326
Cu 3.3422804735786542 2.4741571451023243 2.4954494008456236
Cu -1.4317003581116601 4.0056161526217204 2.5003538039954609
Cu -4.3687846740525291 -0.0472901992016168 2.5020817462351403
Cu -1.4154423149013482 -4.0909502097451087 2.4801840219224798
Cu 1.2172803994741206 -4.0732874683213369 -1.7757819345436938
Cu 4.1535258503157131 -0.0213133539557471 -1.7757382173348653
Cu 1.2034986987231961 4.0190520918008028 -1.7578372480414624
Cu -3.5679721500430248 2.4699287443076963 -1.7564841105751139
Cu -3.5592661481050558 -2.5368279469833941 -1.7697417637723545
Cu -0.1278107607158368 -0.0219680067373473 -4.4022249234369450
Cu 1.6822008313000496 1.2402572888256105 3.9162020946948943
Cu -0.7858697617568647 2.0385990947070867 3.9137013443054918
Cu -2.2978225826230192 -0.0515124568298115 3.9148280035941023
Cu -0.7781577815710717 -2.1279510447367502 3.9050597128727653
Cu 3.4681600122975773 -0.0294670912857922 2.5360153430744505
Cu 1.0017572426289667 -3.4089356006830420 2.5398078294812221
Cu 2.3688629331117426 -3.4000275199847088 0.3421341342146580
Cu 3.8778508889174237 -1.3034782929954702 0.3643479054148195
Cu 0.9871895884226375 3.3400130717267902 2.5546348643794925
Cu 3.8687846199719953 1.2553074793945858 0.3670312336740111
Cu 2.3582989354025772 3.3418598498224665 0.3547043594100843
Cu -2.9941910822093667 2.0495120487833813 2.5514770125681907
Cu -0.1139801116830444 4.1387217941711896 0.3733380650518539
Cu -2.5852716282707395 3.3324504897533882 0.3856556352358838
Cu -2.9861567957812949 -2.1421809965936673 2.5374873596107670
Cu -4.0934528452420036 1.2375977066366248 0.3626933197695592
Cu -4.0859354956012766 -1.3216070938524256 0.3586175889295442
Cu -2.5737605192222941 -3.4097189168843989 0.3687597121845960
Cu -0.1006574147335111 -4.2074378254575135 0.3500624807247481
Cu 2.7788482975595317 -2.1195819387000197 -1.8242467395096051
Cu -1.2039297577358479 -3.4046821444273117 -1.8298523797907702
Cu 0.5688550021916220 -2.1056819912337663 -3.1880365250014759
Cu 2.7710135959657611 2.0716818363326608 -1.8150911246288786
Cu 2.0783354313872677 -0.0214291352266076 -3.1786295626689856
Cu -1.2146027616985760 3.3415924211183037 -1.8134578412295301
Cu 0.5643745034282047 2.0551425986387426 -3.1767600980321808
Cu -3.6859056307364306 -0.0327384520777163 -1.8086413521978488
Cu -1.9064047233455623 1.2503846284714260 -3.1838331889956151
Cu -1.9030858281884515 -1.3032240883388284 -3.1897390396882348

CO/Cu_{55}

C -1.4638003584840755 -4.7904867293828080 -1.0046349388581581

O -1.8021762746870429 -5.9025626479627356 -1.2363317841168753
Cu 0.0597738911384103 0.1995048517547215 0.0418768420422562
Cu 0.0467772072654827 0.1787153346695860 2.4531169662212950
Cu 0.0358961919350449 0.1692781853326810 4.8049322541855961
Cu 1.8323322085577367 -1.1005191745654221 3.6045202005136301
Cu 1.8163730668715290 -1.0467400486865832 1.1233738322491216
Cu 1.7816516926144428 1.4766488588239148 1.1315985317149453
Cu -0.6325286063582995 2.2321730020092545 1.1258887222300429
Cu -2.0985409592125692 0.1766826353952677 1.1138333582422337
Cu -0.5828229236539679 -1.8590805195437434 1.1029434469294159
Cu 0.7547484598862020 -1.8310909406862466 -1.0425324686536479
Cu 2.2191046763613418 0.2222090425725791 -1.0295047632385055
Cu 0.7044542763583079 2.2587970771883370 -1.0211256067407786
Cu -1.6982626225898156 1.4452842999510025 -1.0376922834805025
Cu -1.6582786602708175 -1.0799406470932504 -1.0475581354016583
Cu 0.0717536136329036 0.2209839072617421 -2.3684085861259994
Cu 3.5313505663927618 -2.2749218617781941 2.1786766378684792
Cu 3.4681864181961775 2.7235330509848530 2.1985113242766441
Cu -1.3125373543892203 4.2186163444498517 2.1881772016284375
Cu -4.2086776087611186 0.1426343480255876 2.1573445362392056
Cu -1.2108043837472404 -3.8624008501692848 2.1814768172441243
Cu 1.4707344432100078 -3.8048496492786459 -2.1167886875290813
Cu 4.3272804079647322 0.2538772318989950 -2.0737569006783456
Cu 1.3372694167519963 4.2718359255293441 -2.0642020346403700
Cu -3.4111769972968982 2.6699780196482967 -2.0894375188766143
Cu -3.3648003106440330 -2.3019256183315182 -2.1264425398418485
Cu 0.0798268480058804 0.2307871217643291 -4.7249396358680924
Cu 1.8070809927551768 1.4745650793684264 3.6002130627061395
Cu -0.6671402510533360 2.2500790995766873 3.5943172830699490
Cu -2.1561393771490027 0.1423120595722325 3.5929418356256311
Cu -0.6076082368793061 -1.9140675913698015 3.6024844354285865
Cu 3.6004827449211905 0.2157290968312049 2.2509820287767734
Cu 1.1778822722637079 -3.1653753338759110 2.2207754940727975
Cu 2.5445368042303542 -3.1365270472342228 0.0279086999321461
Cu 4.0529890920096951 -1.0579585042054311 0.0460204504847251
Cu 1.1071014360712297 3.5641947569082548 2.2802760746691111
Cu 4.0084534317910725 1.5182339252991757 0.0692803179032993
Cu 2.4942886276715441 3.5920736302080369 0.0555094128535845
Cu -2.8525232187367076 2.2331965431434524 2.2342237646745788
Cu -0.0098558180487382 4.3738401604516799 0.0494748897502749
Cu -2.4362847062605546 3.5342401533119112 0.0555254401377652
Cu -2.7796879797284046 -1.9319550492179720 2.2037850162671213
Cu -3.9390240201337376 1.4336422888622453 0.0272441966790594
Cu -3.8740977295819139 -1.1380627094640523 0.0139388770696148
Cu -2.3851666785317565 -3.2606855404773252 0.0113465418909865
Cu 0.1314761662871502 -4.0397066600358817 0.0280611633980688
Cu 2.9878942000171471 -1.8407274763867807 -2.1615573301273217
Cu -0.9976881808286040 -3.2228633685667369 -2.2306091243180401
Cu 0.7787051374521579 -1.8559676144327504 -3.5031548173219229

Cu 2.9050541443921269 2.3200243032555199 -2.1355896916485846
Cu 2.2743516444840584 0.2322475938933497 -3.5109542046649573
Cu -1.0661090134026303 3.5612651389713301 -2.1438791402994584
Cu 0.7223419845956121 2.3056404689238583 -3.5018144061648240
Cu -3.4976670401178485 0.1806147199676982 -2.1739196949755653
Cu -1.7291720065975731 1.4808413883665181 -3.5180039365992917
Cu -1.6875807469399648 -1.0858640614266253 -3.5077414268052025

H_2O/Cu_{55}

O -0.1984285421375299 0.1401644438916961 6.5637952559146111
H 0.5596331657113417 -0.2545794165679691 7.0306757373511859
H -0.9746978302376778 -0.3812012774685817 6.8376105611032312
Cu 0.0109445362701471 0.0087400413979380 -0.3614196210365268
Cu 0.0043424795617560 0.0192539928099172 2.0664635514025167
Cu -0.0099135398839098 0.0445356911526025 4.4428429848956155
Cu 1.7609962979229250 -1.2817283129766897 3.1979496381607335
Cu 1.7453254355641108 -1.2518261536449726 0.7195375148112887
Cu 1.7515480604237408 1.2761647040417072 0.6992340607778339
Cu -0.6588325161535448 2.0592573124426443 0.6883554186716477
Cu -2.1431877538501247 0.0129939472965029 0.7008145225059413
Cu -0.6596792190495521 -2.0328553416193214 0.7134859380059134
Cu 0.6816317265237614 -2.0414647527136336 -1.4342703140739324
Cu 2.1650051177442684 0.0048330092979839 -1.4467780850326832
Cu 0.6828992125068972 2.0516307444740396 -1.4575162298530242
Cu -1.7240324524554875 1.2700808966294299 -1.4645449776303980
Cu -1.7281259928156101 -1.2599995486313991 -1.4452278896556994
Cu 0.0179230033504168 0.0001484140699160 -2.7777444633086574
Cu 3.4420626080020065 -2.4859417877074530 1.7882221343849594
Cu 3.4505290853005852 2.5169651824804458 1.7538113321415949
Cu -1.3111120247156220 4.0670016281395887 1.7303987523390636
Cu -4.2539398867101808 0.0175466029844560 1.7501685393233863
Cu -1.3142776382272094 -4.0311322847945901 1.7791217602973268
Cu 1.3366042969692247 -4.0460481556512216 -2.4784548790584076
Cu 4.2738939673633691 -0.0031590156927685 -2.4987812091214838
Cu 1.3413091304844507 4.0493857080432294 -2.5221806495144334
Cu -3.4224495419464240 2.5038292288676272 -2.5310505205044995
Cu -3.4242440700161865 -2.5047870899710438 -2.4990330063739021
Cu 0.0214290219832039 -0.0104053402042181 -5.1342551157000758
Cu 1.7806860304280132 1.3043155730621572 3.1716638152591141
Cu -0.6934334210194600 2.1092503005124268 3.1547006554994907
Cu -2.1998176300841537 0.0039260851670167 3.1720500277937003
Cu -0.6833646457273904 -2.0546930391739462 3.1903763876067459
Cu 3.5530483611903447 0.0170457445243666 1.8430080828063971
Cu 1.0967122748816913 -3.3496490139774182 1.8652729010169109
Cu 2.4563998584357107 -3.3739379410160324 -0.3430161660174659
Cu 3.9699704081781131 -1.2804934544632220 -0.3541341803072039
Cu 1.1025281575657644 3.3921640255971801 1.7971062357281431
Cu 3.9789162056298522 1.3052250680966404 -0.3730163093203930

Cu 2.4829250437480743 3.3784876298328319 -0.3919599139965939
Cu -2.8680761017268184 2.1075414451388705 1.8082246426920436
Cu 0.0069804776324912 4.1835800655328796 -0.4014360253960944
Cu -2.4289072007885522 3.3945695894664665 -0.4049617482189451
Cu -2.8656568865983965 -2.0633053054443216 1.8452614010407964
Cu -3.9496772369754169 1.2928284753926107 -0.3933498377730346
Cu -3.9531168276465216 -1.2951279466095680 -0.3709846125963722
Cu -2.4504073297704556 -3.3674372012229057 -0.3559270739814879
Cu 0.0201828407203476 -4.1658894342979851 -0.3433027784218314
Cu 2.8853330737570633 -2.0865261059438232 -2.5607164502702950
Cu -1.0753769039731575 -3.3746285062267480 -2.5455149034843680
Cu 0.7106511087444879 -2.0882384598997081 -3.9104945151370623
Cu 2.8880389399558508 2.0778147470856343 -2.5909954577482082
Cu 2.2182376290403338 0.0148504384566102 -3.9247775595999412
Cu -1.0735934957477360 3.3685746655501219 -2.6101719458364583
Cu 0.7033069192040385 2.0789506556018531 -3.9350255502590086
Cu -3.5301927899021215 -0.0029849366544381 -2.5865751393266043
Cu -1.7455851191044474 1.3039000132892675 -3.9417923324636002
Cu -1.7598678775306951 -1.2875162477526811 -3.9207423905115046

