Electronic Supplementary Information

Interface Engineering for a Rational Design of Poison-free Bimetallic CO Oxidation Catalysts

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Microkinetic modelling

Fig. S1~S11

XYZ coordinates of selected structure models

Micro kinetic model for bifunctional CO oxidation by Pt@Cu_F NP

CO oxidation by Pt-CO^* and Cu-$2O^*$

The micro-kinetic model[1] for bifunctional CO oxidation by Pt-CO^* and Cu(100)-O^* or Cu(111)-O^* of Pt@Cu_F NP, the results of which are presented in Fig. 3a~c is as follows:

$CO(g) + {}^* \Leftrightarrow CO^*$ (R1)

$O_2(g) + 2^\# \Leftrightarrow 2O^\#$ (R2)

$CO^* + O^\# \Leftrightarrow CO_2{}^* + {}^\#$ (R3, Rate determining step)

$CO_2{}^* \Leftrightarrow CO_2(g) + {}^*$ (R4)

Here, the rate of CO_2 formation is equal to the maximum rate of the reaction R3. Because the first two reactions are in equilibrium, the rate of these reactions can be written as:

$$rate(R1) = k_1^+ p(CO)\theta_* - k_1^- \theta_{CO} \rightarrow \theta_{CO} = \left({}^{k_1^+}\!/_{k_1^-} \right) p(CO)\theta_* = K_1 P(CO)\theta_*$$

$$rate(R2) = k_2^+ p(O_2)\theta_\#^2 - k_2^- \theta_O^2 \rightarrow \theta_O = \sqrt{\left({}^{k_2^+}\!/_{k_2^-} \right) p(O_2)}\theta_\# = \sqrt{K_2 P(O_2)}\theta_\#$$

The maximum rate of R3 is:

$$rate(R3)^{max} = k_3^+ \theta_{CO}\theta_O = k_3^+ K_1 p(CO)\sqrt{K_2 P(O_2)}\theta_*\theta_\#$$

where K_1 and K_2 are the equilibrium constants for R1 and R2, p(CO) and $p(O_2)$ are the partial pressures of CO and O_2. k_i^+ and k_i^- are the forward and the backward rate constant for Ri, respectively.

The overall rate of CO_2 formation, rate(R3)^{max} is:

$$rate(R3)^{max} = k_3^+ \theta_{CO} \theta_O$$

The reaction R1 and R2 concerns the adsorption of CO and O_2, respectively. Therefore, the equilibrium constants K1 and K2 are,

$$K1 = exp\left(\frac{-\Delta G1}{kT}\right) = exp\left(\frac{-(\Delta E1 - T\Delta S1 + \Delta ZPE)}{kT}\right)$$

$\Delta E1 : Energy\ of\ CO\ adsorption$

$\Delta S1 : Entropy\ change\ involved\ in\ CO\ adsorption$

$\Delta ZPE : Zero\ point\ energy\ change\ upon\ CO\ adsorption = -0.07\ eV$

and

$$K2 = exp\left(\frac{-\Delta G2}{kT}\right) = exp\left(\frac{-(\Delta E2 - T\Delta S2 + \Delta ZPE)}{kT}\right)$$

$\Delta E2 : Energy\ of\ O_2\ adsorption$

$\Delta S2 : Entropy\ change\ involved\ in\ O_2\ adsorption$

$\Delta ZPE : Zero\ point\ energy\ change\ upon\ O_2\ adsorption = -0.05\ eV$

The sum of the coverage of adsorbed O, CO and free adsorption sites is equal to 1, so that:

$$\theta_{CO} + \theta_O + \theta_* + \theta_\# = 1$$

where $\theta_{CO}, \theta_O, \theta_*$, and $\theta_\#$ are the coverage of adsorbed CO, adsorbed O, and free sites of the surface for CO (*) and O (#) adsorption.

Because the bifunctional CO oxidation pathways described in Fig. 3a, and b utilizes CO molecules adsorbed on the Pt-edge sites, we regarded the Pt-edge sites as an available CO binding site. For oxygen supplied by Cu(100) or Cu(111), the total number of Cu(100) or Cu(111) atoms were counted and estimated as an active O binding site.

For the reaction at the Pt-Cu(100) interface, the surface fraction of Cu(100) sites (54/102) and Pt edge sites (48/102) of Pt@Cu_F NP was as follows:

$\theta_{CO} + \theta_* = \frac{48}{102} = 0.471$, $\theta_O + \theta_\# = \frac{54}{102} = 0.529$.

The maximum value of θ_{CO} and θ_O can be set to 0.471 and 0.529, respectively.

For the reaction at the Pt-Cu(111) interface, the surface fraction of Cu(111) sites (48/96) and Pt edge sites (48/96) of Pt@Cu_F NP was as follows:

$\theta_{CO} + \theta_* = \frac{48}{96} = 0.50$, $\theta_O + \theta_\# = \frac{48}{96} = 0.50$,

The maximum value of θ_{CO} and θ_O can be set to 0.50.

We found that even at 600K, calculated θ_{CO} and θ_O values are not significantly differing from the values estimated from the site fraction.

Note that we hypothesized that, despite the noticeable level of E_{des} of CO_2 was found, the surface concentration of CO_2 like intermediate (S3 in Fig. 3a, and b), CO_2^* in R4, is marginally small because the partial pressure of the product (p(CO_2)) is low and the prefactor of desorption is generally at least one order or more greater than that of adsorption.[1]

For R3, the maximum rate can be obtained as follows:

$rate(R3)^{max} = k_3^+ \theta_{CO}^{max} \theta_O^{max}$

where,

$$k_3^+ = \frac{kT}{h} exp\left(\frac{-\Delta G3^+}{kT}\right) = \frac{kT}{h} exp\left(\frac{-(E_{act} - T\Delta S3^+)}{kT}\right)$$

E_{act} : $Activation\ energy\ for\ reaction\ 3$

$\Delta S4^+ = 0$

rate(R3)^{max} was calculated at p(CO)=0.01 bar and p(O_2)=0.21 bar. Temperature dependent standard entropy of CO and O_2 was considered and adopted from NIST webbook (http://webbook.nist.gov).

Fig. S1

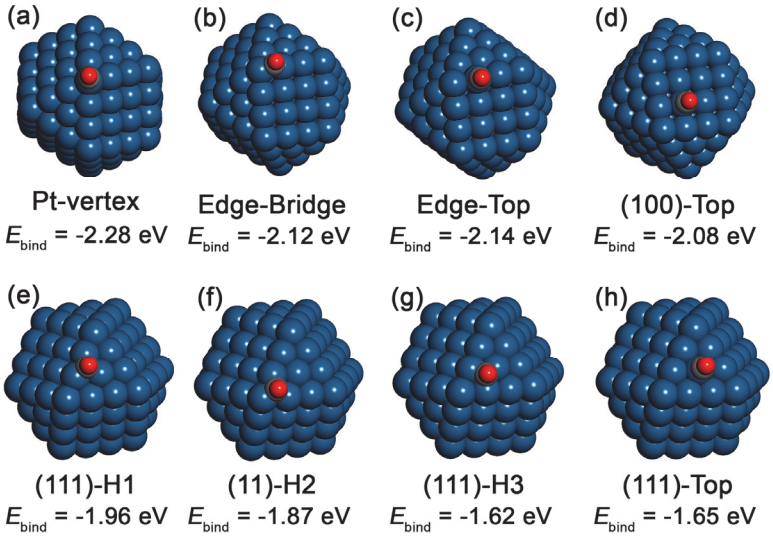

Fig. S1. Optimized adsorption geometry of CO on Pt_{147} NP and corresponding binding energy, E_{bind}.

Fig. S2

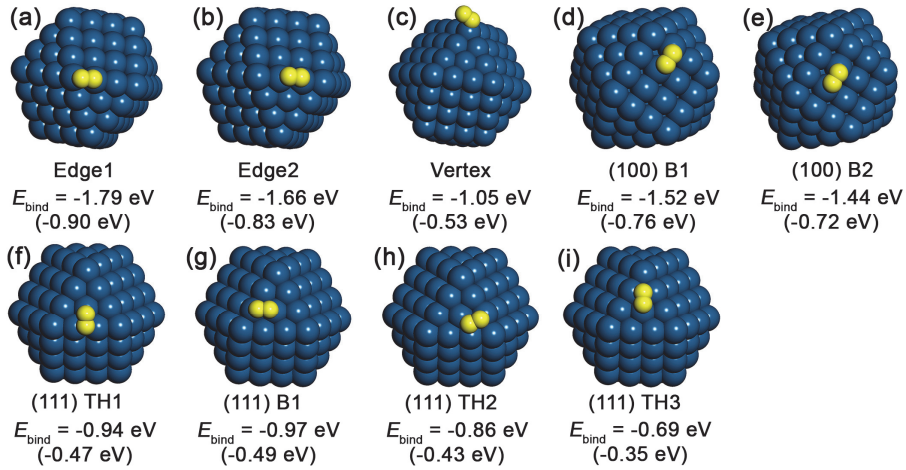

Fig. S2. Optimized molecular adsorption geometry of O_2 on Pt_{147} NP and corresponding binding energy, E_{bind}. Values in the parentheses present the E_{bind} per single binding site.