H_2/Cu_{55}

H 2.2465050473790122 -5.3088538322155472 -2.5358415344960461
H 1.5991875519359515 -5.3396132266707061 -3.0025258453983987
Cu -0.0680376469203335 0.1846367056568022 0.0943803528380023
Cu -0.0880885089758137 0.1917336570381961 2.5057479351398477
Cu -0.1076762638160352 0.1888570611011523 4.8609758659999933
Cu 1.7005760020854119 -1.0649933168295518 3.6667620652266608
Cu 1.6783133076312220 -1.0529419509131284 1.1904447193917844
Cu 1.6452007556244790 1.4760713083253403 1.1949368177234341
Cu -0.7712412490847570 2.2263621479647102 1.1735092144142059
Cu -2.2355694393909711 0.1672191952134624 1.1540765916576126
Cu -0.7236607232758473 -1.8588480618224099 1.1676891507152678
Cu 0.6422811133564560 -1.8670732545875688 -0.9867735241740108
Cu 2.0931340378077752 0.2254627267679000 -0.9539301640078168
Cu 0.5793738342823761 2.2476961024660675 -0.9668611282742288
Cu -1.8205375319352386 1.4429271008257647 -0.9860917604668655
Cu -1.7892960575972763 -1.0888263242905571 -0.9949924398695411
Cu -0.0546686732564309 0.1966198406886502 -2.3063704940144341
Cu 3.3901940936853174 -2.2766715028602929 2.2582695373539314
Cu 3.3261274272869321 2.7346699646919648 2.2686354151425880
Cu -1.4541753393149970 4.2181733526700782 2.2245073864348290
Cu -4.3511591812187511 0.1420938016467169 2.1916419402996778
Cu -1.3596304916258666 -3.8709556664714344 2.2089221854924652
Cu 1.3425681163992069 -3.8697289987236227 -2.0376160632560358
Cu 4.2092352828698694 0.2525190703784731 -1.9915807543317192
Cu 1.2158646925149348 4.2619403829581293 -2.0071407476575596
Cu -3.5324425913848079 2.6678111270705904 -2.0505346795446933
Cu -3.4657096631517734 -2.3497958379236112 -2.0658626949350243

Cu -0.0336522470169681 0.1982248046103018 -4.6600663368507131
Cu 1.6755962077371696 1.4804090885918710 3.6747091354033641
Cu -0.7947177606875083 2.2695619350753877 3.6479997888972089
Cu -2.2913758961774620 0.1624038060852463 3.6262157527590841
Cu -0.7466908167826153 -1.9114879494589956 3.6394168276142791
Cu 3.4618895086313421 0.2308212114221572 2.3258395080708958
Cu 1.0458472786642969 -3.1677259659712074 2.3087123809656118
Cu 2.4411164050582523 -3.1468838165398858 0.1140119783131857
Cu 3.9290413743505943 -1.0319538732143347 0.1453152556784312
Cu 0.9665165961342027 3.5724911596217015 2.3168190283006806
Cu 3.8940731372732915 1.5155864208323582 0.1465869558799780
Cu 2.3489453485581175 3.5923108363737990 0.1239288410060995
Cu -2.9915346776893021 2.2463490297607893 2.2654558105178415
Cu -0.1241521408391158 4.3594120163411318 0.1086091125376694
Cu -2.5770272459658519 3.5404086913362613 0.0904812127264223
Cu -2.9442588221319963 -1.9351256321636492 2.2616128058115530
Cu -4.0688171597129088 1.4240035914829590 0.0591525362562082
Cu -4.0373528668218706 -1.1245409630813157 0.0532698367983953
Cu -2.4956853091804434 -3.2027027881963348 0.0802111937316406
Cu -0.0166062709505671 -3.9655308420400677 0.0956474506818213
Cu 2.8551735444872839 -1.8525430961424436 -2.0557224619371013
Cu -1.0971886047839552 -3.1868375987682751 -2.1169807011657475
Cu 0.6552862171391619 -1.8828695609192647 -3.4430472776600665
Cu 2.8032880487603378 2.3285717801044190 -2.0548583092339836
Cu 2.1489779949570651 0.2325558911254552 -3.4248859095091593
Cu -1.1883602539390539 3.5593182753397969 -2.1053485000043697
Cu 0.6001259248178302 2.3019245360550253 -3.4388190082787329
Cu -3.6055339080677444 0.1567440418796618 -2.1211691802447730
Cu -1.8409903991939063 1.4547795181860721 -3.4629602925216059
Cu -1.8186011085377187 -1.0941661198841888 -3.4745147819480380

C 147-atom Substrates

CO_2/Co_{147}

C 2.6929742127360705 -2.9306923618359826 6.8285861956163920
O 1.7471057392003462 -3.6665661972147867 7.1615187354739440
O 3.8188334861941891 -2.6016432668951257 7.2825279198434005
Co -2.6270825105117543 -3.3889101099445540 -2.0629538399472813
Co 3.0669274520626928 -0.9816740512673355 -2.4703839438424562
Co -2.5407532068854235 1.1768292173689454 -3.9874825247713113
Co -2.3678114865577649 2.6735614691014153 5.9693154265421109
Co -3.1621371667719123 4.9771924447481952 -2.2247606783349627
Co 2.5731814883995532 -5.1774432817842628 -2.0696420772385733
Co 3.8503110490427104 -1.8631105930892320 -4.5216504826286235
Co 0.8444286965257890 -2.0538617012053106 -0.0803974313519919
Co 6.9176800907574520 -0.4028681352120275 -0.9447083877851364
Co 3.7733786505205669 2.9809031056402810 3.7094867283050665

Co 4.7892988614100105 -1.2047911018153343 3.4418422040954053
Co 2.7028539031178749 -6.4085096950051614 0.0660295708060860
Co 3.5352439705166536 -0.6426005883446525 1.5259218611310339
Co -2.3435133027352348 -3.2012938339982377 0.3982896876653979
Co -0.4177347391852179 -3.8537916306287316 -1.0367132226650599
Co -2.8230891665275966 -2.1221045365036555 4.9310476735875985
Co -0.9612625490983621 2.1781032888809504 -0.2114804026364087
Co 5.8903595296127635 -0.8066269473265616 1.2458361874347836
Co -4.7342433599033056 -3.0782327227431470 0.6661548609273732
Co -2.5961893419874205 -1.1119477569455987 -3.0404880796133322
Co 0.2448793961840986 -1.1291691073721239 -6.1962529686876957
Co -3.3435743420356365 -4.7343402054735755 1.9010248949746549
Co -3.9677597011678034 1.9831029679005612 4.2305071208630816
Co -3.8869925119654258 -2.8395439816156158 -4.0118541372681733
Co -3.6530904413484495 0.7766538361521262 -1.8119481502729708
Co 5.9253808272731092 1.4974538753170374 0.2874333436046694
Co 4.2883828368877523 2.9681160984522648 -3.4146541636779619
Co -1.3107226404894576 -1.6240717560948339 -1.0800831962322806
Co -1.8596282054153268 -4.2797926054631814 -4.1378642056922503
Co 3.2851778709514621 1.4352357214924718 -1.9200352756094479
Co -0.5680118422811072 -2.5522582867623775 -3.1635488760787402
Co 1.0101817293187807 5.3135658897766520 -3.2076586106150944
Co -1.4272713653659879 -5.4298170550542375 0.4728443879310356
Co -0.8012513465968601 -3.5668333552691829 4.7976982729188817
Co 4.5237740837942422 -2.8396248938652402 1.5872333699001870
Co -2.6027666802830352 0.2805731376656123 5.4785454982683826
Co 4.0369454504374627 -3.1914043081140053 -2.4246342440925885
Co -5.7397159266205664 -1.1679143755263144 1.8957698667845797
Co 3.2292610091662084 4.8657008917141642 -2.1802690098644892
Co 1.7335811154123779 4.4167223555169723 3.8431161828780178
Co 3.3784129545325028 -3.2277048678702744 3.7523811244895362
Co 0.1955121624350093 -3.4409056309322934 -5.2184975465339027
Co 5.6326876440006020 1.2837113919820389 -2.1879903861803807
Co 2.7230364074119859 2.2401974376504183 -5.2072992438655410
Co 0.6910439374015787 3.6929017883164357 -5.0850811724084757
Co 2.2249539378822716 -0.0902057294830804 -0.4017773790804717
Co -3.1829124692669657 1.0954760292937806 2.1813254576130969
Co -3.3943655787000870 -1.3194332915060720 1.6239306537811320
Co -1.9128262012491701 4.3953249452554068 -0.2781000569642120
Co 0.8040432716210185 -5.8255270490171274 1.5061249083873856
Co -1.6065536560157261 1.8158797364053092 3.9472747561221362
Co 4.8782628153602667 3.3693285794678953 1.5044261007850155
Co -1.8334283134897551 -2.0125078878856608 -5.1468809890856138
Co -4.6247297859027299 2.9840987941567714 -1.8962173873138084
Co 2.4216128212899255 -3.8843350355206381 -4.1857853674127918
Co 3.0688473576304505 -4.8432302490497579 1.9173080682859514
Co -2.8313208747004182 6.5255349824661568 -0.3413305455003638
Co -3.3317975651041603 2.3927935307843060 0.0538868469325634
Co 2.2262174729395761 3.3338692706032851 -0.6844341250280176

Co 2.5089282027018247 3.5172971278103282 1.7724017893606281
Co -2.0339225702010637 -2.9920533411196835 2.8549796339679312
Co -1.7746326138552764 3.1200149390160319 1.8440179992905836
Co -1.7068456789871993 -5.5886615989641406 -1.9950091533577534
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CO/Co_{147}

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Co -2.5907868134386081 5.1536630502675616 1.8789344863977777
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Co 0.5175054894282645 0.2462950376272431 3.9267519267696160
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Co -3.0564047810134509 5.0405840197363601 -2.1774172511498122
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Co -2.8872602430070300 -4.5164872937179288 4.3910278644483327
Co -0.2219086133368964 1.2362235404078896 5.9973335066911906
Co 5.6974528171394159 -2.4515958204822410 -0.5224753798994438
Co -0.4594876620970328 -1.1899040058292820 5.4858308273588161
Co 1.4533529312259597 5.5445179225929566 -0.6508321320285243

Co 3.0546240016836350 4.6095405130953946 -4.4946316884348247
Co -0.8949693836220622 -1.4455621723585079 1.4021394963251055
Co -2.5605695117481599 5.2765995822307925 1.8927126108793049
Co -0.7738742093234889 5.9396245065360143 -1.6810514924919620
Co 0.5472277098621416 0.3663803506644046 3.9373074422589620
Co 0.8333590170098001 -0.8040902612429547 -2.0521478285897858

CO_2/Ni_{147}

C 2.3062376137619589 -3.1981875073859158 6.9505313909153079
O 1.6007990820806208 -3.9656183319171161 7.5741837825961644
O 3.4697153923367363 -2.6866931841954855 7.1267003487222835
Ni -2.5959247067763354 -3.3670357211257085 -2.0514969557184477
Ni 3.0860489428623952 -0.9658362171044218 -2.4688171061226671
Ni -2.5056471276667751 1.1791171228859645 -3.9630594524418092
Ni -2.3430880961026874 2.6600284145437381 5.8842020708940703
Ni -3.1727528221130679 4.9626829028242323 -2.2376900736190612
Ni 2.5879601775423322 -5.1543578537757169 -2.1072728779258916
Ni 3.8791350625769407 -1.8421496368062684 -4.5080981796708137
Ni 0.8639940901706120 -2.0653699539611350 -0.0891562386196461
Ni 6.8506959432687049 -0.3859015788113028 -0.9301859652421005
Ni 3.7919746863918946 2.9545234568450809 3.7291341847993871
Ni 4.8091277713624754 -1.1991333364691115 3.4355335894672980
Ni 2.6812198652828054 -6.3250963611636370 0.0376891329524707
Ni 3.5539502934350828 -0.6519811750577847 1.5358888247265094
Ni -2.3477774321357452 -3.2089482657652293 0.3882076321260607
Ni -0.4074842180078280 -3.8514761499347672 -1.0502459777568136
Ni -2.8344634271419533 -2.0908487024045357 4.9172751919550324
Ni -0.9675726244212453 2.2007979555235431 -0.2079258910510131
Ni 5.8966738135132575 -0.8044803904448897 1.2829622310988649
Ni -4.8180858235182225 -3.1321961568307000 0.6701384086880769
Ni -2.5934734239588080 -1.1102132506012286 -3.0506036409640327
Ni 0.2274084570467833 -1.1252928193768084 -6.1979001024675018
Ni -3.3508309006253043 -4.7421043457469985 1.8501117399462610
Ni -3.9846901294852310 1.9819004565827427 4.2041756901759406
Ni -3.8880705801398423 -2.8156205074623695 -4.0246879999040539
Ni -3.6539401031290031 0.7806592476985338 -1.8190115986494497
Ni 5.9330689609280700 1.5225382974649482 0.3021347773900083
Ni 4.3208465148051509 2.9605865413729644 -3.4035531399806831
Ni -1.3167970050544928 -1.6355331070518233 -1.0976328676925182
Ni -1.8300908042337329 -4.2758238197057592 -4.1539797065115840
Ni 3.3102255853549627 1.4498106693424160 -1.9089610839071538
Ni -0.5617507172431007 -2.5490000601096856 -3.1736053384422647
Ni 0.9887214556251537 5.3261937543218085 -3.2010418320451177
Ni -1.4467439511455293 -5.5189061017920853 0.4675306000518299
Ni -0.7711048879731599 -3.5576243325520536 4.8068569443576816
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Ni 3.2511050363815683 4.8842786651282175 -2.1496713580436730
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Ni 2.7200122136210965 2.2259232718377464 -5.2177867637871618
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Ni 2.2549067618995617 -0.0830085364408291 -0.4044957204159403
Ni -3.1852823001216235 1.1012780128157742 2.1753441187528866
Ni -3.4041877907157261 -1.3240332944356998 1.6196371210991003
Ni -1.8971874080321958 4.3616785845195034 -0.2632286066165344
Ni 0.7874525942964916 -5.8196567261926724 1.4998174559193798
Ni -1.5836903424853750 1.7895535411365215 3.9143678124174990
Ni 4.8996089361280957 3.3626797840775744 1.5008404379479465
Ni -1.8619297992901138 -2.0436632892582511 -5.2321228664886030
Ni -4.7021608175088208 3.0325329975979476 -1.9285152128284562
Ni 2.4409092620144435 -3.8979623671422772 -4.1760807306613099
Ni 3.0710229056866263 -4.8308968148587441 1.9352746363674420
Ni -2.7903409152462144 6.4622443372947247 -0.3402323859464873
Ni -3.3383509905496100 2.3947692090656605 0.0505483232598747
Ni 2.2496329224382321 3.3467827200368530 -0.6706568249104923
Ni 2.4958191704324939 3.4808081540695528 1.7812303564798802
Ni -1.9912510687033536 -2.9587092558347794 2.8184037781781499
Ni -1.7683457838202401 3.1285078733138656 1.8524088785734911
Ni -1.6751162230037002 -5.5921019907266025 -2.0060768145104517
Ni -3.6405421144607102 -4.9396165860151067 -0.5533126509038169
Ni -4.9200180846259691 1.3356773812992775 -3.7196369655145243
Ni 0.4886258050805997 -6.0224512945995601 -0.9983145521132910
Ni 1.9321290681919263 3.1050840193889333 -3.0891408404287510
Ni -3.8467915530782850 -0.5827784373165098 -4.9662213300453386
Ni -5.0033897088951473 -3.2270025870526835 -1.8031240827266117
Ni -4.2892297165640239 4.5537650897133277 -0.0166669757984112
Ni -3.8467995707881988 -5.0338182028232215 -2.9915352066449459
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Ni -2.5473327168605087 4.0308088112950236 3.8702020878519225
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Ni 0.3075611145847847 3.9847156610406005 0.7544630303839178
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Ni 3.5355196873323536 5.0734709491628580 0.2533370529222554
Ni 4.5883737303562837 -0.2400204150074494 -0.6451307885176985
Ni -1.0965926090428573 -5.1969075787659813 2.8971647074359486
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Ni 1.6419837482057837 -0.1247933956738317 5.7643025697931680
Ni 3.5957494116959170 1.6520910665881261 0.5598552729399269
Ni -1.2724411022218967 0.6160469951795174 -2.0424973604004069

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Ni 0.2153921780897416 -2.0314989791270781 3.3020443831975781
Ni -0.8177236559997156 0.9316974206051744 1.8648187294130163
Ni -2.2334704054226124 2.8077410097500413 -2.1439088687849801
Ni 2.1347568377994297 -2.6680104873821260 1.8495602162121472
Ni -4.4206060885562390 -2.8270800027349718 3.0994941090162809
Ni -4.6908066683863581 0.3603722732654515 0.3810117892119091
Ni -3.7234078424667638 1.7031161601856319 -5.8167200953815676
Ni -6.9584422339817849 0.5227932731990402 0.6277618285613393
Ni 1.7354590638150547 0.7257352805467648 -3.7041670392313768
Ni -0.0489511698844458 0.0682549181339522 -0.1484020901089858
Ni 1.1562358286758136 -4.3030719626380849 3.4410239474330400
Ni -2.3563453901356199 0.2157555090823804 0.1094808304556439
Ni 0.9371848811575638 1.5766038711175798 -1.6115828410204163
Ni -0.2978507115827438 3.5849007512027304 4.9157905930406125
Ni 0.0173554043575788 3.7863394291111252 -1.7073234357338509
Ni 1.4951143946190042 -1.6739673398731973 -4.2040929775251596
Ni -0.1190900011518383 -3.6445638789749046 1.4218757795577486
Ni 0.4884184435256806 1.3092130560404653 -5.7807754973491408
Ni 4.1865637434879561 0.5796802120057399 -4.0745683318799779
Ni -5.5153504772055131 1.2740079947195349 2.4582944919112024
Ni 0.3771315532860995 -4.8513889920233169 -3.1845309153188057
Ni 3.7450426609121807 0.7018170055391612 4.6688084929826283
Ni 1.7913624785813473 -4.2234043966228976 -0.0086933357814638
Ni 2.2373764655008999 -2.5264235298248257 -6.1891268833971678
Ni -4.2844631182236608 -0.4438005996911421 3.7713250838766279
Ni 5.4085530614441977 -1.1369848459275276 -2.7600243500165909
Ni -3.4820216598012337 3.3863777251921707 -4.0566411303377192
Ni -0.5932566399015444 6.1583150059121730 0.6931072621367049
Ni -5.9900220687589965 0.9387842957325484 -1.5800445252047410
Ni 3.2373196583904442 -2.2672502025904735 -0.3504062762974522
Ni 4.1826172218011619 -4.4208576008306073 -0.2920750989966325
Ni -5.6681210908784108 2.5801460368559996 0.3099357059819698
Ni -5.0725569499075052 -0.9809485349024428 -2.8519855814215060
Ni 2.5065885282970122 -0.1304294055670463 -5.7586615735015450
Ni 1.6669274983843301 -2.9962761543319330 -2.1427347152037064
Ni 1.7609910045717874 2.1896064316192820 4.9344277380005117
Ni 3.6421059701399270 -1.5972208384617299 5.5795435003719387
Ni 1.4675835809564912 -2.6397212292464522 5.3250009053899134
Ni -1.2644478912059400 4.4487351503341568 -3.7382265456201438
Ni -1.8278821693175953 -0.5976212422563419 3.4091188581679162
Ni 1.5707409030906621 5.7249020419402044 1.7021410802253103
Ni -0.2933727726631223 2.1687902420767071 -3.5807032863623474
Ni -3.6955742672485488 -1.5186711684589702 -0.8536532168288573
Ni -0.4830593008552642 4.9936365640661009 2.8830240227568162
Ni 1.1720521894914868 -0.4807800796613496 1.7445595510521930
Ni 4.9749567409881159 1.1141725597259098 2.5576749862569543
Ni -0.5170516818063466 -0.2554196970195826 -4.1410260189960670

Ni 0.4567964557565540 2.6886363151408608 2.8807095313967679
Ni -2.9859023512094431 -4.4375530493354729 4.2461511554982767
Ni -0.3344791793032380 1.2642435962427263 5.8990778765602023
Ni 5.5676961898684851 -2.4490289689257381 -0.6161194050576346
Ni -0.5907802163425078 -1.1790483344121645 5.4730697517173867
Ni 1.3468688849971460 5.6613425711348730 -0.7663347182852320
Ni 2.8870359665842411 4.5758739109562541 -4.5480221470107676
Ni -1.0381516301811502 -1.4361082883196168 1.3084241918237329
Ni -2.6973439702786361 5.2954335802167520 1.8062161319293550
Ni -0.8912062530830303 5.9495452198900054 -1.7986193916738036
Ni 0.4226342120132400 0.3896819899807695 3.8425389060988935
Ni 0.7171773177745052 -0.7970571618125003 -2.1630345776484847

CO/Ni_{147}

C 0.2580390597861729 7.0983688075973914 -0.5836090661078528
O 0.4053745930425383 8.2793126983920384 -0.6914484753921832
Ni -2.5492962958967218 -3.5230719440562073 -1.9076811619041547
Ni 3.1307994735925835 -1.1450309374218730 -2.3166587121278579
Ni -2.4658190135909042 1.0041167717410324 -3.8043181655609790
Ni -2.2934758187210118 2.4738798517296434 6.0548044968040688
Ni -3.1043491838462911 4.8051889493618249 -2.0729970670531328
Ni 2.6442907964920228 -5.3260050032016668 -1.9526844613574272
Ni 3.9265561380910579 -2.0084836576373317 -4.3566236523580075
Ni 0.9080046019323108 -2.2443150041542466 0.0695058276835168
Ni 6.8945221640203753 -0.5587610639116866 -0.7749852757952718
Ni 3.8266658012803902 2.7730257173206994 3.8987812965909350
Ni 4.8643720136317432 -1.3804451769630246 3.5825945843724076
Ni 2.7351752734383608 -6.5032254078699987 0.1911816047189580
Ni 3.6011993228822368 -0.8305190500733285 1.6743896878286788
Ni -2.2990484990176925 -3.3805536639991915 0.5355802495450739
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Ni -0.9175881734028971 2.0323210035070334 -0.0520093728236120
Ni 5.9392896006710307 -0.9765708252178146 1.4409127860066737
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Ni -3.3018153413580040 -4.9221484201172023 2.0031962898621263
Ni -3.9285835611982911 1.8058632812093116 4.3670750750284366
Ni -3.8419154766911268 -2.9774273653032060 -3.8769454176150568
Ni -3.6047753353224139 0.6142352807410235 -1.6601993477046255
Ni 5.9715072300850540 1.3469084153593425 0.4564772706134221
Ni 4.3643106001924989 2.8014420305339733 -3.2338847801607655
Ni -1.2691932673085708 -1.8033465185848290 -0.9451111917402983
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Ni 3.3537532136691586 1.2727415247485898 -1.7541401417297060
Ni -0.5146593430716030 -2.7189862978099710 -3.0248774577291342
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Ni -2.5685011910527753 0.0833086711392155 5.6229353173707706
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Ni 3.4300995326528749 -3.4330330805882827 3.9133705894376880
Ni 0.2320650447264647 -3.6077566630498032 -5.0677104287915009
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Ni -3.1335809818550140 0.9254015705100850 2.3345633012663640
Ni -3.3605703115813133 -1.4924114143042080 1.7740233593425525
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Ni -1.9784058820958559 -3.1439848881217070 2.9590488188214854
Ni -1.7128118343752474 2.9508339915070319 2.0152759272271088
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Ni -2.5010757876670238 3.8518419051075985 4.0381279112110224
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Ni 0.3617854906152280 3.8165892043891598 0.9177859943180751
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Ni 3.5547875837189595 4.9158348851291729 0.4173551465366316
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Ni -1.0481884820626464 -5.3748215120905076 3.0498794236758746
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Ni -2.1844646151615605 2.6386689694390184 -1.9930907430339153
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Ni -4.3782924975508788 -3.0079644956535594 3.2567350348753683
Ni -4.6327766623308904 0.1947860598258523 0.5302314430066206
Ni -3.6797755832018728 1.5530788563354356 -5.6638893194698436
Ni -6.8978080608815970 0.3564724438003488 0.7892233882729094
Ni 1.7792880425170998 0.5502795383592521 -3.5539952285018264
Ni -0.0030990118792887 -0.1051446675388166 0.0083774250537460
Ni 1.2102093450489662 -4.4982763273981385 3.5967456225943351
Ni -2.3041776404877226 0.0454836734679270 0.2682242024904427
Ni 0.9779437674933130 1.4038535614124279 -1.4599701310426851
Ni -0.2510068494713574 3.3981246249417261 5.0845638318830408
Ni 0.0705107293759615 3.6249809775479971 -1.5524903307562443
Ni 1.5392227794054931 -1.8448500032074431 -4.0473584049063316
Ni -0.0755590537891418 -3.8288356204938121 1.5709693689514148
Ni 0.5333482745934947 1.1555880154826281 -5.6219712842470155
Ni 4.2274553011585372 0.4157956253006628 -3.9197383630099893
Ni -5.4609035269023858 1.0965850463901312 2.6210797603627261
Ni 0.4277122481877622 -5.0210459378747547 -3.0372880413578138
Ni 3.7860693379468437 0.5344687557495599 4.8368252636905344
Ni 1.8170266317558945 -4.4102993911292883 0.1283962190609233
Ni 2.2828560922659178 -2.6847361724728409 -6.0396584232641670
Ni -4.2398645354779152 -0.6231182115891191 3.9336721525746214
Ni 5.4587126446208822 -1.2945281386236978 -2.6147181588497594
Ni -3.4365268664714557 3.2307665823842528 -3.8928118048817102
Ni -0.5521389994356986 6.0251442909075053 0.8443539777821272
Ni -5.9392079430007803 0.7808445569072574 -1.4191629843261231
Ni 3.2780873061861127 -2.4525863002469181 -0.1949941389452362
Ni 4.2315809556690551 -4.5897858804472040 -0.1354947828717790
Ni -5.6200326551678303 2.4143676656423065 0.4734118212120355
Ni -5.0225787689629673 -1.1437643373475457 -2.6968161914692539
Ni 2.5512535691941882 -0.2872854079867864 -5.6084757928247102
Ni 1.7098312289822775 -3.1694398331002231 -1.9889747211559088
Ni 1.7994301251804199 1.9969183207080339 5.0954265380167421
Ni 3.6694420133872554 -1.7603274211735795 5.6846182841352144
Ni 1.4642153333409298 -2.7844260154314888 5.3717992119360316
Ni -1.2172369012555899 4.2941067768125203 -3.5641060101814279
Ni -1.7859521919521431 -0.7721223993982139 3.5712584608804101
Ni 1.6251995188928281 5.5388130171706118 1.9093262772203980
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Ni -0.4397274872353070 4.8114741063211719 3.0438192775739918
Ni 1.2244898587566464 -0.6606945683266433 1.9020965532729956
Ni 5.0143180004399968 0.9378249203065471 2.7150892984531034
Ni -0.4718958941939929 -0.4199765717241977 -3.9869993103759280
Ni 0.5123408967754121 2.5117570131486615 3.0411554756649419
Ni -2.9403716649080831 -4.6268334138255387 4.4042634859029697
Ni -0.2842883234237819 1.0710102110475930 6.0591164833132858
Ni 5.6178309994640845 -2.6213278703907776 -0.4584790256582392
Ni -0.5472067412917533 -1.3610327560667532 5.6404158678566807
Ni 1.4037235629471234 5.5779688851894713 -0.6036089259522153
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Ni 0.4715383250483732 0.2054070878053950 4.0029148151905343
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H_2O/Ni_{147}