Fig. S3

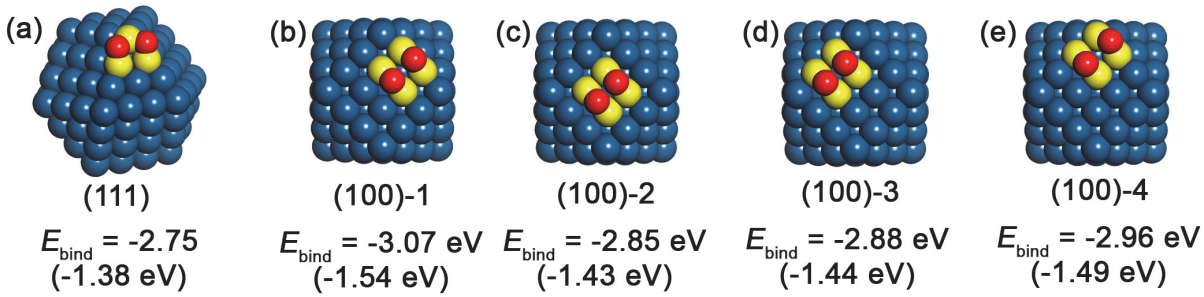

Fig. S3. Optimized dissociative adsorption geometry of O_2 on Pt_{147} NP and corresponding binding energy, E_{bind}. Values in the parentheses present the E_{bind} per single binding site.

Fig. S4

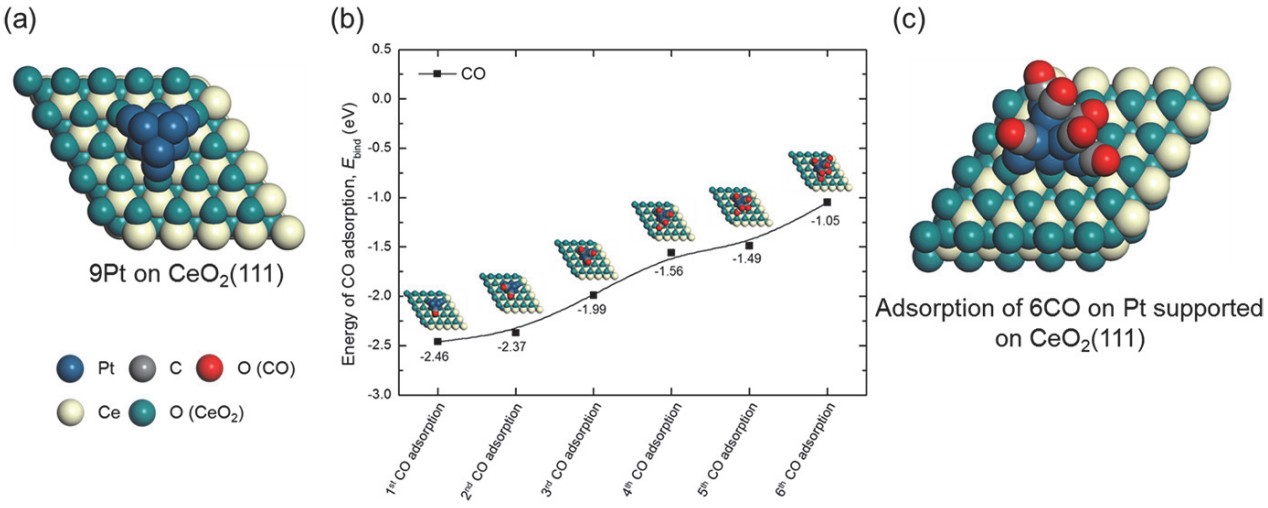

Fig. S4. Coverage dependent E_{bind} of CO molecules on CeO_2(111) supported Pt_9 NP. (a) The initial geometry of Pt_9/CeO_2, (b) The E_{bind} presented as a function of CO coverage, and (c) Pt_9/CeO_2 with 6 CO molecules. We found that Pt_9 cannot stably bind more than 6 CO molecules. The open Pt sites at the Pt-CeO_2 perimeter could not bind CO molecules. Rather, the NP was disordered.

Fig. S5

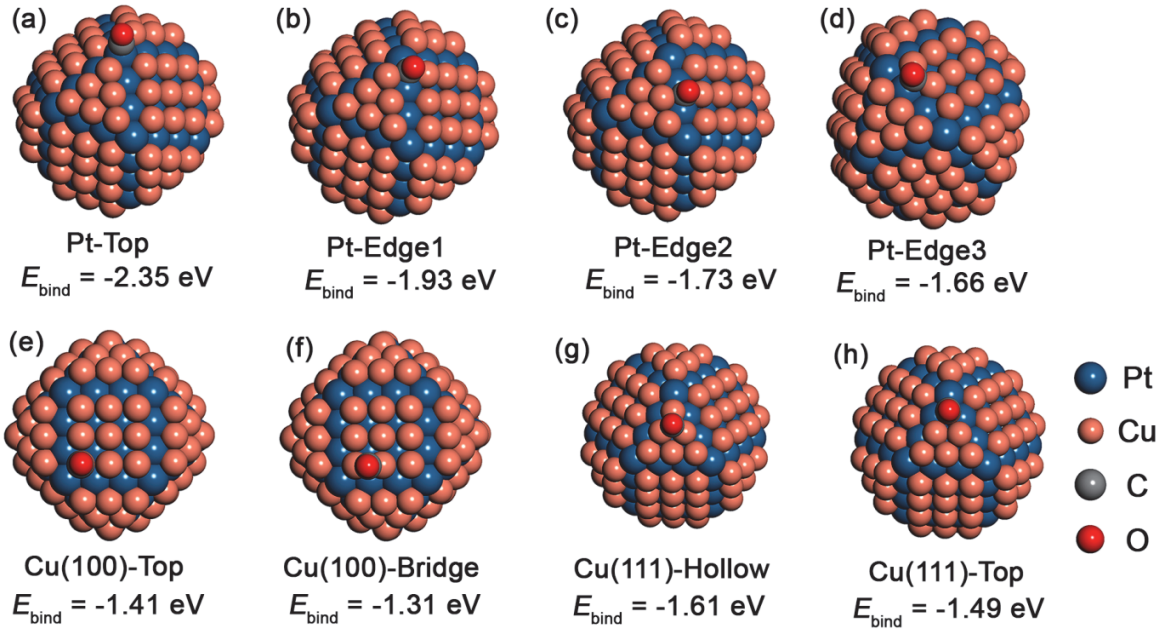

Fig. S5. Optimized adsorption geometry of CO on Pt@Cu_F NP and corresponding binding energy, E_{bind}.

Fig. S6

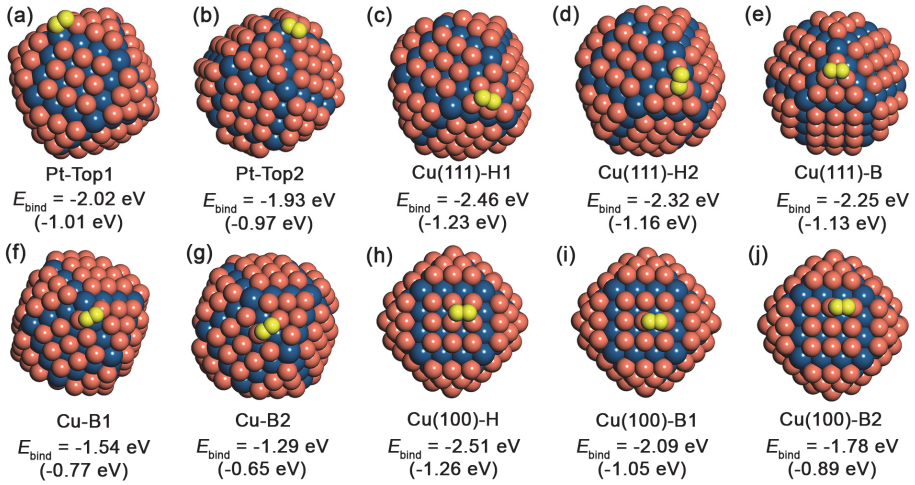

Fig. S6. Optimized adsorption geometry of O_2 on Pt@Cu_F NP and corresponding binding energy, E_{bind}. Values in the parentheses present the E_{bind} per single binding site.

Fig. S7

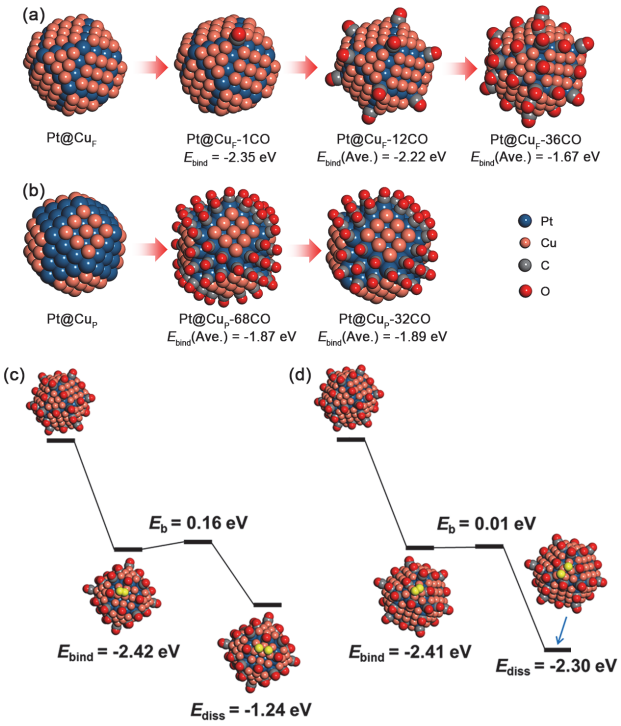

Fig. S7. CO saturated NPs for CO oxidation calculations: (a) Pt@Cu_F, (b) Pt@Cu_P. Because Pt preferentially binds CO all available Pt sites were covered with CO. The last image of (b) presents the half-NP model. (c) and (d) presents the dissociation of molecularly bound O_2 on Cu(100) and Cu(111) in the presence of pre-adsorbed CO molecules. Yellow spheres in (c) and (d) denotes oxygen atoms.