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Ni 3.3082334550912016 -1.0532230634151953 -2.3541175093255906
Ni -2.2872227578669881 1.0963091806928880 -3.8357142490092309
Ni -2.0993946719081613 2.5596281436575272 6.0193435083172373
Ni -2.9424274751413195 4.8786323658947230 -2.1118650574158191
Ni 2.8189783181377668 -5.2431197778604286 -1.9909600297384091
Ni 4.1074883281142629 -1.9290718433441243 -4.3871011286431116
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Ni 4.0140059524588612 2.8585536527124886 3.8601655595152491
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Ni 2.9127412637076810 -6.4211195030487520 0.1550086717147393
Ni 3.7820083149783663 -0.7394791363724270 1.6414199662665387
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Ni 4.8262169210332511 -2.9935684424234204 1.7497066824159302
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Ni 0.1822071666764121 -0.0211355421244309 -0.0272809874698527
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Ni 0.7195253998990893 1.2324710286413407 -5.6643942134577960
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Ni 0.6084176629128875 -4.9406747478708279 -3.0717432317457405
Ni 3.9739493441419484 0.6201280891756770 4.8010252876394457
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Ni -4.8366096440578472 -1.0660447378390772 -2.7326260803731848
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Ni 1.8915592972181849 -3.0786336042801636 -2.0287144170061207
Ni 1.9911639689409537 2.0863306209721602 5.0669850040671616

Ni 3.8488165044917091 -1.6754645770880630 5.6525559668355552
Ni 1.6516220600869580 -2.7022263003888938 5.3338524307414330
Ni -1.0339374818563913 4.3722302072090358 -3.6153378872018576
Ni -1.5950388462183362 -0.6842923657207437 3.5357204626836700
Ni 1.8034962127077934 5.6371373298796374 1.8325273767665378
Ni -0.0701310624925478 2.0876391498309750 -3.4637486034779648
Ni -3.4604267433261144 -1.6016299026407763 -0.7310212421783242
Ni -0.2476507753721764 4.8999942293521279 3.0179703054908007
Ni 1.4034245048022436 -0.5720133144458400 1.8711180719055740
Ni 5.1961196604868656 1.0214549902688059 2.6791497351560953
Ni -0.2933452207413572 -0.3333161081272477 -4.0275337553061332
Ni 0.6940246795521898 2.5973484610326736 3.0081950345479842
Ni -2.7515265768566017 -4.5439931248383134 4.3733604461903184
Ni -0.0962873065094299 1.1548403731213943 6.0264956375928058
Ni 5.7915986333681930 -2.5406371823304110 -0.4878776929821806
Ni -0.3564418484946537 -1.2762620638910249 5.6118824959093159
Ni 1.5736440301310211 5.5771151832941417 -0.6361138238109698
Ni 3.1117870337089228 4.5012203223807541 -4.4293210730876327
Ni -0.7956861837948814 -1.5328898056960378 1.4420583071065800
Ni -2.4616758741049440 5.2019723880241822 1.9395450013554056
Ni -0.6636121830965553 5.8667689606119291 -1.6728035021805046
Ni 0.6550598732322022 0.2960596789021875 3.9728238661297808
Ni 0.9400186931629924 -0.8803231901623955 -2.0488205023120272

H_2/Ni_{147}

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H -5.6544609702722699 5.0884228816066193 0.2670383292631578
Ni -2.4986207311431325 -3.4859425667977479 -1.9094032746317708
Ni 3.1978998906723630 -1.1139027720502792 -2.3295463228132589
Ni -2.3939258126259113 1.0489010297905925 -3.8092114000205668
Ni -2.2035586127410660 2.5098032838335165 6.0419282037346358
Ni -3.0255759885602789 4.8310781951037249 -2.0920555770283640
Ni 2.7029340720814790 -5.2983458101710541 -1.9653991385172791
Ni 3.9903629190937862 -1.9872086620823413 -4.3630823922852784
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Ni 3.9213411243327467 2.7940540552993367 3.8827475619176206
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Ni 3.6699232938469635 -0.8000789113086922 1.6687120205897701
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Ni 3.4313068463051399 1.3061601422187388 -1.7684281369599972
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Ni 2.5487204363912053 -4.0332236517309674 -4.0334817584434308
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Ni -3.2062570149141729 2.3053898833986080 0.1977188657690516
Ni 2.3814288602785441 3.1980031633969439 -0.5339536517425910
Ni 2.6360386075651601 3.3408576999357535 1.9126721710219876
Ni -1.9289844779531828 -3.0918178526306881 2.9572372791027637
Ni -1.6260781735269265 2.9956909609713933 1.9926443043364799
Ni -1.5639108292855470 -5.7267669937350085 -1.8630601643964626
Ni -3.5199747279673139 -5.0801054901854243 -0.4076033545664667
Ni -4.7916918075169628 1.1994123896652296 -3.5837837449275338
Ni 0.6016655267019406 -6.1590383113237266 -0.8610565448905364
Ni 2.0568612211338579 2.9573868001177583 -2.9625559482207797
Ni -3.7235153488674935 -0.7116591820540549 -4.8294950801128218
Ni -4.8880974501419736 -3.3603190166869941 -1.6537274532173218
Ni -4.2068823938101403 4.4846548502944055 0.1391300914483365

Ni -3.7325857477703983 -5.1665468793804807 -2.8449721642370980
Ni 4.8513039487675851 3.1170990402897631 -0.8200777061854702
Ni 2.6209669453163698 1.0896310247615379 2.9037775916419046
Ni 3.8841001185333441 5.0129396671033906 2.8443774847715861
Ni -1.6235856918279368 0.1512767252426745 -5.9307942730565530
Ni -2.4093146217312800 3.8900721208009652 4.0298498367219686
Ni 2.5219723872928488 -1.1940573667247403 3.8195256824842740
Ni 0.4508595604699955 3.8405463529393180 0.9020291773200836
Ni -1.3897772962222901 2.5999313129000750 -5.3666464390058231
Ni 3.6738580852031388 4.9242429152082652 0.4027847570762999
Ni 4.7067940489110756 -0.3902228126037782 -0.5258406389844342
Ni -0.9825687184754925 -5.3398099399609116 3.0371749897466098
Ni -5.9057226045044731 -1.5148912995742831 -0.4497094246781611
Ni 1.7693429471897932 -0.3050663967254755 5.9269781767193583
Ni 3.7250088335323985 1.5015791943404362 0.7002166934771262
Ni -1.1534118331972365 0.4798214600377912 -1.8946251957115763
Ni -4.0738457910664740 3.2205637889565999 2.3213366891217091
Ni 1.3475861879187436 1.6238885975026915 0.9468093744709116
Ni 0.3111357863938110 -2.1809145966163954 3.4307967011891152
Ni -0.6879590848229962 0.7930050205272073 2.0134483502553500
Ni -2.1021403786802093 2.6767074439509302 -2.0012188561627018
Ni 2.2490259566211845 -2.8230195217769074 1.9965546557089604
Ni -4.3092639131421109 -2.9712798949236361 3.2468885404676322
Ni -4.5495307741023154 0.2792764927439830 0.5220452217670005
Ni -3.5904369317870044 1.5785761505459530 -5.6834988556913899
Ni -6.8199514884363985 0.3902992471163082 0.7792594346449574
Ni 1.8532579743754982 0.5802019560601389 -3.5653245972497203
Ni 0.0728949216833486 -0.0729711596071623 -0.0014440338081353
Ni 1.2776987449970929 -4.4724259689671619 3.5810486798440677
Ni -2.2263731156054640 0.0832534019394095 0.2592468895930066
Ni 1.0588879667404314 1.4327559708255957 -1.4724328223230967
Ni -0.1551532529107613 3.4290871931041194 5.0726764792507550
Ni 0.1564680664854347 3.6444826282253517 -1.5667276508411287
Ni 1.5904449594164130 -1.8131045462858872 -4.0679885024107598
Ni -0.0102035468834768 -3.7935261146601102 1.5636669949070114
Ni 0.6207707106389082 1.1779429007159687 -5.6349448634955754
Ni 4.3095796750089930 0.4350116621198212 -3.9209093076551893
Ni -5.3869167008183565 1.1284085662369971 2.6214868311232702
Ni 0.4892842910445864 -4.9912643946039150 -3.0427494725331643
Ni 3.8721919830506200 0.5565172536708458 4.8209592615634236
Ni 1.9091428530004533 -4.3694096003234417 0.1235000524663374
Ni 2.3503202730065591 -2.6619803970388936 -6.0496592388082195
Ni -4.1615888096537557 -0.5888653560616105 3.9206557096567218
Ni 5.5267934927469531 -1.2868455206082023 -2.6191334117106524
Ni -3.3471339267870848 3.2568577676176313 -3.9186895178501895
Ni -0.4515403970960920 6.0141258603046435 0.8488280307503248
Ni -5.8662650980648090 0.8066667954405887 -1.4377748959412897
Ni 3.3508088996374013 -2.4162511541048377 -0.2063866214053528
Ni 4.3007058155195041 -4.5722953703930385 -0.1488680439508406

Ni -5.5572088592884192 2.4466106133334327 0.4656242027492612
Ni -4.9462718127124576 -1.1130188296277779 -2.7038642858746358
Ni 2.6377110960765151 -0.2689438465899004 -5.6144156653041781
Ni 1.7743852991933136 -3.1364318444087775 -1.9987645516099852
Ni 1.8902672216655583 2.0278244920878006 5.0852583452220035
Ni 3.7414729752436435 -1.7352668241918399 5.6746958023751946
Ni 1.5394239978466084 -2.7591909318820709 5.3601955666286436
Ni -1.1238868543361809 4.3172411904868371 -3.5911260985712405
Ni -1.7123601190598607 -0.7213241563318086 3.5618442457182060
Ni 1.7193290051710235 5.5766355916966557 1.8541040267817648
Ni -0.1706719710907705 2.0285727742881270 -3.4358551886089028
Ni -3.5811236994864828 -1.6395931158162487 -0.6989778577811673
Ni -0.3402180669653298 4.8450815013393287 3.0388241178099316
Ni 1.2939588672901345 -0.6304644915611156 1.8945585336260338
Ni 5.0935033092285993 0.9578637532678045 2.6968837532073890
Ni -0.4048641701624759 -0.3878505562477819 -3.9950686554097188
Ni 0.5981005785137519 2.5423357702949443 3.0251718479985019
Ni -2.8711234323103891 -4.5941638057453451 4.3970470658152667
Ni -0.2085207654186067 1.0990571779324654 6.0475806712883351
Ni 5.6820091866747111 -2.6015179644396018 -0.4683529454883869
Ni -0.4713405435537047 -1.3334227349665055 5.6275173277405441
Ni 1.4894367221994418 5.5153529447437677 -0.6147220535148527
Ni 3.0276467963536100 4.4370210403242085 -4.4073106160396929
Ni -0.9168237541296931 -1.5781619209251581 1.4683341163882195
Ni -2.5461995895438636 5.1535085098714211 1.9558641688812342
Ni -0.7470234972754848 5.8162541971120758 -1.6464342625800938
Ni 0.5434226038164442 0.2456549959112956 3.9923952316992430
Ni 0.8318352363274596 -0.9381832382479297 -2.0190421941979100

CO_2/Cu_{147}

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O -0.6843654298815330 7.8300170467905685 -4.6175220014951082
O -2.6974467965846887 6.7997201965616227 -5.2440400735916901
Cu -2.5902177497668002 -3.6737874870712774 -1.8623121830113654
Cu 3.2444392800981583 -1.2110875698205879 -2.2834842088831406
Cu -2.4895969900914841 0.9866295289115364 -3.8009515161516991
Cu -2.3365182841317043 2.5293647055412105 6.3519549814263421
Cu -3.1654680639362245 4.8990381579972730 -2.0194347196743405
Cu 2.7523176898529349 -5.5308152158267037 -1.9004519321647766
Cu 4.0645172357656945 -2.1156658802326707 -4.3992882456795401
Cu 0.9746274451987510 -2.3535540502731211 0.1578211942269790
Cu 7.1749083850272806 -0.6205643975579523 -0.7132528963014177
Cu 3.9786508909485545 2.8302749868754744 4.0798829923617141
Cu 5.0281327130034397 -1.4598348004271271 3.7742433006442049
Cu 2.8629311114361840 -6.7704909528692339 0.2921044055075840
Cu 3.7250955574747917 -0.8835881669570930 1.8001191598218638
Cu -2.3201090372075517 -3.5082343658345998 0.6443888477442322
Cu -0.3376264263040624 -4.1643463113450707 -0.8295143041858992

Cu -2.8251869010847357 -2.3933961934391026 5.3040044453514872
Cu -0.9057231776083611 2.0526368478071566 0.0442276620464947
Cu 6.1486824127325805 -1.0519862474752593 1.5455263736966436
Cu -4.8424474333388492 -3.4275332284629791 0.9357743575907680
Cu -2.5692421515096195 -1.3566848167639687 -2.8642144441689004
Cu 0.3452184224889021 -1.3712047945161638 -6.1196785435796137
Cu -3.3584813724270339 -5.1018920234273555 2.1724228069554368
Cu -3.9987986920847098 1.8168618693441072 4.5989534431053372
Cu -3.9088250969791063 -3.1251715161974354 -3.8829471468887400
Cu -3.6578962060601610 0.5820234142283754 -1.5975266742952803
Cu 6.1925752195960833 1.3241429354777752 0.5522581126089726
Cu 4.5267673620579751 2.8464808720039105 -3.2526458281250736
Cu -1.2724020165720764 -1.9068037858054352 -0.8752579294503857
Cu -1.8137120188937135 -4.6131193744329257 -4.0173607383654266
Cu 3.4756953646066284 1.2710444797924025 -1.7081792407389955
Cu -0.4924392097431497 -2.8315167953438682 -3.0001722115176648
Cu 1.1257952468346828 5.2553084759783966 -3.0366045263917609
Cu -1.4000705630765082 -5.8727624132391458 0.7212534305590110
Cu -0.7306662281354411 -3.8841422323351820 5.1708608211016704
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Cu -2.5993672068285871 0.0665768338276766 5.8717099634449763
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Cu 3.4331048640783588 4.8009236388681140 -1.9716971645094810
Cu 1.8804410967159944 4.3200000542074717 4.2141395881308235
Cu 3.5536384556964324 -3.5515491786870812 4.1121516550383248
Cu 0.2976116241606734 -3.7437000209933347 -5.1222220002593106
Cu 5.8941533950724923 1.1230115885893970 -2.0005487826402559
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Cu 0.8000223001373447 3.5887846851757348 -4.9687542399019478
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Cu -3.1755518873290982 0.9131609511424797 2.4851081994515400
Cu -3.4052377461706294 -1.5693858325898615 1.9090857276278763
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Cu 0.9091451117476311 -6.2073471164302116 1.7792845301648197
Cu -1.5531030709382139 1.6423311460813470 4.2745941300517094
Cu 5.1194879359871948 3.2499780046193472 1.8129545026067757
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Cu -4.7273751866811251 2.8907451495063143 -1.7065034917540800
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Cu -2.7943879915847281 6.4693890896548920 -0.0908131546584456
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Cu 2.3927138453173087 3.2084906245653126 -0.4433795650457139
Cu 2.6585470192378327 3.3783284230466712 2.0619386300488722
Cu -2.0060220942611870 -3.2709939942741788 3.1371086954776217
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Cu -1.6545640782592423 -5.9598308446359543 -1.8262096466862261
Cu -3.6571874549928811 -5.3006603697315651 -0.3392025631271056

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Cu 2.0769427631243116 2.9735221242513616 -2.9371599402612514
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Cu -5.0505965238002481 -3.5475095277711435 -1.6147374641320402
Cu -4.3093105011043376 4.4795069735569362 0.2466299102791668
Cu -3.8938378528508761 -5.4187339519062974 -2.8473413771707099
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Cu 2.6350807355467301 1.0621860618498269 3.0649896474471121
Cu 3.9639470729444368 5.1258127377289346 3.0445451488951303
Cu -1.7128650296745196 0.0909546542598401 -5.9830135947181766
Cu -2.5331560441900689 3.9120914846292791 4.2569958819113882
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Cu 0.4049837736308458 3.8659600833661836 1.0322023168346630
Cu -1.4803254532388317 2.5933227900606393 -5.4008722171935899
Cu 3.7267055063422188 5.0013319648439492 0.5377525867621495
Cu 4.8037785406582776 -0.4638676265381964 -0.4484187503131260
Cu -1.0590411761726883 -5.5534048878681173 3.2386199440324930
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Cu 1.7856114575153310 -0.3836701992409953 6.1857067270379522
Cu 3.7707064291932149 1.4734876530659229 0.8191063537589691
Cu -1.2204594341719821 0.4141080958175545 -1.8400126211537664
Cu -4.2309246915339314 3.2252583470313270 2.4754518501334997
Cu 1.3409705381803010 1.6099529685624505 1.0759526921919000
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Cu -2.2012157629359757 2.6560733358448982 -1.9259060563581605
Cu 2.2644078823992890 -2.9599925953854993 2.1325379122524240
Cu -4.4534728150072977 -3.1446671868248441 3.4526795554323106
Cu -4.7356212357586971 0.1622781906076941 0.6505126855663196
Cu -3.7436935272843965 1.5544952795169122 -5.7397166687221040
Cu -7.1068069635309667 0.3218529687826178 0.9125223150006153
Cu 1.8644156265750698 0.5258230976260273 -3.5458583017352128
Cu 0.0352463690417864 -0.1500985126697326 0.1014062767997675
Cu 1.2701632088312704 -4.6376215556544995 3.7618220407356926
Cu -2.3417664139078389 0.0064408543879411 0.3711639415943311
Cu 1.0526540794989185 1.4052363097199081 -1.4113664037293732
Cu -0.2299966600744353 3.4540119971060252 5.3214670965554429
Cu 0.1133707262357229 3.6580927615086272 -1.4892246833277893
Cu 1.6228778442593492 -1.9374318156981420 -4.0736949190861456
Cu -0.0398418584827459 -3.9601734994141720 1.6960236182463198
Cu 0.5988127292697704 1.1323118419454454 -5.6638286832688802
Cu 4.3733909622318325 0.3786451590417693 -3.9123692285642440
Cu -5.5931537352120548 1.0797807095824783 2.7769740991382030
Cu 0.4740932515513642 -5.1801728935611022 -3.0109969565983352
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Cu 1.9212083071200565 -4.5739125685701740 0.2190665251473778
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Cu -4.3027187342613020 -0.6786984928020344 4.1126581387632477

Cu 5.6612816039017329 -1.3808636118027693 -2.5776492327278624
Cu -3.4885285989563179 3.2546908684298423 -3.9083993657289788
Cu -0.5389060940430418 6.1140715570567856 0.9727171361997464
Cu -6.0810517462997149 0.7477246737602282 -1.3448493469506209
Cu 3.3981934614658589 -2.5438142628065461 -0.1119917835333268
Cu 4.3760952164703246 -4.7804313075686533 -0.0472972261189066
Cu -5.7501518387772510 2.4199243872478560 0.5841081383512110
Cu -5.1053546287626919 -1.2200983993217751 -2.6594277720496473
Cu 2.6720716619100244 -0.3616365745263826 -5.6721817316837901
Cu 1.7884460412283871 -3.2877450192333679 -1.9484823176103283
Cu 1.8807877932605648 2.0107220759021098 5.3029904058661028
Cu 3.8183822678325079 -1.8472533178071699 5.9408570618957670
Cu 1.5528673663373915 -2.8906289218685184 5.6038580966549159
Cu -1.1956323718202460 4.3137691041863029 -3.5441322852352171
Cu -1.7934274608870500 -0.8228594015731797 3.7461160387751615
Cu 1.7219328012987767 5.6659921011221925 2.0236149839124327
Cu -0.2060825599531207 1.9983089600927850 -3.4095359748354097
Cu -3.7017574400222730 -1.7727312034949565 -0.6165006156370936
Cu -0.4068506202261791 4.8861884173221526 3.2114030325841281
Cu 1.2898825433592485 -0.7138268640210391 2.0423149904846709
Cu 5.1703402355683048 0.9201876777219632 2.8605952415293459
Cu -0.4391706413885951 -0.4794569382999617 -3.9873572024990835
Cu 0.5592856327416852 2.5372297092836393 3.2007655312414354
Cu -3.0085732930409077 -4.8217649882957776 4.6535143411771180
Cu -0.2757575627108687 1.0792318863037602 6.3190299595127275
Cu 5.8182369628262993 -2.7226702417561355 -0.3856829359102034
Cu -0.5269581716121573 -1.4287886365202296 5.8652672062198414
Cu 1.4693437834536491 5.5710177865323978 -0.5208532084357462
Cu 3.0804962141715184 4.5283633705276189 -4.4506650515013009
Cu -0.9812003831834540 -1.7047366526675340 1.6135789087439325
Cu -2.6890121769045598 5.2305725743555032 2.1017127457574336
Cu -0.8410203981655476 5.9013885634540735 -1.5726773682608801
Cu 0.5089905628331365 0.1814940207690638 4.1893873180091727
Cu 0.8237015147312838 -1.0408721743922575 -1.9797305008284352

CO/Cu_{147}

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Cu -2.6788358642128896 -3.5975875032443385 -1.8881809267284630
Cu 3.1525322368036437 -1.1465890753204957 -2.2980382761371674
Cu -2.5968455596044477 1.0577525921289164 -3.8369151367989720
Cu -2.4161548647407640 2.5862727038408009 6.3393451043460605
Cu -3.2601311110922828 4.9693110964865967 -2.0403043923376187
Cu 2.6616411333122922 -5.4622084744132504 -1.9169953478220312
Cu 3.9735290232703253 -2.0504423183224652 -4.4137197594146498
Cu 0.8894708031092202 -2.2837606174361018 0.1437313760800738
Cu 7.0858577629885389 -0.5597630653475834 -0.7230768850343801
Cu 3.8934648271537573 2.8850986417642122 4.0721317710122840

Cu 4.9417354448592636 -1.4050214670370484 3.7728041216346426
Cu 2.7721094745623418 -6.7025205195064688 0.2724558718838743
Cu 3.6384150230384233 -0.8225305236296261 1.7948161999057017
Cu -2.4064499049116397 -3.4323847483349712 0.6183047984068740
Cu -0.4245430027168031 -4.0911710905801479 -0.8487791727731442
Cu -2.9120893617536066 -2.3207396331080319 5.2830342227697500
Cu -0.9966967506203033 2.1170820550056852 0.0247051801013184
Cu 6.0612411335004399 -0.9873888313054686 1.5383062132437346
Cu -4.9334385537067069 -3.3482740042141166 0.9141054990580679
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Cu 5.0206280786601640 0.9312161487811581 2.6846767973003955
Cu -0.5927722646452965 -0.4445584091126045 -4.1727250302891123
Cu 0.3986652739845352 2.5409786942664843 3.0195060274382781
Cu -3.1531951068966197 -4.8022867268854830 4.4777915493106999
Cu -0.4199535847024572 1.0929774960647012 6.1403691930216304
Cu 5.6752873487549866 -2.7053347535677243 -0.5606026886465677
Cu -0.6698391759232328 -1.4132918235548966 5.6876657280594349
Cu 1.3100720089805500 5.5910949374135841 -0.7110857014493747
Cu 2.9306829871337228 4.5470780574532688 -4.6364871271808106
Cu -1.1235932211222135 -1.6828526927046070 1.4390967924489908
Cu -2.8361030355002566 5.2434627976899035 1.9188248778045791
Cu -0.9931098601774099 5.9279832525171843 -1.7590822860270681
Cu 0.3677498229564701 0.1923554074430205 4.0133347879045900
Cu 0.6775630767186364 -1.0148247265956154 -2.1624399445753713