Fig. S8

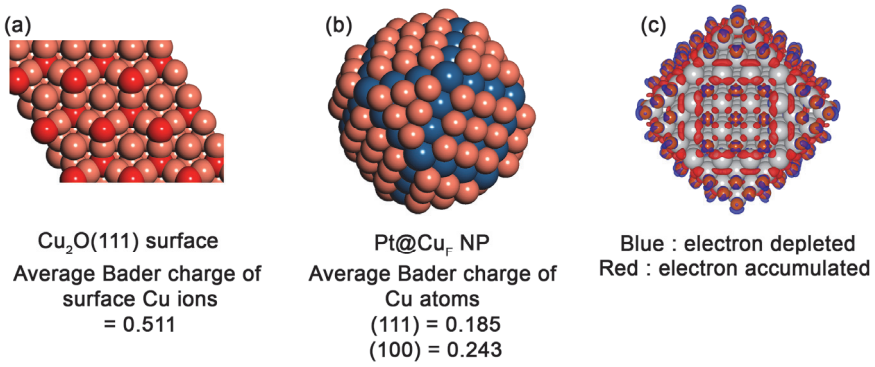

Fig. S8. Electronic analysis of $Cu_2O(111)$ surface and Pt@Cu NP. (a) Bader charge analysis of $Cu_2O(111)$ surface. Red spheres represent oxygen atoms. (b) Bader charge analysis of $Pt@Cu_F$ NP. Cu atoms are reduced. (c) Electron density difference map upon Cu deposition on Pt_{147} NP. Cu donates electron density to Pt. Blue and red area represents the electron depleted or accumulated orbitals, respectively. Grey and dark orange spheres represent Pt and Cu.

Fig. S9

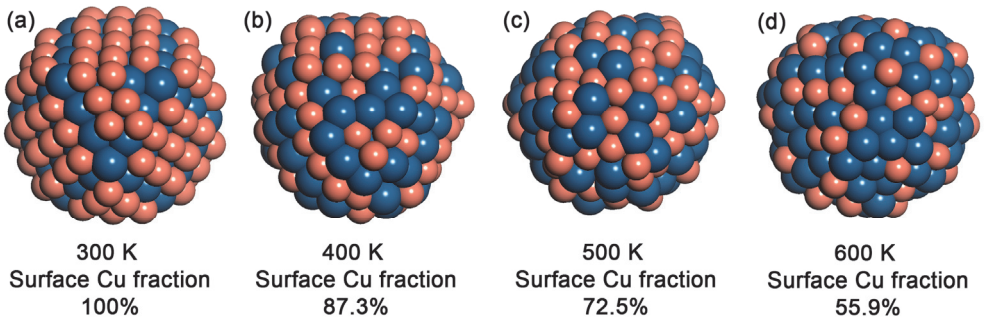

Fig. S9. Snapshots of $Pt@Cu_F$ NPs after 300 ns of MD simulation at corresponding temperature. (a) 300 K, (b) 400 K, (c) 500 K, and (d) 600 K. Numbers below show the fraction of the remaining surface Cu atoms after 300 ns of MD simulation.

Fig. S10

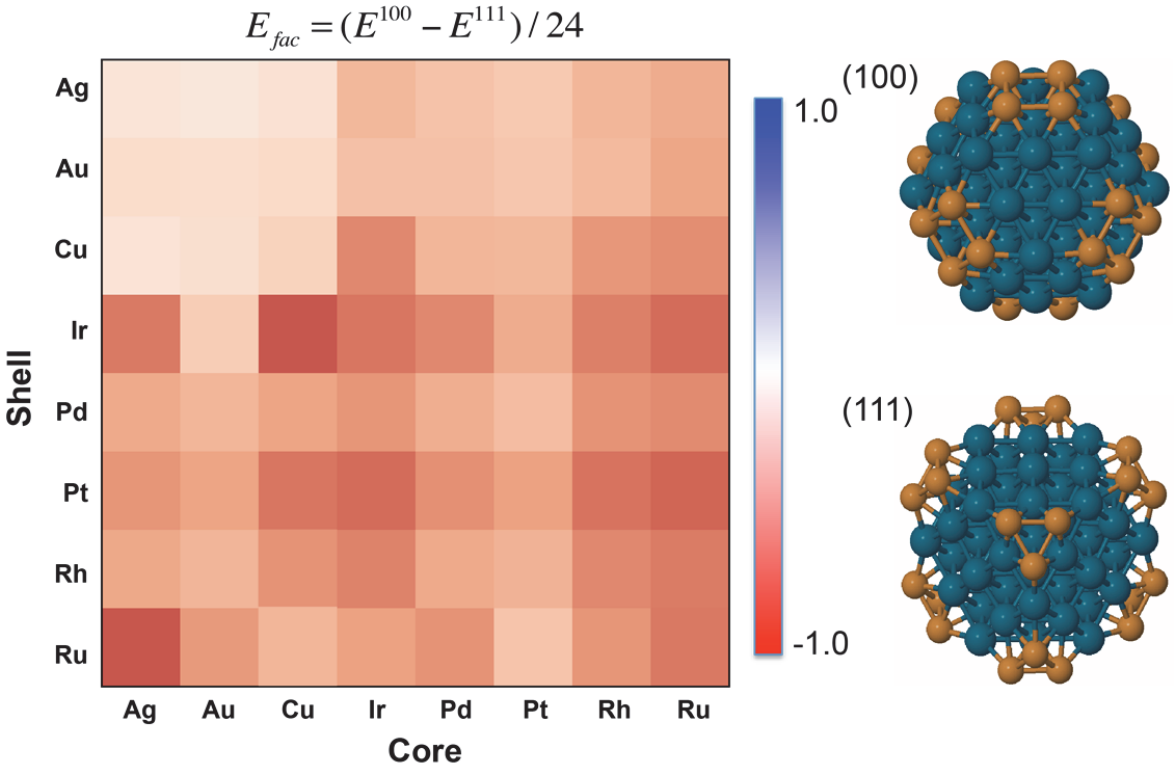

Fig. S10. E_{fac} over tested 56 X@Y core@shell NPs. Negative (red) E_{fac} indicates (100) shells are more stable than (111) shells. Positive (blue) E_{pref} denotes the reverse case. E^{100} and E^{111} are the total energy of X@Y NPs with geometries showing on the right side, respectively. All the X@Y NPs prefer to occupy (100) facets first.

Fig. S11

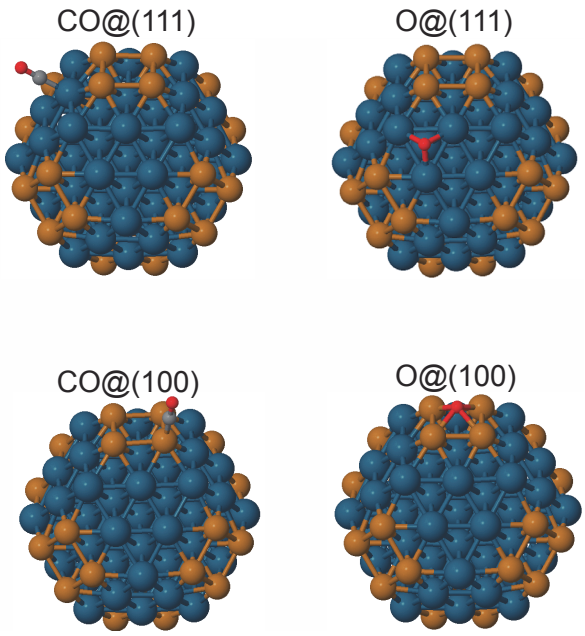

Fig. S11. Binding geometries of O and CO at (111) and (100) facets on X@Y_P NPs

References

1 I. Chorkendorf and J. W. Niemantsverdriet, *Concepts of Modern Catalysis and Kinetics*; Wiley-VCH: Weinheim, 2007.

XYZ coordinates of selected structure models

1. CO saturated Pt_{147} NP

Pt	12.4327789	9.9558193	12.3429221
Pt	16.3967493	13.9538000	16.3215974
Pt	12.4421572	17.9690605	16.3088032
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C	6.8788511	16.3929442	9.5459596
C	12.0165445	18.7221291	6.7606299
C	9.6730856	16.3887541	6.7604768
C	9.6526280	11.5404730	6.7691849
C	11.9942798	9.2306766	6.7388714
C	16.8176247	6.4029932	9.5419084
C	19.1597541	6.3928749	11.8700112
C	11.9920604	6.3904645	9.5719413
C	9.6426762	6.4152558	11.8669467
C	9.6432732	6.4040324	16.7707699
C	11.9817232	6.4007333	19.1005684
C	6.8546215	9.2213038	16.7708888
C	6.8547516	11.5613132	19.0931317
C	6.8749069	11.5392811	9.5476680
C	6.8587990	9.2186516	11.8767658
C	6.8800822	18.7531949	16.7740908
C	6.8596352	16.3953603	19.0832635
C	14.3621587	6.8334304	7.1944981
C	7.2936372	6.8324951	14.3221281
C	16.8352984	18.7069465	21.9052664
C	16.8143491	13.9333909	22.3616277
C	14.3579915	16.3913958	22.3518337
C	11.9830552	13.9417120	22.3501859
C	14.3501572	11.5621702	22.3626572
C	14.4693302	21.9728063	11.9361754
C	16.8423251	21.9645879	14.3142804
C	14.4644580	21.9799069	16.6934999
C	12.0794409	21.9901411	14.3129848
C	14.4598476	11.5580706	6.2972332
C	16.8370626	13.9276675	6.3031591
C	14.4659724	16.3151986	6.2807514
C	12.0798708	13.9337260	6.2751037
C	16.8228450	5.9340088	14.3171721
C	14.4456961	5.9226535	11.9445940
C	11.9870742	5.9357485	14.3147679