H_2/Cu_{147}

H 3.2556407015806754 -3.4453383895046814 -7.4816119464133646

H 2.7011042335473547 -3.0492864990577937 -7.8800490790105204
Cu -2.6723824247095247 -3.4734669701860055 -1.8565631518887107
Cu 3.1654619782666997 -1.0121247757645087 -2.2641504262522871
Cu -2.5834409671152327 1.1963291900945818 -3.8120933522502805
Cu -2.3907629321198325 2.7068833243883930 6.3255207322717188
Cu -3.2481242535354680 5.0989895837841130 -2.0226901218481976
Cu 2.6692744461489712 -5.3357604470632944 -1.8839432388838449
Cu 3.9894762341996284 -1.9121346575004745 -4.3711910909066694
Cu 0.8989702064093167 -2.1606495882989831 0.1736271810379886
Cu 7.0992385776243196 -0.4283024582033845 -0.7021675726451978
Cu 3.9084148934467517 3.0126315649618420 4.0869209683168251
Cu 4.9583401181956575 -1.2773031699577868 3.7958618555251173
Cu 2.7827125439264000 -6.5796985922649274 0.3047992380115979
Cu 3.6536614523271576 -0.6970531485130984 1.8164632946789971
Cu -2.3971567708625976 -3.3150442054523777 0.6478203775399205
Cu -0.4149824201162698 -3.9680394969176302 -0.8211887642269114
Cu -2.9021003578419076 -2.2049530704222913 5.3043794456535114
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Cu 6.0765022113363472 -0.8642267795814451 1.5596005251930911
Cu -4.9212455214835469 -3.2318528801904680 0.9366952413381543
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Cu -4.5291626104820475 -2.9521483842308669 3.4522667043698774
Cu -4.8115536569182158 0.3555888963281440 0.6364360404203120
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Cu 1.7808677706091747 0.7303571055227986 -3.5313094490820007

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Cu 0.0330361046007146 3.8586119794218163 -1.4977052635919745
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Cu -0.1164898359592671 -3.7710634261710880 1.7066265244470153
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Cu 4.2936934200924703 0.5783821085847339 -3.9025464335424287
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Cu 5.5841232296022820 -1.1819224281894325 -2.5615800434383389
Cu -3.5710821800627786 3.4601098684661515 -3.9210556371148129
Cu -0.6080889129606643 6.3030033953842759 0.9700801532524320
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Cu 4.2961711331522423 -4.5898243221096502 -0.0350283696703780
Cu -5.8234465713555812 2.6137510922501894 0.5822712947536843
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Cu 1.8189827931613931 2.1918096472800603 5.3059854218007301
Cu 3.7573573458836442 -1.6698636596697272 5.9771401646452533
Cu 1.4875187483790160 -2.7048537016578842 5.6162038965028351
Cu -1.2803522302889556 4.5435048429317444 -3.5616375455647820
Cu -1.8634161526806072 -0.6405214028900208 3.7425082300865280
Cu 1.6553454980975497 5.8503364163061153 2.0238705998935278
Cu -0.2962985332706062 2.2036965729390268 -3.4115179322041222
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Cu 1.2261793586160463 -0.5295756354310375 2.0566251801123197
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Cu -0.5305054465632096 -0.2697996044896842 -3.9787754367261376
Cu 0.4969281725365720 2.7209241638373265 3.1972800169342439
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Cu -0.3364311276516881 1.2590075624138861 6.3133176483384803
Cu 5.7421314318646832 -2.5317209941571748 -0.3724738168654512
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Cu 1.3957849640914868 5.7663744371385564 -0.5203929409613975
Cu 3.0007077849211994 4.7265939348475392 -4.4456730891855996
Cu -1.0542731772563165 -1.5159356732529394 1.6166337914285667
Cu -2.7508840264512511 5.4209507986087733 2.0955083131658188
Cu -0.9139651067797182 6.1065158730797400 -1.5774371080463923
Cu 0.4500797261397610 0.3612569945582483 4.1888398302463674

Cu 0.7449712489763113 -0.8429681069763904 -1.9720021065003042

D Substrates Using the Slab Model

CO_2/Co(0001)
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-3.6990350946536101 6.4069167229204034 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.9693238884347757
C O Co
1 2 45
Selective dynamics
Direct
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0.8909120656136058 0.1130539700607809 0.2932887552049904 T T T
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CO/Co(0001)
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-3.6990350946536101 6.4069167229204034 0.0000000000000000
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C O Co
1 1 45
Selective dynamics
Direct
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H_2O/Co(0001)
1.00000000000000
7.3980701893072203 0.0000000000000000 0.0000000000000000
-3.6990350946536101 6.4069167229204034 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.9693238884347757
O H Co
1 2 45
Selective dynamics
Direct
0.2431391441430189 0.4432111458587665 0.3816674074602308 T T T
0.3892753932446276 0.5527996102676691 0.3854847822235345 T T T
0.2453008739633414 0.3128208514182333 0.3858981850377472 T T T
0.2225388256743264 0.1087622277655861 0.2937576110466743 T T T
0.5555827618621699 0.1109604331931413 0.2948970726239767 T T T
0.8878968045742569 0.1093045518917969 0.2942864327543849 T T T
0.2223806923986426 0.4441679018632507 0.2990306130303808 T T T
0.5576291150814924 0.4443273686776760 0.2939518602796575 T T T
0.8877298165478564 0.4439703422186259 0.2944093983696498 T T T
0.2230504590777651 0.7793091515462806 0.2943445760096958 T T T
0.5581297170968010 0.7799836642299671 0.2938258760805081 T T T
0.8890088011056140 0.7776468411148167 0.2950058171650332 T T T
0.1121574088278742 0.2244182252359979 0.2225795103680297 T T T
0.4446769004864867 0.2218694259068632 0.2216963903008008 T T T
0.7775929655734640 0.2218591121146642 0.2219912400745119 T T T
0.1122618030605394 0.5542760631743804 0.2227738577440895 T T T
0.4417732402376671 0.5540967435507409 0.2226151090877783 T T T
0.7781147800730291 0.5557523601409533 0.2218783617416792 T T T
0.1106914837588557 0.8882274779019742 0.2217560402676348 T T T

0.4444997622939584 0.8889798998744513 0.2217488729334497 T T T
0.7783594862574625 0.8886078509482233 0.2217533488734809 T T T
0.2218845959736818 0.1109919491747068 0.1475690354418555 T T T
0.5556593514797761 0.1109668752890856 0.1469676428458627 T T T
0.8892365267396651 0.1110743983557707 0.1475870228646236 T T T
0.2220253441617985 0.4442292587954753 0.1470988775534415 T T T
0.5551915578053956 0.4443589301975586 0.1476109732104162 T T T
0.8891598401366788 0.4443312137020052 0.1476648050883266 T T T
0.2219328825778154 0.7771360851253913 0.1476115447553756 T T T
0.5553767875263482 0.7771952319505185 0.1475813470412393 T T T
0.8887577770029557 0.7773898882312698 0.1469276256654446 T T T
0.1111111111111143 0.2222222222222214 0.0726695292043260 F F F
0.4444444444444429 0.2222222222222214 0.0726695292043260 F F F
0.7777777777777786 0.2222222222222214 0.0726695292043260 F F F
0.1111111111111143 0.5555555555555571 0.0726695292043260 F F F
0.4444444444444429 0.5555555555555571 0.0726695292043260 F F F
0.7777777777777786 0.5555555555555571 0.0726695292043260 F F F
0.1111111111111143 0.8888888888888857 0.0726695292043260 F F F
0.4444444444444429 0.8888888888888857 0.0726695292043260 F F F
0.7777777777777786 0.8888888888888857 0.0726695292043260 F F F
0.2222222222222214 0.1111111111111143 0.0000000000000000 F F F
0.5555555555555571 0.1111111111111143 0.0000000000000000 F F F
0.8888888888888857 0.1111111111111143 0.0000000000000000 F F F
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0.8888888888888857 0.7777777777777786 0.0000000000000000 F F F

H_2/Co(0001)
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-3.6990350946536101 6.4069167229204034 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.9693238884347757
H Co
2 45
Selective dynamics
Direct
0.4960581525989438 0.4472210323191337 0.3543128858187125 T T T
0.6212120207037409 0.4469855502900560 0.3540854858239331 T T T
0.2213557003747515 0.1102372194274673 0.2941928448148353 T T T
0.5560103166371101 0.1102015524040147 0.2941897700525775 T T T
0.8893244754155771 0.1115492479759985 0.2942858005159472 T T T
0.2221482624359874 0.4447398281716519 0.2945578816132945 T T T
0.5557465913039745 0.4440727548405708 0.2981899903790964 T T T
0.8898230996697424 0.4447709651144074 0.2945163164275538 T T T
0.2225315761700341 0.7779595551713061 0.2949467288295641 T T T
0.5560782863182153 0.7789837089275179 0.2942059605666733 T T T

0.8901461793228999 0.7790709367169750 0.2941550642623348 T T T
0.1110671792225595 0.2223597511902694 0.2218745994570815 T T T
0.4457811730523759 0.2245249687452352 0.2223532257847486 T T T
0.7783163210753511 0.2223564608473795 0.2218702568418650 T T T
0.1114858149155741 0.5558509479011019 0.2221907625015844 T T T
0.4454853983835435 0.5549155515898767 0.2222105164876575 T T T
0.7765544076286232 0.5549705578756510 0.2221895796075684 T T T
0.1116801106980470 0.8889573370502079 0.2219760461515309 T T T
0.4442629652775437 0.8888867176842773 0.2219932111836215 T T T
0.7782169156802017 0.8894325408496452 0.2217319021966737 T T T
0.2227078085756045 0.1115524977118647 0.1477405113232300 T T T
0.5557035754723285 0.1115618806716018 0.1477388429934354 T T T
0.8891751654645581 0.1114712005210098 0.1470424870612581 T T T
0.2224655198042343 0.4450254177245002 0.1477561382588015 T T T
0.5560671658522827 0.4451890722164217 0.1469289678754229 T T T
0.8894065683222454 0.4450434624926061 0.1477369776761875 T T T
0.2224877131114416 0.7781826801524373 0.1470416959563134 T T T
0.5556466002647373 0.7782491704393721 0.1477362949393778 T T T
0.8894643268616322 0.7782565683636442 0.1477167003445584 T T T
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0.4444444444444429 0.2222222222222214 0.0726695292043260 F F F
0.7777777777777786 0.2222222222222214 0.0726695292043260 F F F
0.1111111111111143 0.5555555555555571 0.0726695292043260 F F F
0.4444444444444429 0.5555555555555571 0.0726695292043260 F F F
0.7777777777777786 0.5555555555555571 0.0726695292043260 F F F
0.1111111111111143 0.8888888888888857 0.0726695292043260 F F F
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0.7777777777777786 0.8888888888888857 0.0726695292043260 F F F
0.2222222222222214 0.1111111111111143 0.0000000000000000 F F F
0.5555555555555571 0.1111111111111143 0.0000000000000000 F F F
0.8888888888888857 0.1111111111111143 0.0000000000000000 F F F
0.2222222222222214 0.4444444444444429 0.0000000000000000 F F F
0.5555555555555571 0.4444444444444429 0.0000000000000000 F F F
0.8888888888888857 0.4444444444444429 0.0000000000000000 F F F
0.2222222222222214 0.7777777777777786 0.0000000000000000 F F F
0.5555555555555571 0.7777777777777786 0.0000000000000000 F F F
0.8888888888888857 0.7777777777777786 0.0000000000000000 F F F

CO_2/Ni(111)
1.00000000000000
7.3727437355057734 0.0000000000000000 0.0000000000000000
-3.6863718677528867 6.3849833705405779 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.0330334201612921
C O Ni
1 2 45
Selective dynamics
Direct
0.6436822775424488 0.4462125707541560 0.3692883686211776 T T T
0.8163143609827277 0.4466292772861735 0.3712629082683449 T T T

0.5194909550674041 0.4462355081409045 0.3985439007211242 T T T
0.2212765264935754 0.1106064175103079 0.2964737528946247 T T T
0.5519530287299717 0.1062842238500543 0.2961660776823972 T T T
0.8881661958598257 0.1092948217689557 0.2965735252053310 T T T
0.2237522685430836 0.4448518893212426 0.2967824569437315 T T T
0.5554355429251241 0.4440651781171706 0.3006336338226933 T T T
0.8891632807003953 0.4441101416081632 0.3015927269065513 T T T
0.2231612778155714 0.7785644827710166 0.2964203292404348 T T T
0.5546317842935022 0.7775505307480288 0.2967555172542495 T T T
0.8892010173105307 0.7812666341935126 0.2960802908409284 T T T
0.9988532643586939 0.0003374301634722 0.2224283804348436 T T T
0.3321211476231306 0.0004368847229513 0.2224373454003777 T T T
0.6659324547459661 0.0002993832966989 0.2225456959776481 T T T
0.9980341313041736 0.3350009881264375 0.2240857367129616 T T T
0.3328460207954971 0.3340928055152496 0.2228249634249547 T T T
0.6657723784522086 0.3345453373415924 0.2234205294152559 T T T
0.9978389793888144 0.6646435438265380 0.2232478400513517 T T T
0.3324666623842378 0.6665947853904882 0.2225062741478173 T T T
0.6649893837264580 0.6653102495270301 0.2227988871885211 T T T
0.1096108543188071 0.2218887202797241 0.1483516301424570 T T T
0.4434009178343543 0.2223561535119369 0.1485305175420449 T T T
0.7772839191206595 0.2227812726963323 0.1487737056544943 T T T
0.1100313432289661 0.5551395436437778 0.1486323676720185 T T T
0.4434842926141758 0.5553771191832255 0.1484361547480203 T T T
0.7772044945646601 0.5557275858756289 0.1485846199254841 T T T
0.1103034524627187 0.8890904992782533 0.1484013458599231 T T T
0.4436523737147556 0.8889872837784865 0.1483226833121616 T T T
0.7770836519849151 0.8892817572906990 0.1482201415928248 T T T
0.2222222222222214 0.1111111111111143 0.0740727112510271 F F F
0.5555555555555571 0.1111111111111143 0.0740727112510271 F F F
0.8888888888888857 0.1111111111111143 0.0740727112510271 F F F
0.2222222222222214 0.4444444444444429 0.0740727112510271 F F F
0.5555555555555571 0.4444444444444429 0.0740727112510271 F F F
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0.5555555555555571 0.7777777777777786 0.0740727112510271 F F F
0.8888888888888857 0.7777777777777786 0.0740727112510271 F F F
0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.3333333333333357 0.0000000000000000 0.0000000000000000 F F F
0.6666666666666643 0.0000000000000000 0.0000000000000000 F F F
0.0000000000000000 0.3333333333333357 0.0000000000000000 F F F
0.3333333333333357 0.3333333333333357 0.0000000000000000 F F F
0.6666666666666643 0.3333333333333357 0.0000000000000000 F F F
0.0000000000000000 0.6666666666666643 0.0000000000000000 F F F
0.3333333333333357 0.6666666666666643 0.0000000000000000 F F F
0.6666666666666643 0.6666666666666643 0.0000000000000000 F F F