C	14.4381479	5.9194079	16.6946414
C	6.3822865	13.9505568	16.6848558
C	6.4056381	11.5626559	14.3091288
C	6.4006368	13.9431194	11.9343013
C	6.4177081	16.4086823	14.3075654
C	22.4427409	13.9204725	11.9416027
C	22.4294040	11.5431450	14.3182533
C	22.4410083	13.9205816	16.7071356
C	22.4544570	16.3089518	14.3184305
C	19.5737007	19.0903195	19.4614998
C	19.5943134	19.0610962	9.1835103
C	9.2951969	19.0967589	9.1693969
C	9.2744931	19.1229291	19.4459663
C	9.2360918	8.8369956	19.4491365
C	19.5305137	8.7971277	19.4651832
C	19.5454477	8.7988704	9.1878564
C	9.2911225	8.8183983	9.1792873
O	14.4760981	21.8964680	22.2906375
O	6.4894716	21.9171662	14.3044589
O	6.4914505	13.9237140	22.2972820
O	6.4828411	6.0027903	14.3211647
O	6.4968085	13.9272076	6.3643089
O	14.4767310	21.9044496	6.3816249
O	22.3705706	21.8964709	14.3210659
O	22.3249249	13.9202239	22.3100479
O	22.3784543	13.9080950	6.3940992
O	22.3209712	5.9761688	14.3212930
O	14.3221037	6.0136840	6.3747492
O	17.1222720	19.2289141	22.9009513
O	14.3279059	6.0382822	22.3075070
O	19.6861016	16.6915925	22.8931978
O	17.1394710	22.5009282	19.6286909
O	19.6915303	22.4976101	17.0909464
O	22.9480436	19.2585713	17.0850482
O	22.9465426	16.6870151	19.6490325
O	22.9385536	19.2593843	11.5368001
O	22.9554214	16.6844527	9.0241171
O	19.6964137	22.5040911	11.5738712
O	17.1767694	22.4943034	9.0337112
O	17.1961199	19.2558670	5.7944730
O	19.6939375	16.6771892	5.7676144
O	9.1457085	22.5056200	11.5452999
O	11.7146217	22.5071663	9.0170135
O	11.7183842	19.2531776	5.7730139
O	9.1456587	16.6880917	5.7713048
O	5.9107895	19.2834101	11.5276645
O	5.8942967	16.6904574	9.0089803
O	5.8716005	16.6962250	19.6117589
O	5.9026266	19.2902745	17.0939132
O	11.7078673	22.5217011	19.6039704
O	9.1243797	22.5043882	17.0765442
O	11.6469465	19.2871836	22.8564912
O	9.1209958	16.6939910	22.8847821
O	11.6416679	8.7095161	22.8974839
O	9.1137692	11.2698429	22.8897835
O	5.8670461	11.2735420	19.6295280
O	5.8663649	8.7052563	17.0913691
O	11.6909605	5.4125512	19.6346783
O	9.1166190	5.4181770	17.0819414
O	19.6829501	11.2092682	22.8909325
O	17.1010671	8.7040364	22.9093366
O	22.9351854	8.6429069	17.0816754
O	22.9150718	11.1744257	19.6586300
O	19.6796327	5.4053897	17.0910575
O	17.1028541	5.4272393	19.6675577
O	19.6862639	5.4118034	11.5440677
O	17.1093796	5.4195375	8.9999459
O	22.9320876	11.1447960	9.0326808
O	22.9205017	8.6252348	11.5607604
O	19.6898677	11.1613028	5.7851783
O	17.1302269	8.6158319	5.7988835
O	9.1164920	11.2435408	5.7840655
O	11.7062118	8.7237993	5.7355944
O	5.8922938	11.2409799	9.0079543
O	5.8675756	8.7046779	11.5620787
O	11.7024396	5.3944416	9.0521549
O	9.1121623	5.4358358	11.5425162
O	17.0819192	13.9131477	23.4910460
O	14.3224731	16.6705677	23.4780702
O	11.7145939	13.9184117	23.4792959
O	14.3137507	11.3059728	23.4942162
O	5.2911852	16.6880731	14.2999925
O	5.2662206	13.9165714	11.6912701
O	5.2453390	13.9290527	16.9166830
O	5.2746615	11.3026084	14.3018238
O	14.4897091	16.5350309	5.1413442
O	11.8695053	13.9124906	5.1338267
O	17.0988968	13.9100055	5.1725864
O	14.4877635	11.3045037	5.1649820
O	23.5929585	16.5342490	14.3062095
O	23.5768230	13.9059336	11.6950662
O	23.5787670	13.9057750	16.9359456
O	23.5628598	11.2936556	14.3065806
O	14.4696018	4.7811513	16.9189645
O	17.0907047	4.8046726	14.3061009
O	11.7173125	4.8067804	14.3044592
O	14.4775766	4.7886856	11.6993923
O	14.4882192	23.1180222	16.9189473
O	11.8630247	23.1302321	14.3043688
O	14.4929665	23.1076630	11.6944326
O	17.0998746	23.0963260	14.3029355
O	20.2540383	19.7637505	20.1142108
O	20.2809565	19.7087227	8.5116518
O	8.6206925	19.7562877	8.4968783
O	8.6007871	19.8015310	20.1000900
O	8.5440013	8.1764489	20.1026855
O	20.1991699	8.1156889	20.1215530
O	20.2083105	8.1256040	8.5172256
O	8.6279053	8.1430668	8.5111276

2. Pt@Cu_F NP

Pt	9.809987	10.871198	15.265907
Pt	9.826775	10.845858	8.505436
Pt	9.798906	10.893620	22.028572
Pt	4.223979	10.868011	15.253990
Pt	12.602670	10.872328	15.272982
Pt	12.654505	10.895866	8.382325
Pt	12.623032	10.846586	22.159683
Pt	7.016767	10.869546	15.259048
Pt	6.999780	10.892302	8.369512
Pt	6.975095	10.844162	22.148991
Pt	15.395258	10.874186	15.280328
Pt	11.185927	3.553694	15.256723
Pt	2.784308	13.340219	15.210883
Pt	11.204982	13.290732	15.261740
Pt	11.281136	13.269318	8.371193
Pt	11.168417	13.368238	22.151668
Pt	5.654611	3.670169	15.279353
Pt	13.973950	3.673960	15.301682
Pt	5.623821	13.284702	15.224855
Pt	5.640917	13.291356	22.040221
Pt	13.992533	13.289294	15.244009
Pt	13.954032	13.297359	22.056316
Pt	8.442366	3.552846	15.249930
Pt	8.412564	13.289135	15.255612
Pt	8.369683	13.267890	8.365230
Pt	8.426223	13.365114	22.147568
Pt	16.830438	13.347474	15.240823
Pt	9.812941	6.039547	15.255065
Pt	9.797111	6.090413	22.069280
Pt	9.806616	15.703428	15.275994
Pt	9.822688	15.645542	8.458188
Pt	4.156978	6.022696	15.301977
Pt	12.605958	6.037026	15.288858
Pt	4.155485	15.716270	15.205573
Pt	12.598302	15.709640	15.256987
Pt	7.019482	6.034663	15.273925
Pt	15.467068	6.029838	15.332907
Pt	7.015560	15.706374	15.244651
Pt	15.459325	15.722880	15.228684
Pt	2.784944	8.396660	15.292934
Pt	11.207877	8.453448	15.277029
Pt	11.200721	8.374752	8.390688
Pt	11.252622	8.469674	22.165422
Pt	11.176481	18.190856	15.277264
Pt	5.625276	8.453511	15.289373
Pt	5.669369	8.444766	8.473639
Pt	13.996816	8.458082	15.310257
Pt	13.988199	8.450263	8.495731
Pt	5.649677	18.069932	15.232088
Pt	13.962351	18.074975	15.248131
Pt	8.414978	8.451970	15.269308
Pt	8.457156	8.372485	8.384113
Pt	8.342534	8.468958	22.156698
Pt	16.837954	8.404812	15.328724
Pt	8.434507	18.189628	15.270922
Pt	2.779948	11.669439	17.591052
Pt	11.201555	11.686660	17.546700
Pt	11.236489	11.672692	10.719254
Pt	5.619152	11.658985	17.539874
Pt	5.584417	11.704577	10.669275
Pt	13.990014	11.663810	17.560012
Pt	14.055344	11.709543	10.689873
Pt	8.408636	11.685083	17.540074
Pt	8.403990	11.670765	10.712751
Pt	16.829043	11.677355	17.623336
Pt	9.808525	4.504729	17.538369
Pt	9.803608	14.130135	17.554568
Pt	9.818792	14.078090	10.694123
Pt	12.635382	4.401828	17.635251
Pt	4.281375	14.064751	17.499500
Pt	12.572317	14.115361	17.549437
Pt	12.674223	14.098304	10.676600
Pt	6.981294	4.399615	17.620777
Pt	7.033934	14.111432	17.536659
Pt	6.964332	14.094502	10.665022
Pt	15.326006	14.070828	17.522681
Pt	11.223235	6.865501	17.568723
Pt	11.204662	6.761854	10.699655
Pt	11.179998	16.567622	17.582304
Pt	11.272828	16.540771	10.666859
Pt	5.572055	6.840335	17.600313
Pt	5.621984	6.751878	10.688444
Pt	14.041105	6.844627	17.621423
Pt	14.025652	6.756165	10.711466
Pt	5.603098	16.563250	17.581563
Pt	13.999984	16.569300	17.597433
Pt	8.391331	6.864399	17.560981
Pt	8.442936	6.759454	10.691993
Pt	8.421253	16.564548	17.576203
Pt	8.361626	16.539990	10.660279
Pt	9.806430	9.267155	17.550001
Pt	9.821810	9.219167	10.725071
Pt	4.190134	9.228295	17.589970
Pt	4.167284	9.269785	10.675241
Pt	12.621714	9.255924	17.576503
Pt	12.615324	9.244572	10.718807
Pt	6.990816	9.253174	17.562148
Pt	7.028660	9.241362	10.704822
Pt	15.421280	9.235335	17.615823
Pt	15.477450	9.275580	10.704149
Pt	9.800832	12.521874	19.808919
Pt	9.813451	12.474817	12.980780
Pt	4.148020	12.468096	19.830999
Pt	4.200439	12.507732	12.918487
Pt	12.593157	12.501620	19.827469
Pt	12.628179	12.489332	12.969373
Pt	7.008792	12.497980	19.814655
Pt	6.999436	12.486270	12.956364
Pt	15.455023	12.475360	19.856177
Pt	15.428560	12.513192	12.944444
Pt	11.258176	5.199175	19.868006
Pt	11.200586	5.175861	12.956932
Pt	11.177548	14.981634	19.841494
Pt	11.226743	14.877877	12.969181
Pt	5.616861	5.175751	12.932413
Pt	14.020623	5.179149	12.955322