CO/Ni(111)
7.3727437355057734 0.0000000000000000 0.0000000000000000

-3.6863718677528867 6.3849833705405779 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.0330334201612921
C O Ni
1 1 45
Selective dynamics
Direct
0.4483014735238360 0.5596200881188820 0.3486776344997037 T T T
0.4498829387539615 0.5609945860439371 0.3926372269734362 T T T
0.2226130606366086 0.1104087700654831 0.2966554034202945 T T T
0.5575269404874810 0.1133745117970490 0.2968452340515620 T T T
0.8907960623283409 0.1134267907995393 0.2968442591376564 T T T
0.2239607626577266 0.4464911152391570 0.2998295344220769 T T T
0.5576744166791693 0.4463868988364288 0.2996266508112221 T T T
0.8907138145279027 0.4463307722046332 0.2968599887777587 T T T
0.2225773604031877 0.7810421000275772 0.2966760968237943 T T T
0.5578721384910323 0.7808226794510278 0.2994018821009758 T T T
0.8933045650186155 0.7811709644976207 0.2966575280379533 T T T
0.0008709794690223 0.0016912309786925 0.2227464277528767 T T T
0.3351881801003404 0.0016700795875668 0.2227776563074807 T T T
0.6676952754365727 0.0010343303175911 0.2230387921890056 T T T
0.0018410172119522 0.3351466161957959 0.2231269883299295 T T T
0.3347847660665308 0.3354457295707644 0.2227995322856391 T T T
0.6675530825034732 0.3350456680157942 0.2230768719614441 T T T
0.0008861436988358 0.6675215290946712 0.2227553911891953 T T T
0.3347491653275159 0.6676604583625489 0.2227316961828929 T T T
0.6672549421437944 0.6678279406439667 0.2227123874677765 T T T
0.1113025362977309 0.2229274141640158 0.1484903545970621 T T T
0.4452262675799474 0.2229031182766220 0.1485061584693629 T T T
0.7782837205743042 0.2228551659074298 0.1481479844681562 T T T
0.1112738400670284 0.5559433132669603 0.1484685978581130 T T T
0.4450004692791443 0.5563074662908379 0.1485407966429843 T T T
0.7783623225511962 0.5559401858578948 0.1484893697188617 T T T
0.1116922532536996 0.8897064692941155 0.1484823439879759 T T T
0.4452642967252379 0.8899134859891994 0.1484596539871737 T T T
0.7784127339641780 0.8899612755422661 0.1484585814019709 T T T
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0.5555555555555571 0.1111111111111143 0.0740727112510271 F F F
0.8888888888888857 0.1111111111111143 0.0740727112510271 F F F
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0.5555555555555571 0.7777777777777786 0.0740727112510271 F F F
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0.3333333333333357 0.0000000000000000 0.0000000000000000 F F F
0.6666666666666643 0.0000000000000000 0.0000000000000000 F F F
0.0000000000000000 0.3333333333333357 0.0000000000000000 F F F
0.3333333333333357 0.3333333333333357 0.0000000000000000 F F F

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0.0000000000000000 0.6666666666666643 0.0000000000000000 F F F
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0.6666666666666643 0.6666666666666643 0.0000000000000000 F F F

H_2O/Ni(111)
1.00000000000000
7.3727437355057734 0.0000000000000000 0.0000000000000000
-3.6863718677528867 6.3849833705405779 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.0330334201612921
O H Ni
1 2 45
Selective dynamics
Direct
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0.3906744458363135 0.5220344458285332 0.3850739374175721 T T T
0.2075394934083480 0.2924151379447524 0.3849659501868494 T T T
0.2212564459814063 0.1079584203135402 0.2962017592715754 T T T
0.5549245049378951 0.1099457053036326 0.2968111058000537 T T T
0.8872888384608801 0.1082366728746178 0.2966122174760002 T T T
0.2213324996128659 0.4441323770739492 0.3013636358148367 T T T
0.5571236086340904 0.4438549447460119 0.2962400803663133 T T T
0.8867134452224912 0.4436276232224509 0.2967858897454334 T T T
0.2215056807685864 0.7783391599859937 0.2967390745124753 T T T
0.5575010620223529 0.7785417099767877 0.2964057001365671 T T T
0.8880073891891497 0.7768344637647723 0.2973152994301260 T T T
-0.0005453484859088 -0.0009243729800726 0.2226520855443382 T T T
0.3333547157186810 -0.0008921078533097 0.2224649518582555 T T T
0.6664109206705958 -0.0004663661881292 0.2224364883164460 T T T
0.0014585275674518 0.3335077545327336 0.2238209858029213 T T T
0.3320495322827677 0.3332285556762907 0.2234469278226544 T T T
0.6664019982191652 0.3321587162707726 0.2224842616113942 T T T
-0.0004422824822095 0.6658433556153773 0.2228548232149937 T T T
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0.6662593425741232 0.6658172119317828 0.2225932229303149 T T T
0.1108978595232194 0.2220229684406822 0.1486181875000603 T T T
0.4441786513029718 0.2218689350886609 0.1485166920354211 T T T
0.7779128051548787 0.2219650513588082 0.1484735487812749 T T T
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0.4438422130335163 0.5549842681256336 0.1485848811772816 T T T
0.7777034775691604 0.5551410536947914 0.1483698802294518 T T T
0.1108506192321156 0.8883127355980132 0.1483854391549437 T T T
0.4441850689981830 0.8881808189246304 0.1484667239636833 T T T
0.7775786848066176 0.8884212896088337 0.1483017346787995 T T T
0.2222222222222214 0.1111111111111143 0.0740727112510271 F F F
0.5555555555555571 0.1111111111111143 0.0740727112510271 F F F
0.8888888888888857 0.1111111111111143 0.0740727112510271 F F F
0.2222222222222214 0.4444444444444429 0.0740727112510271 F F F
0.5555555555555571 0.4444444444444429 0.0740727112510271 F F F

0.8888888888888857 0.4444444444444429 0.0740727112510271 F F F
0.2222222222222214 0.7777777777777786 0.0740727112510271 F F F
0.5555555555555571 0.7777777777777786 0.0740727112510271 F F F
0.8888888888888857 0.7777777777777786 0.0740727112510271 F F F
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0.3333333333333357 0.0000000000000000 0.0000000000000000 F F F
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0.3333333333333357 0.3333333333333357 0.0000000000000000 F F F
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0.6666666666666643 0.6666666666666643 0.0000000000000000 F F F

H_2/Ni(111)
1.00000000000000
7.3727437355057734 0.0000000000000000 0.0000000000000000
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0.0000000000000000 0.0000000000000000 27.0330334201612921
H Ni
2 45
Selective dynamics
Direct
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0.6090218411301862 0.4416275629217506 0.3572135963855579 T T T
0.2189134247870327 0.1082293219010678 0.2965258893259343 T T T
0.5541752442675352 0.1085087164036834 0.2965980391210426 T T T
0.8878343185374052 0.1109428361129291 0.2965822418526923 T T T
0.2195704103537471 0.4448846314236108 0.2969522036519796 T T T
0.5543928642023914 0.4441731843430629 0.3010434591982390 T T T
0.8902161935855075 0.4448559465948448 0.2970103973829426 T T T
0.2211846488863220 0.7775821736329610 0.2969349831876982 T T T
0.5540571868613929 0.7799540794367628 0.2965834159468732 T T T
0.8903894817323513 0.7795747235691681 0.2965478472345890 T T T
-0.0007905816504156 -0.0001439002124318 0.2224993833658731 T T T
0.3327274182880918 -0.0000539431253919 0.2226053186122711 T T T
0.6661511060174287 0.0000526082725733 0.2225338578799985 T T T
-0.0005694483429329 0.3334378361341259 0.2227208717934371 T T T
0.3343674303424247 0.3341581870573802 0.2234322850365839 T T T
0.6652010882802677 0.3344586024220528 0.2235429213642374 T T T
-0.0008537921197257 0.6663603656440660 0.2226496185364490 T T T
0.3327189922091044 0.6663159290807146 0.2226410969943766 T T T
0.6649597333644979 0.6647531778351774 0.2233374160592107 T T T
0.1105257661602729 0.2221129038091143 0.1484885081385053 T T T
0.4444315249786093 0.2225193962419271 0.1486259338304567 T T T
0.7776872198415643 0.2222193862176345 0.1485087892991936 T T T
0.1107852033791023 0.5554800308775221 0.1483285156735286 T T T
0.4442670494714280 0.5553652573899259 0.1485647949186910 T T T
0.7772070914438759 0.5553976374163351 0.1485771441329472 T T T

0.1108201816476777 0.8888802875791985 0.1482733820737491 T T T
0.4441531849895458 0.8888083728642581 0.1482942239831120 T T T
0.7775873852750274 0.8891514392979821 0.1484409420250433 T T T
0.2222222222222214 0.1111111111111143 0.0740727112510271 F F F
0.5555555555555571 0.1111111111111143 0.0740727112510271 F F F
0.8888888888888857 0.1111111111111143 0.0740727112510271 F F F
0.2222222222222214 0.4444444444444429 0.0740727112510271 F F F
0.5555555555555571 0.4444444444444429 0.0740727112510271 F F F
0.8888888888888857 0.4444444444444429 0.0740727112510271 F F F
0.2222222222222214 0.7777777777777786 0.0740727112510271 F F F
0.5555555555555571 0.7777777777777786 0.0740727112510271 F F F
0.8888888888888857 0.7777777777777786 0.0740727112510271 F F F
0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.3333333333333357 0.0000000000000000 0.0000000000000000 F F F
0.6666666666666643 0.0000000000000000 0.0000000000000000 F F F
0.0000000000000000 0.3333333333333357 0.0000000000000000 F F F
0.3333333333333357 0.3333333333333357 0.0000000000000000 F F F
0.6666666666666643 0.3333333333333357 0.0000000000000000 F F F
0.0000000000000000 0.6666666666666643 0.0000000000000000 F F F
0.3333333333333357 0.6666666666666643 0.0000000000000000 F F F
0.6666666666666643 0.6666666666666643 0.0000000000000000 F F F

CO_2/Cu(111)
1.00000000000000
7.5604597440039107 0.0000000000000000 0.0000000000000000
-3.7802298720019554 6.5475502025969803 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.2884825520348429
C O Cu
1 2 45
Selective dynamics
Direct
0.3925604264256219 0.4430664442434463 0.4215834315936930 T T T
0.5497332998144542 0.4471599688072944 0.4216739845227253 T T T
0.2354446887019983 0.4390978074302068 0.4217883761086120 T T T
0.2223539135542238 0.1112549964899505 0.3015183761543658 T T T
0.5556514385991098 0.1111030267160393 0.3017106237191858 T T T
0.8888648725926808 0.1111000600159738 0.3017117762838240 T T T
0.2222581773252554 0.4445965892206887 0.3013505882103770 T T T
0.5558034744546956 0.4445831727935309 0.3013016294580163 T T T
0.8890219500234922 0.4445701996834167 0.3015822403382092 T T T
0.2223889837426840 0.7780714492796831 0.3017173778711054 T T T
0.5556893679868754 0.7779641686283192 0.3015372572581794 T T T
0.8891327810969027 0.7780845936594816 0.3017157484025757 T T T
0.0000665117001925 0.0001672100928809 0.2257823106466199 T T T
0.3335261903644967 0.0001651868346832 0.2257802707698881 T T T
0.6668464611857587 0.0002538734574686 0.2258165126994353 T T T
-0.0000939191048189 0.3333354662787589 0.2257452412248272 T T T
0.3333768888204331 0.3333299341848153 0.2256737542799769 T T T
0.6668640418828149 0.3333296677838961 0.2257483369218824 T T T