Pt	5.599221	14.988277	19.827528
Pt	5.579970	14.897295	12.914731
Pt	13.998235	14.993609	19.843782
Pt	14.044759	14.901113	12.934243
Pt	8.346348	5.200317	19.860243
Pt	8.437230	5.175396	12.949350
Pt	8.417960	14.978502	19.835439
Pt	8.397466	14.876566	12.963140
Pt	9.803076	7.662133	19.835576
Pt	9.817503	7.611463	12.977788
Pt	9.811116	17.238036	12.989407
Pt	4.293338	7.674005	13.009710
Pt	12.658088	7.646537	19.867903
Pt	12.587119	7.630880	12.997431
Pt	12.636483	17.342986	12.906896
Pt	6.946803	7.644685	19.853886
Pt	7.046977	7.628204	12.982809
Pt	15.340727	7.680074	13.038401
Pt	6.987350	17.340505	12.895378
Pt	2.790893	10.067980	12.911350
Pt	11.217390	10.070270	19.818453
Pt	11.211954	10.057485	12.992054
Pt	5.568315	10.034858	19.842055
Pt	5.630050	10.079643	12.972336
Pt	14.035317	10.038571	19.861675
Pt	14.001030	10.084233	12.992822
Pt	8.387114	10.068908	19.811625
Pt	8.419313	10.055782	12.985305
Pt	16.840867	10.075408	12.945509
Pt	18.126403	10.877820	15.287531
Pt	1.493707	10.868731	15.247915
Cu	13.884568	13.192547	8.579019
Cu	12.452233	15.548726	8.605760
Cu	15.212119	10.780151	8.632331
Cu	15.291060	14.019773	10.805312
Cu	13.877979	16.382970	10.820684
Cu	16.634344	11.612191	10.842167
Cu	16.625055	14.801056	13.082272
Cu	15.194115	17.156005	13.107999
Cu	17.955070	12.385687	13.134956
Cu	5.738437	8.552817	21.953807
Cu	4.418022	10.964841	21.901637
Cu	7.169354	6.192808	21.922924
Cu	4.330825	7.728243	19.734207
Cu	2.987842	10.132001	19.691819
Cu	5.743271	5.360495	19.712562
Cu	2.992828	6.939780	17.452955
Cu	1.664297	9.360136	17.397580
Cu	4.422282	4.586277	17.418876
Cu	16.620746	6.947752	17.487948
Cu	17.948733	9.370699	17.440710
Cu	15.194565	4.592040	17.450012
Cu	15.276012	7.732174	19.757269
Cu	16.614330	10.137622	19.725154
Cu	13.862479	5.362890	19.733913
Cu	13.856478	8.554713	21.972051
Cu	15.182202	10.969144	21.924104
Cu	12.424796	6.192677	21.934195
Cu	2.999412	14.792510	13.053245
Cu	4.429627	17.151114	13.087292
Cu	1.673428	12.378596	13.097927
Cu	4.347870	14.013962	10.778305
Cu	5.757658	16.378099	10.802875
Cu	3.004369	11.604165	10.812171
Cu	5.765836	13.188653	8.561100
Cu	7.192197	15.545174	8.595170
Cu	4.441543	10.772019	8.603924
Cu	9.831076	6.162234	8.593590
Cu	12.591579	6.223158	8.643544
Cu	7.067724	6.219408	8.628180
Cu	9.825704	4.536208	10.822277
Cu	12.587923	4.582054	10.855132
Cu	7.060586	4.578522	10.841521
Cu	9.818212	2.995364	13.101989
Cu	12.582819	3.055722	13.152402
Cu	7.056413	3.053875	13.137461
Cu	9.791153	15.579578	21.941630
Cu	12.551781	15.523361	21.903621
Cu	7.037551	15.518529	21.894463
Cu	9.792418	17.204705	19.714626
Cu	12.553700	17.163300	19.688658
Cu	7.037531	17.160220	19.678449
Cu	9.796653	18.748328	17.424460
Cu	12.557262	18.689284	17.388260
Cu	7.043368	18.685676	17.378361
Cu	8.524206	10.155328	24.173854
Cu	9.799446	12.367925	24.170918
Cu	7.204635	12.389608	24.114311
Cu	9.789682	7.891123	24.126037
Cu	11.071233	10.156521	24.179057
Cu	12.391597	12.395036	24.120527
Cu	11.104053	11.570728	6.358692
Cu	9.832248	9.365140	6.363750
Cu	12.428486	9.336230	6.423770
Cu	9.829196	13.830946	6.399130
Cu	8.556515	11.569729	6.353808
Cu	7.235754	9.331847	6.411933
Cu	3.374038	16.061419	18.901471
Cu	2.101398	13.851497	18.905506
Cu	3.431820	14.560182	21.022163
Cu	3.440577	17.549324	16.770634
Cu	2.106551	15.319948	16.816171
Cu	0.843010	13.048110	16.779374
Cu	16.249507	5.682676	11.639788
Cu	17.520746	7.891071	11.634004
Cu	16.193688	7.181032	9.515835
Cu	16.185909	4.199092	13.771331
Cu	17.517956	6.428035	13.722124
Cu	18.778183	8.698178	13.759584
Cu	3.393745	5.678633	11.601364
Cu	2.112861	6.421693	13.680218
Cu	3.447951	4.194233	13.731374
Cu	3.459872	7.174946	9.480007
Cu	2.120442	7.884435	11.591621
Cu	0.851224	8.689867	13.714249
Cu	8.531895	2.731330	18.951063
Cu	9.811478	1.987733	16.875039
Cu	7.217449	2.027360	16.824116
Cu	9.796194	3.542825	21.067503
Cu	11.080323	2.731730	18.956191
Cu	12.406361	2.029616	16.835521
Cu	9.809572	19.754516	13.653369
Cu	11.087442	19.009834	11.572216
Cu	12.401197	19.715206	13.699110
Cu	7.216574	19.713139	13.688280
Cu	8.542652	19.009401	11.567000
Cu	9.819024	18.195081	9.456026
Cu	17.501452	15.330617	16.846984
Cu	16.222380	16.072085	18.925757
Cu	16.166850	17.557003	16.793572
Cu	18.764914	13.062303	16.816421
Cu	17.500284	13.865880	18.935885
Cu	16.164020	14.570823	21.046774

3. 36-CO saturated Pt@Cu_F NP with dissociatively adsorbed O_2 on Cu(100)

Pt	9.1617710	10.1297310	14.2514360
Pt	9.1566730	10.1177190	7.4552880
Pt	9.1653270	10.1900310	21.0564580
Pt	3.3333160	10.1505140	14.2439770
Pt	11.9932570	10.1531030	14.2409670
Pt	12.0471160	10.1601440	7.2260660
Pt	12.0487180	10.1606720	21.2723640
Pt	6.3307050	10.1464440	14.2420790
Pt	6.2658340	10.1508860	7.2290040
Pt	6.2804970	10.1562890	21.2752090
Pt	14.9903760	10.1655270	14.2421510
Pt	10.5803390	2.6926420	14.2592420
Pt	1.9782920	12.6576110	14.1989180
Pt	10.5828560	12.5612200	14.2258750
Pt	10.6346320	12.6024750	7.2125210
Pt	10.5720880	12.7245120	21.2559630
Pt	4.8634870	2.7045350	14.3026550
Pt	13.4754220	2.7157360	14.2974420
Pt	4.9405290	12.5739000	14.2237720
Pt	4.8760250	12.6927790	21.2473420
Pt	13.3770040	12.5842250	14.2218060
Pt	13.4467580	12.7030010	21.2476040
Pt	7.7579670	2.6893080	14.2612240
Pt	7.7357920	12.5579000	14.2264000
Pt	7.6671770	12.5992160	7.2142480
Pt	7.7514210	12.7201560	21.2581460
Pt	16.3409050	12.6746840	14.1962090
Pt	9.1672860	5.3068690	14.2888590
Pt	9.1700550	5.2261880	21.3096860
Pt	9.1563300	14.9294790	14.1771380
Pt	9.1425240	15.0874830	7.1988510
Pt	3.4066830	5.1977500	14.3245710
Pt	12.0777510	5.1234700	14.2810990
Pt	3.3876940	15.1060610	14.1887540
Pt	12.0808180	15.1738140	14.1896410
Pt	6.2570880	5.1162680	14.2833600
Pt	14.9287110	5.2145750	14.3196820
Pt	6.2305340	15.1687400	14.1914120
Pt	14.9268490	15.1188110	14.1807820
Pt	1.9980940	7.6351650	14.3102080
Pt	10.5788610	7.7049190	14.2663860
Pt	10.5726600	7.5933890	7.2449710
Pt	10.6514060	7.7088180	21.2980770
Pt	10.5514300	17.5900150	14.3210600
Pt	4.9649390	7.7305840	14.2569880
Pt	4.8616420	7.6186400	7.2426200
Pt	13.3654460	7.7409020	14.2544740
Pt	13.4631420	7.6362290	7.2406620
Pt	4.9095910	17.5996000	14.2701240
Pt	13.3990920	17.6048330	14.2605140
Pt	7.7510860	7.7014110	14.2666870
Pt	7.7519940	7.5872680	7.2465750
Pt	7.6839090	7.7077130	21.2992140
Pt	16.3339610	7.6554880	14.3052290
Pt	7.7546990	17.5914220	14.3312030
Pt	1.9955640	10.9673090	16.6266770
Pt	10.5740850	10.9511450	16.5540870
Pt	10.5538990	10.9403210	9.6730840
Pt	4.9582310	10.9762710	16.5202550
Pt	4.9711350	10.9176610	9.6837090
Pt	13.3665590	10.9860640	16.5188100
Pt	13.3412140	10.9322210	9.6814940
Pt	7.7526010	10.9482300	16.5554850
Pt	7.7590610	10.9359710	9.6737230
Pt	16.3288220	10.9830860	16.6259290
Pt	9.1691970	3.7538310	16.5551000
Pt	9.1604020	13.3091100	16.5051870
Pt	9.1519400	13.4875660	9.4737240
Pt	12.0620760	3.5608320	16.6666140
Pt	3.6124320	13.3749940	16.4985900
Pt	11.9679630	13.3596990	16.5111080
Pt	11.9355210	13.3569750	9.6680270
Pt	6.2775380	3.5546870	16.6693230
Pt	6.3501170	13.3520010	16.5108700
Pt	6.3693870	13.3486060	9.6727870
Pt	14.7076380	13.3853630	16.4955080
Pt	10.5640390	6.1191060	16.5641140
Pt	10.5675720	6.1133820	9.7220520
Pt	10.5444920	15.6860980	16.4038300
Pt	10.6241970	15.9286010	9.5339920
Pt	4.9880270	6.1363110	16.5430440
Pt	4.8865830	5.9373110	9.5948730
Pt	13.3472100	6.1452860	16.5401380
Pt	13.4447950	5.9521470	9.5931690
Pt	4.9119320	15.9711060	16.5714460
Pt	13.4025510	15.9745630	16.5680810
Pt	7.7709020	6.1162890	16.5652490
Pt	7.7622800	6.1086270	9.7228300
Pt	7.7695340	15.6778160	16.4041240
Pt	7.6687110	15.9261670	9.5332120

Pt	9.1654390	8.5169620	16.5700110	Cu	17.2976710	8.6446940	16.4382220	Cu	9.1472690	17.6190030	8.3906640
Pt	9.1607290	8.5177930	9.6899420	Cu	14.5733930	3.9050950	16.4666770	Cu	16.9472280	14.6613000	15.9035400
Pt	3.5871890	8.5651880	16.5272310	Cu	14.5875370	7.0610230	18.6899730	Cu	15.7135540	15.3732990	17.8816610
Pt	3.4009030	8.4974770	9.5784720	Cu	15.8924200	9.2910960	18.6986720	Cu	15.6237480	16.9081240	15.8013210
Pt	11.9539600	8.5583300	16.5345120	Cu	13.3283430	4.8061160	18.7200880	Cu	18.2484040	12.4101640	15.8280180
Pt	12.0714770	8.4544520	9.5097940	Cu	13.3265640	7.8055140	20.8183130	Cu	16.9357780	13.2701460	17.9089240
Pt	6.3769000	8.5526500	16.5359350	Cu	14.5559310	10.2577240	20.8848790	Cu	15.5964020	13.9543470	20.0455600
Pt	6.2498710	8.4445420	9.5108560	Cu	11.8392330	5.4950100	20.9225010	C	3.9189850	13.2188940	22.7432490
Pt	14.7435370	8.5772330	16.5242750	Cu	2.4063040	14.0297700	11.8890510	C	14.3977660	7.0973900	5.7353740
Pt	14.9208430	8.5198970	9.5754710	Cu	3.7766000	16.4487650	12.0835190	C	14.3439880	19.1995680	14.2262570
Pt	9.1647270	11.7916640	18.8295200	Cu	1.0143960	11.6677340	12.0675180	C	3.9223730	1.1086760	14.3137680
Pt	9.1573550	11.7679160	11.9360080	Cu	3.7251440	13.2542260	9.7918990	C	9.1288670	16.1536820	5.6852410
Pt	3.4296800	11.8101050	18.9105290	Cu	4.9964500	15.5125670	9.7694750	C	9.1714250	4.1568210	22.8223090
Pt	3.5634440	11.7465070	11.9611590	Cu	2.4156690	11.0256010	9.7882540	C	14.3772410	13.2195380	22.7638810
Pt	12.0586120	11.8805270	18.9900900	Cu	4.9929850	12.5089450	7.6785310	C	3.9385170	7.0739370	5.7323370
Pt	11.9554440	11.7533760	11.9548110	Cu	6.4716100	14.8137150	7.5850560	C	14.4114770	1.1171450	14.3074160
Pt	6.2667900	11.8711790	18.9909660	Cu	3.7551340	10.0579090	7.6066820	C	3.9708520	19.1980790	14.2340100
Pt	6.3593110	11.7458520	11.9565200	Cu	9.1665730	5.3212600	7.7317200	C	19.6237780	10.1664720	14.2480700
Pt	14.8956760	11.8206210	18.9106520	Cu	11.8993690	5.4633630	7.6402450	C	-1.7763393	10.0286295	14.1948300
Pt	14.7523000	11.7611160	11.9586610	Cu	6.4333630	5.4514070	7.6413050	C	16.8418300	11.2288660	18.6010770
Pt	10.6540710	4.3892410	18.9664780	Cu	9.1682110	3.8743480	9.8704890	C	1.4842880	11.2134600	18.6022940
Pt	10.5711840	4.5099930	12.0218970	Cu	11.7520260	3.8423600	9.8530400	C	1.4599030	9.0845970	9.9061580
Pt	10.5471680	14.2276160	18.7596880	Cu	6.5858220	3.8330900	9.8549770	C	16.8611140	9.1102500	9.9026890