0.0001529378509706 0.6668625173470567 0.2258893747424807 T T T
0.3334840852672096 0.6669997506712932 0.2257302085119256 T T T
0.6669400184964009 0.6669860218218546 0.2257341647293828 T T T
0.1112446719579514 0.2223209825988794 0.1508187884268818 T T T
0.4444697833085393 0.2223321232731663 0.1508197276202767 T T T
0.7778864137420193 0.2223537766768360 0.1508220888637410 T T T
0.1110405104129305 0.5556675597074900 0.1508332654963228 T T T
0.4445589720238822 0.5556956080604907 0.1508018055637206 T T T
0.7780006244589295 0.5556589215733383 0.1508345611380705 T T T
0.1111687964942436 0.8889284724902797 0.1508508291392620 T T T
0.4446244723023582 0.8889815769382939 0.1508313692441774 T T T
0.7777459898667871 0.8889844064107216 0.1508304748453795 T T T
0.2222222222222214 0.1111111111111143 0.0758738322541390 F F F
0.5555555555555571 0.1111111111111143 0.0758738322541390 F F F
0.8888888888888857 0.1111111111111143 0.0758738322541390 F F F
0.2222222222222214 0.4444444444444429 0.0758738322541390 F F F
0.5555555555555571 0.4444444444444429 0.0758738322541390 F F F
0.8888888888888857 0.4444444444444429 0.0758738322541390 F F F
0.2222222222222214 0.7777777777777786 0.0758738322541390 F F F
0.5555555555555571 0.7777777777777786 0.0758738322541390 F F F
0.8888888888888857 0.7777777777777786 0.0758738322541390 F F F
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0.6666666666666643 0.0000000000000000 0.0000000000000000 F F F
0.0000000000000000 0.3333333333333357 0.0000000000000000 F F F
0.3333333333333357 0.3333333333333357 0.0000000000000000 F F F
0.6666666666666643 0.3333333333333357 0.0000000000000000 F F F
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0.6666666666666643 0.6666666666666643 0.0000000000000000 F F F

CO/Cu(111)
1.00000000000000
7.5604597440039107 0.0000000000000000 0.0000000000000000
-3.7802298720019554 6.5475502025969803 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.2884825520348429
C O Cu
1 1 45
Selective dynamics
Direct
0.4491236277841788 0.5610430235618701 0.3558974087143274 T T T
0.4514946795117876 0.5642333654457796 0.3990198198549141 T T T
0.2214351135978275 0.1093276538805075 0.3012461478760619 T T T
0.5555525525156669 0.1117717474730959 0.3020149807196358 T T T
0.8900539516418139 0.1119998139235742 0.3020412925435999 T T T
0.2219827676209316 0.4448594065556641 0.3040906627419013 T T T
0.5569005737584644 0.4446228606823903 0.3037812360146008 T T T
0.8897753357018524 0.4455074091779532 0.3021136389563450 T T T
0.2213289267376287 0.7795286476465533 0.3011523464389382 T T T

0.5572887453863944 0.7808032847332498 0.3031842657608118 T T T
0.8918725225706472 0.7795995605853921 0.3011122104341286 T T T
-0.0002976796177097 0.0005268256589452 0.2257537201196779 T T T
0.3341726072597023 0.0005143122470336 0.2257590313764310 T T T
0.6661522052787320 -0.0011623011410320 0.2264373900255314 T T T
0.0022976115711487 0.3346710625152954 0.2266448549915842 T T T
0.3338714423385472 0.3343752552927590 0.2256804661822767 T T T
0.6659397812401400 0.3345684055228625 0.2265779600692409 T T T
-0.0003384706500836 0.6659528313884545 0.2257404357497544 T T T
0.3338390934530839 0.6664031516736996 0.2254935547740609 T T T
0.6660024955576630 0.6664452926685690 0.2254049663046351 T T T
0.1108136595638337 0.2220536514686834 0.1509325649307120 T T T
0.4445476581120908 0.2220389953751845 0.1509283250165276 T T T
0.7778718817099862 0.2223546560402197 0.1515968131916350 T T T
0.1107587943137915 0.5553891577124669 0.1508765704237593 T T T
0.4443620969983458 0.5554559399856658 0.1506753968932673 T T T
0.7779856974310215 0.5553885235146886 0.1508468229332001 T T T
0.1110940837233886 0.8888758689899751 0.1509843115848024 T T T
0.4445702194241270 0.8892648191810347 0.1508578399657475 T T T
0.7780350675277680 0.8892995070461371 0.1508321381822808 T T T
0.2222222222222214 0.1111111111111143 0.0758738322541390 F F F
0.5555555555555571 0.1111111111111143 0.0758738322541390 F F F
0.8888888888888857 0.1111111111111143 0.0758738322541390 F F F
0.2222222222222214 0.4444444444444429 0.0758738322541390 F F F
0.5555555555555571 0.4444444444444429 0.0758738322541390 F F F
0.8888888888888857 0.4444444444444429 0.0758738322541390 F F F
0.2222222222222214 0.7777777777777786 0.0758738322541390 F F F
0.5555555555555571 0.7777777777777786 0.0758738322541390 F F F
0.8888888888888857 0.7777777777777786 0.0758738322541390 F F F
0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.3333333333333357 0.0000000000000000 0.0000000000000000 F F F
0.6666666666666643 0.0000000000000000 0.0000000000000000 F F F
0.0000000000000000 0.3333333333333357 0.0000000000000000 F F F
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0.6666666666666643 0.3333333333333357 0.0000000000000000 F F F
0.0000000000000000 0.6666666666666643 0.0000000000000000 F F F
0.3333333333333357 0.6666666666666643 0.0000000000000000 F F F
0.6666666666666643 0.6666666666666643 0.0000000000000000 F F F

H_2O/Cu(111)
1.00000000000000
7.5604597440039107 0.0000000000000000 0.0000000000000000
-3.7802298720019554 6.5475502025969803 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.2884825520348429
O H Cu
1 2 45
Selective dynamics
Direct
0.8474274825937734 0.4430234707849382 0.3895817445180882 T T T

0.8137717306374475 0.5522129866637354 0.3904840465789504 T T T
0.7142417523070024 0.3179300320783303 0.3906474270372050 T T T
0.2215623373267943 0.1112374774705863 0.3015925711705132 T T T
0.5528352894842034 0.1090626278508202 0.3006790375835595 T T T
0.8875012398451904 0.1097030544910655 0.3014088981958082 T T T
0.2226175050058947 0.4445707330957167 0.3015091377119258 T T T
0.5529905911333864 0.4448090764309342 0.3007688018775373 T T T
0.8887256298084845 0.4446863977364929 0.3042338772107411 T T T
0.2224397014076551 0.7791080691286680 0.3013825531662391 T T T
0.5549067192107181 0.7777513129496918 0.3020121056445245 T T T
0.8876343560509510 0.7796297736868397 0.3007928274467257 T T T
0.9996303293439607 0.0004988950477731 0.2253354525526591 T T T
0.3320458736809832 0.9998032312070817 0.2253015276624712 T T T
0.6660181078559625 -0.0000695006134680 0.2255561048376684 T T T
0.9986340433586045 0.3341307440853090 0.2265606289865950 T T T
0.3321673619490065 0.3331189406681732 0.2253818215580981 T T T
0.6672835878319812 0.3340831731286175 0.2260714351570401 T T T
0.9986336325311279 0.6653410240638623 0.2263160694002010 T T T
0.3325396269985301 0.6666418929595609 0.2257870183866779 T T T
0.6658734012104954 0.6667484507150709 0.2254605084870639 T T T
0.1103537937114852 0.2229498074967801 0.1508391896662552 T T T
0.4448341778975347 0.2226631613744964 0.1507896432900367 T T T
0.7777115538717904 0.2224655792589517 0.1508661177718571 T T T
0.1105288566713153 0.5553292408071449 0.1509277002909616 T T T
0.4437993838556683 0.5553841535297162 0.1507636752546393 T T T
0.7777237718419453 0.5557534965526844 0.1508081338153835 T T T
0.1102454460519549 0.8879745622907964 0.1508340361768451 T T T
0.4440332163041334 0.8890266267463796 0.1507817960736086 T T T
0.7775998752526847 0.8890624528224264 0.1507179683422258 T T T
0.2222222222222214 0.1111111111111143 0.0758738322541390 F F F
0.5555555555555571 0.1111111111111143 0.0758738322541390 F F F
0.8888888888888857 0.1111111111111143 0.0758738322541390 F F F
0.2222222222222214 0.4444444444444429 0.0758738322541390 F F F
0.5555555555555571 0.4444444444444429 0.0758738322541390 F F F
0.8888888888888857 0.4444444444444429 0.0758738322541390 F F F
0.2222222222222214 0.7777777777777786 0.0758738322541390 F F F
0.5555555555555571 0.7777777777777786 0.0758738322541390 F F F
0.8888888888888857 0.7777777777777786 0.0758738322541390 F F F
0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.3333333333333357 0.0000000000000000 0.0000000000000000 F F F
0.6666666666666643 0.0000000000000000 0.0000000000000000 F F F
0.0000000000000000 0.3333333333333357 0.0000000000000000 F F F
0.3333333333333357 0.3333333333333357 0.0000000000000000 F F F
0.6666666666666643 0.3333333333333357 0.0000000000000000 F F F
0.0000000000000000 0.6666666666666643 0.0000000000000000 F F F
0.3333333333333357 0.6666666666666643 0.0000000000000000 F F F
0.6666666666666643 0.6666666666666643 0.0000000000000000 F F F

H_2/Cu(111)

1.00000000000000
7.5604597440039107 0.0000000000000000 0.0000000000000000
-3.7802298720019554 6.5475502025969803 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.2884825520348429
H Cu
2 45
Selective dynamics
Direct
0.3304261498383215 0.4427934644617291 0.4227263532424188 T T T
0.3703355875237325 0.4437877779032950 0.3971847647292805 T T T
0.2226988082447906 0.1111026538066817 0.3015200376949550 T T T
0.5560606843455497 0.1112636982675057 0.3015038805127404 T T T
0.8893395417295213 0.1112050472595671 0.3015158257993875 T T T
0.2226805175649013 0.4446382924805067 0.3015577916409074 T T T
0.5562837073301864 0.4446411230259091 0.3014443665506502 T T T
0.8893811310720977 0.4446314741274273 0.3016217210480727 T T T
0.2227320182393213 0.7780802106670215 0.3015271380383924 T T T
0.5562226089910599 0.7780761679574116 0.3015419924280433 T T T
0.8894630586984033 0.7779957977346973 0.3015316496624590 T T T
0.0003167742713357 0.0001248356512666 0.2257208347686584 T T T
0.3336745545019582 0.0000600468756851 0.2257136117733285 T T T
0.6671472746623688 0.0003338486335490 0.2256639966655513 T T T
0.0005016684545791 0.3336204326787836 0.2257649363663511 T T T
0.3336939405871736 0.3333673364361328 0.2256591580724117 T T T
0.6671805590845657 0.3335778842039425 0.2256938573710940 T T T
0.0003812913412307 0.6668332542002681 0.2257210708610878 T T T
0.3338078397033153 0.6669009801166188 0.2257410851619343 T T T
0.6669947020736100 0.6669070274138289 0.2257061446587307 T T T
0.1110993206646173 0.2221347504829909 0.1507918687959907 T T T
0.4447008431494220 0.2221532103236279 0.1507856609199653 T T T
0.7782734536907320 0.2225602673859724 0.1507833795899438 T T T
0.1113741742234855 0.5557265464589725 0.1508085281060079 T T T
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0.7778493724770694 0.5556496420461841 0.1507898453673043 T T T
0.1114413556371344 0.8891319903100546 0.1507872734434970 T T T
0.4446003469872768 0.8889466721580106 0.1507782735163791 T T T
0.7779478571032981 0.8890415988603075 0.1507694345141036 T T T
0.2222222222222214 0.1111111111111143 0.0758738322541390 F F F
0.5555555555555571 0.1111111111111143 0.0758738322541390 F F F
0.8888888888888857 0.1111111111111143 0.0758738322541390 F F F
0.2222222222222214 0.4444444444444429 0.0758738322541390 F F F
0.5555555555555571 0.4444444444444429 0.0758738322541390 F F F
0.8888888888888857 0.4444444444444429 0.0758738322541390 F F F
0.2222222222222214 0.7777777777777786 0.0758738322541390 F F F
0.5555555555555571 0.7777777777777786 0.0758738322541390 F F F
0.8888888888888857 0.7777777777777786 0.0758738322541390 F F F
0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.3333333333333357 0.0000000000000000 0.0000000000000000 F F F
0.6666666666666643 0.0000000000000000 0.0000000000000000 F F F

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0.3333333333333357 0.6666666666666643 0.0000000000000000 F F F
0.6666666666666643 0.6666666666666643 0.0000000000000000 F F F