Pt	10.5573750	14.1809590	11.9296350	Cu	9.1689610	2.3678840	11.9603670	C	4.4292340	3.9661700	9.9404080
Pt	4.8849200	4.3282700	11.9100830	Cu	11.9090190	2.3322460	12.1256670	C	6.1937700	11.8115500	6.0211850
Pt	13.4509770	4.3405750	11.9068510	Cu	6.4308950	2.3249620	12.1282510	C	12.0997660	17.3179270	9.8689050
Pt	4.9258850	14.4128610	18.9036410	Cu	9.1580580	14.9771090	20.7643330	C	13.8976830	16.3647960	18.5213370
Pt	4.9525220	14.1737970	11.9422010	Cu	11.8562470	14.8767730	20.8663090	C	12.1287970	8.5006360	22.4822670
Pt	13.3875640	14.4235220	18.9022060	Cu	6.4589090	14.8670410	20.8684110	C	6.2080260	2.9991430	18.6449010
Pt	13.3561590	14.1833640	11.9377490	Cu	9.1447550	16.5499130	18.6999970	C	6.2061480	8.4968560	22.4854210
Pt	7.6851430	4.3868160	18.9681650	Cu	11.7140290	16.5523760	18.7063710	C	12.1112800	11.8215200	6.0190360
Pt	7.7637180	4.5066880	12.0233270	Cu	6.5774460	16.5333990	18.7188820	C	6.1926500	17.3127170	9.8742930
Pt	7.7680940	14.2157380	18.7604450	Cu	9.1694120	18.0584310	16.7193820	C	13.9081440	3.9820940	9.9367130
Pt	7.7512370	14.1774770	11.9304730	Cu	11.8125910	18.0283640	16.5290760	C	12.1339120	3.0042910	18.6418290
Pt	9.1676170	6.8163350	19.0316140	Cu	6.5296720	18.0116280	16.5601600	C	4.4184880	16.3585010	18.5259840
Pt	9.1647160	6.9263100	11.9973510	Cu	7.9458890	9.5056150	23.2925530	C	16.8666820	5.7270410	14.7641330
Pt	9.1497730	16.5476480	11.9681110	Cu	9.1651410	11.6163220	23.2760530	C	1.4520950	14.5909250	13.7437880
Pt	3.6103600	6.9261380	12.0051940	Cu	6.5628400	11.7095250	23.2410300	C	9.1532050	19.0176730	14.7529210
Pt	11.9473220	6.9637380	18.8324880	Cu	9.1682270	7.2084570	23.2749780	C	1.4686120	5.7066090	14.7711300
Pt	11.9716300	6.9191060	11.9847250	Cu	10.3877230	9.5060190	23.2914450	C	9.1703180	1.2665430	13.8179340
Pt	12.0270260	16.7505760	11.8408260	Cu	11.7627420	11.7124310	23.2387810	C	16.8644760	14.6078330	13.7391100
Pt	6.3875950	6.9575900	18.8346160	Cu	10.3736590	10.8087550	5.2187260	C	9.1636880	6.6886610	6.0559030
Pt	6.3570650	6.9111370	11.9860850	Cu	9.1576740	8.6937800	5.2327010	C	9.1614640	13.6276220	22.4431540
Pt	14.7188180	6.9432320	12.0012060	Cu	11.7612860	8.6018620	5.2628160	O	3.2916230	13.5516510	23.7176050
Pt	6.2763100	16.7447740	11.8455740	Cu	9.1490470	13.1087490	5.2396890	O	15.0090260	6.7493160	4.7557610
Pt	1.9879380	9.3303090	11.8741790	Cu	7.9348940	10.8058610	5.2212450	O	14.9720890	20.2279570	14.1826010
Pt	10.5585850	9.3664000	18.8357270	Cu	6.5575750	8.5935800	5.2665030	O	3.3034830	0.0737390	14.3258160
Pt	10.5770730	9.3304790	11.9494590	Cu	2.5998920	15.3619190	17.8817630	O	9.1160590	16.8500430	4.7008660
Pt	4.9936130	9.3868950	18.8134550	Cu	1.3843340	13.2535490	17.9088270	O	9.1722880	3.4617510	23.8075780
Pt	4.9485870	9.3250550	11.9651130	Cu	2.7179620	13.9416220	20.0442870	O	14.9838970	13.5451540	23.7536670
Pt	13.3372910	9.3955240	18.8110980	Cu	2.6894650	16.9011920	15.8032460	O	3.3355980	6.7209500	4.7493230
Pt	13.3732350	9.3373130	11.9629630	Cu	1.3699540	14.6471750	15.9047640	O	15.0252050	0.0792190	14.3175150
Pt	7.7722950	9.3629900	18.8366060	Cu	0.0729350	12.3912820	15.8302090	O	3.3483620	20.2300480	14.1911650
Pt	7.7447830	9.3264430	11.9497150	Cu	15.7313860	4.9456070	10.6048760	O	20.8296160	10.1681980	14.2420920
Pt	16.3332920	9.3522620	11.8708550	Cu	16.9467570	7.0610530	10.5912970	O	-2.9820103	10.0101585	14.1837720
Pt	17.7716470	10.1672420	14.2517580	Cu	15.6477420	6.3885100	8.4413910	O	17.8566090	11.0266340	19.3108260
Pt	0.5525940	10.1435370	14.2562910	Cu	15.6542490	3.4133590	12.7107660	O	0.4711960	11.0094390	19.3140570
Cu	13.3139500	12.5211000	7.6739400	Cu	16.9490120	5.6667100	12.5930440	O	0.4445760	9.3040160	9.2025870
Cu	11.8098940	14.8244320	7.5792060	Cu	18.2450870	7.9228570	12.6817750	O	17.8759040	9.3334890	9.1995390
Cu	14.5585600	10.0813830	7.6038600	Cu	2.6030500	4.9245540	10.6094460	O	4.0997200	2.9732490	9.2484550
Cu	14.5809220	13.2721470	9.7881050	Cu	1.3860160	5.6400450	12.5993380	O	5.4988790	12.2041080	5.0533360
Cu	13.3002000	15.5233430	9.7636580	Cu	2.6869380	3.3904540	12.7166020	O	12.8046720	18.0811430	9.1653240
Cu	15.8967260	11.0493700	9.7828510	Cu	2.6808530	6.3609450	8.4451940	O	14.3425660	17.3420660	19.1653580
Cu	15.9051840	14.0441640	11.8865520	Cu	1.3803010	7.0355840	10.5962860	O	12.8399080	8.1059880	23.4374600
Cu	14.5292850	16.4579610	12.0717650	Cu	0.0851470	7.8878990	12.6876320	O	5.5235290	2.2172210	19.3468710
Cu	17.3037800	11.6896100	12.0618030	Cu	7.9501380	1.8929990	17.9680660	O	5.5005970	8.1025100	23.4447620
Cu	5.0097090	7.7969990	20.8218670	Cu	9.1703130	1.1737090	15.9835560	O	12.8032920	12.2163740	5.0500480
Cu	3.7725730	10.2474800	20.8852090	Cu	6.5618240	1.1726760	15.8824510	O	5.4801520	18.0724130	9.1746440
Cu	6.5009190	5.4913600	20.9256840	Cu	9.1709800	2.7075740	20.1195440	O	14.2419900	2.9915650	9.2434870
Cu	3.7469910	7.0519380	18.6938100	Cu	10.3921080	1.8960030	17.9670330	O	12.8193190	2.2221110	19.3425190
Cu	2.4385180	9.2811510	18.7006970	Cu	11.7778320	1.1784580	15.8810910	O	3.9558640	17.3285020	19.1692270
Cu	5.0093970	4.7984700	18.7241330	Cu	9.1483720	19.0996260	12.5506860	O	17.8901630	5.1384780	15.1867140
Cu	2.4312640	6.2773050	16.6237250	Cu	10.3631610	18.4140050	10.5479370	O	0.4409600	15.1718320	13.2800290
Cu	1.0332770	8.6238790	16.4423730	Cu	11.7158880	19.1075000	12.6613710	O	9.1558650	20.2315890	15.0617380
Cu	3.7659140	3.8933610	16.4745570	Cu	6.5771550	19.1019320	12.6717370	O	0.4472710	5.1171380	15.1974890
Cu	15.9045280	6.2928720	16.6173930	Cu	7.9277290	18.4120100	10.5515890	O	9.1712960	0.0870230	13.3912120

O	17.8781910	15.1902490	13.2836800
O	9.1652500	5.8742800	5.1017520
O	9.1612480	14.4149070	23.4191020
O	10.6943390	18.0947960	18.1214620
O	7.6581480	18.0511220	18.1642510

4. 36-CO saturated $Pt@Cu_F$ NP with dissociatively adsorbed O_2 on Cu(111)

Pt	9.1635080	10.1658120	14.2478800
Pt	9.1528740	10.1158960	7.4515940
Pt	9.1654430	10.1975850	21.0422690
Pt	3.3372230	10.1491130	14.2470910
Pt	11.9822180	10.1689560	14.2503350
Pt	12.0434960	10.1591370	7.2232110
Pt	12.0566500	10.1534880	21.2722860
Pt	6.3411340	10.1568360	14.2497060
Pt	6.2630090	10.1551900	7.2277770
Pt	6.2750780	10.1484660	21.2734440
Pt	14.9791690	10.1649020	14.2468790
Pt	10.5805150	2.7007560	14.2587380
Pt	1.9825900	12.6568550	14.1944970
Pt	10.5641240	12.6167710	14.2253620
Pt	10.6239220	12.5964410	7.1944540
Pt	10.5705320	12.7199630	21.2552860
Pt	4.8622350	2.7023960	14.2969720
Pt	13.4746340	2.7175480	14.2907560
Pt	4.9547410	12.5775970	14.2387960
Pt	4.8594290	12.6711180	21.2577710
Pt	13.3545520	12.5942790	14.2355190
Pt	13.4631370	12.6814300	21.2575450
Pt	7.7584350	2.6972370	14.2597320
Pt	7.7442240	12.6074290	14.2267670
Pt	7.6740780	12.6013700	7.1990880
Pt	7.7474150	12.7159870	21.2572940
Pt	16.3291900	12.6742100	14.1937890
Pt	9.1680340	5.3163690	14.2833950
Pt	9.1700170	5.2278490	21.3062690
Pt	9.1566450	15.0193580	14.2082350
Pt	9.1560870	15.0612800	7.1651950
Pt	3.4061830	5.1986730	14.3190490
Pt	12.0778950	5.1244660	14.2792640
Pt	3.3854000	15.1056060	14.1922840
Pt	12.0659560	15.2083780	14.2158150
Pt	6.2556740	5.1149710	14.2816010
Pt	14.9272650	5.2165670	14.3100530
Pt	6.2321300	15.1820140	14.2362310
Pt	14.9167340	15.1146290	14.1793320
Pt	1.9967110	7.6384470	14.3016820
Pt	10.5773110	7.7239910	14.2656810
Pt	10.5697740	7.5976810	7.2439120
Pt	10.6447450	7.7115340	21.2898850
Pt	10.5685050	17.6312770	14.2201280
Pt	4.9652750	7.7310890	14.2614380
Pt	4.8576340	7.6272220	7.2417780
Pt	13.3651920	7.7428590	14.2593190
Pt	13.4621770	7.6410330	7.2407480
Pt	4.8201860	17.5950140	14.2414600
Pt	13.4740930	17.6164760	14.2068040
Pt	7.7507110	7.7168950	14.2636440
Pt	7.7498410	7.5926250	7.2461900
Pt	7.6907110	7.7093570	21.2899220
Pt	16.3366140	7.6604610	14.2992360
Pt	7.7445480	17.5781560	14.2691340
Pt	1.9932970	10.9630350	16.6211360
Pt	10.5756810	10.9896860	16.5433190
Pt	10.5500090	10.9456030	9.6676860
Pt	4.9609650	10.9779350	16.5289170
Pt	4.9801780	10.9271430	9.6902910
Pt	13.3641470	10.9925630	16.5278080
Pt	13.3302810	10.9342780	9.6866840
Pt	7.7499200	10.9869520	16.5454540
Pt	7.7579700	10.9393870	9.6693770
Pt	16.3299270	10.9805170	16.6222730
Pt	9.1718900	3.7674280	16.5544290
Pt	9.1578410	13.3896680	16.5012100
Pt	9.1535890	13.4743490	9.4679620
Pt	12.0603920	3.5653480	16.6659820
Pt	3.6049650	13.3636760	16.4967320
Pt	11.9598780	13.4083960	16.5073850
Pt	11.9418560	13.3565370	9.6692030
Pt	6.2804120	3.5593040	16.6671120
Pt	6.3541070	13.3999610	16.5126160
Pt	6.3769770	13.3612980	9.6798000
Pt	14.7098120	13.3812270	16.4942680
Pt	10.5626520	6.1321700	16.5576820
Pt	10.5641690	6.1187190	9.7242040
Pt	10.5566610	15.8179620	16.4721670
Pt	10.6347230	15.8870500	9.5472450
Pt	4.9894110	6.1363010	16.5409410
Pt	4.8866890	5.9459230	9.5973760
Pt	13.3449420	6.1472930	16.5379850
Pt	13.4428520	5.9605230	9.5954890
Pt	4.8604750	15.9701370	16.6015800
Pt	13.4315580	15.9798250	16.5951870
Pt	7.7712100	6.1310820	16.5588940
Pt	7.7612890	6.1138250	9.7240240
Pt	7.7582430	15.8047680	16.4982500
Pt	7.7259310	15.9373980	9.5673420
Pt	9.1674000	8.5467090	16.5609940
Pt	9.1589320	8.5218500	9.6867110
Pt	3.5851340	8.5605350	16.5269380
Pt	3.4043740	8.5117640	9.5762300
Pt	11.9535970	8.5678600	16.5345500
Pt	12.0696910	8.4555820	9.5090890
Pt	6.3807670	8.5611570	16.5346180
Pt	6.2476120	8.4468230	9.5114060
Pt	14.7475950	8.5746880	16.5257750
Pt	14.9157120	8.5293040	9.5739930
Pt	9.1614500	11.7919680	18.8078230
Pt	9.1518430	11.7847580	11.9318080
Pt	3.4036330	11.7900340	18.9197600
Pt	3.5767500	11.7497150	11.9726190
Pt	12.0686310	11.8616960	18.9884670
Pt	11.9407510	11.7624730	11.9623290
Pt	6.2530950	11.8569170	18.9918210
Pt	6.3695900	11.7545740	11.9642130
Pt	14.9180320	11.8025800	18.9221080
Pt	14.7353130	11.7582770	11.9723320
Pt	10.6516540	4.3882600	18.9663930
Pt	10.5701350	4.5148680	12.0200310
Pt	10.5613640	14.1957420	18.7771450
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Pt	4.8867260	4.3298810	11.9085530
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Pt	4.8803270	14.3525840	18.9096440
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Pt	13.4343690	14.3616500	18.9072900
Pt	13.3256870	14.1948580	11.9528200
Pt	7.6907940	4.3859910	18.9661770
Pt	7.7633420	4.5116840	12.0211830
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Pt	7.7681880	14.2084870	11.9408840
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Pt	9.1652050	6.9333860	11.9978440
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Pt	3.6151700	6.9405880	12.0033340
Pt	11.9441000	6.9621380	18.8245470
Pt	11.9670760	6.9228430	11.9875330
Pt	12.0289480	16.7784680	11.8338340
Pt	6.3914750	6.9549470	18.8267720
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Pt	14.7135400	6.9568270	12.0008470
Pt	6.3152890	16.7640800	11.8712820
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Pt	10.5703560	9.3393490	11.9481090
Pt	4.9873030	9.3788420	18.8093630
Pt	4.9597780	9.3285960	11.9722500
Pt	13.3452540	9.3894830	18.8103960
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Pt	7.7699020	9.3741270	18.8255000
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Pt	16.3272370	9.3591320	11.8702820
Pt	17.7670850	10.1739230	14.2449860
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Cu	13.3074720	12.5199950	7.6737550
Cu	11.8162140	14.8057200	7.5712370
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Cu	5.0129600	7.7861280	20.8177620
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Cu	6.5039630	5.4931810	20.9203420
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Cu	2.4306350	9.2656320	18.6987870
Cu	5.0122180	4.7979470	18.7247720
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Cu	1.0297440	8.6240340	16.4316770
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Cu	14.5886410	7.0555920	18.6891210
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Cu	2.4240170	11.0414320	9.7968010
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Cu	6.5184350	14.8330550	7.6105480
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Cu	9.1643170	5.3267280	7.7320610
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Cu	6.5872410	3.8385430	9.8503810
Cu	9.1678630	2.3721410	11.9582320
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Cu	6.4332440	2.3268660	12.1260190
Cu	9.1606460	14.9867810	20.7733720
Cu	11.8911150	14.8532130	20.8612070
Cu	6.4249700	14.8484210	20.8645620
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Cu	6.4108420	17.9707580	16.3983150
Cu	7.9484780	9.5057540	23.2830940
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Cu	6.5608980	11.7029110	23.2395210
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Cu	11.7666410	11.7113720	23.2353270
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Cu	9.1537320	8.6903770	5.2246760
Cu	11.7581090	8.6000800	5.2586700
Cu	9.1487010	13.0920620	5.2040780
Cu	7.9284600	10.8016670	5.2151170
Cu	6.5542970	8.5942960	5.2647270
Cu	2.5899170	15.3542170	17.9020450
Cu	1.3709800	13.2413590	17.9112060
Cu	2.6738640	13.9196370	20.0582100
Cu	2.6450190	16.8951390	15.8152350
Cu	1.3672380	14.6367400	15.9112190

Cu	0.0709680	12.3853910	15.8231930	O	3.3295760	20.2637060	14.1276990
Cu	15.7276880	4.9555660	10.6065650	O	20.8251200	10.1682260	14.2384580
Cu	16.9452820	7.0691040	10.5918110	O	-3.2320881	10.0357000	14.2327620
Cu	15.6452520	6.3982260	8.4436810	O	17.8761000	10.9979210	19.2954970
Cu	15.6577040	3.4176700	12.7027870	O	0.4508270	10.9677950	19.2983700
Cu	16.9497950	5.6739120	12.5901200	O	0.4462610	9.3053550	9.2032760
Cu	18.2468040	7.9339300	12.6732330	O	17.8730770	9.3316450	9.1986750
Cu	2.6075580	4.9319470	10.6112890	O	4.1102370	2.9792890	9.2433440
Cu	1.3867630	5.6453900	12.5967010	O	5.4814580	12.2124050	5.0632450
Cu	2.6857300	3.3945890	12.7113240	O	12.9075140	17.9108730	9.1105660
Cu	2.6823290	6.3746610	8.4475160	O	14.2048790	17.3295590	19.2610670
Cu	1.3830680	7.0419990	10.5960330	O	12.8228890	8.0944660	23.4408710
Cu	0.0841460	7.8932930	12.6761790	O	5.5148500	2.2307250	19.3467520
Cu	7.9510670	1.8988330	17.9681140	O	5.5158240	8.0907930	23.4463600
Cu	9.1710870	1.1866100	15.9820280	O	12.8130570	12.2144330	5.0529880
Cu	6.5622260	1.1779910	15.8794750	O	5.4152300	17.9153440	9.1763780
Cu	9.1719670	2.7004410	20.1204190	O	14.2336860	2.9975810	9.2421090
Cu	10.3923570	1.8995100	17.9680140	O	12.8268840	2.2302380	19.3418910
Cu	11.7757450	1.1828030	15.8815760	O	4.1011750	17.3158220	19.2729940
Cu	9.1591240	19.2225670	12.6099510	O	17.8850600	5.1414240	15.1896310
Cu	10.4659470	18.4539430	10.4663860	O	0.4343480	15.1696690	13.2921810
Cu	11.7645870	19.1574720	12.6152410	O	9.1239200	20.1188080	15.3129110
Cu	6.3049810	19.1791640	12.8259250	O	0.4505780	5.1248850	15.2085860
Cu	7.8246930	18.5961960	10.4099040	O	9.1735210	0.0959750	13.3852830
Cu	9.1984420	17.4841440	8.0919050	O	17.8759270	15.1918850	13.3025520
Cu	16.9394200	14.6610510	15.9091570	O	9.1624920	5.8761410	5.1009370
Cu	15.7153340	15.3749470	17.8987580	O	9.1584820	14.4216760	23.4086280
Cu	15.6388570	16.9074580	15.8031800	O	9.2542870	19.0169590	9.1182720
Cu	18.2434120	12.4146550	15.8211330	O	7.6156940	19.9779920	11.8011460
Cu	16.9397100	13.2639470	17.9100240				
Cu	15.6376670	13.9353110	20.0618870				
C	3.9113830	13.2085540	22.7542740				
C	14.3963890	7.1020500	5.7353970				
C	14.4208800	19.2085300	14.1830180				
C	3.9183540	1.1089510	14.3136670				
C	9.1371730	16.2040150	5.7060100				
C	9.1698740	4.1567880	22.8175860				
C	14.3801190	13.2048720	22.7787330				
C	3.9376240	7.0835360	5.7294770				
C	14.4081110	1.1180320	14.3088730				
C	3.9482710	19.2287080	14.1559650				
C	19.6192430	10.1689090	14.2410250				
C	-2.0264201	10.0540760	14.2394650				
C	16.8590220	11.2152200	18.5935110				
C	1.4628040	11.1967280	18.5927960				
C	1.4654560	9.1001080	9.9048240				
C	16.8549020	9.1224360	9.9010100				
C	4.4253440	3.9740250	9.9394360				
C	6.1887730	11.8158990	6.0202040				
C	12.1161510	17.2694350	9.8486440				
C	13.8922870	16.3340540	18.5645680				
C	12.1270040	8.4939460	22.4765500				
C	6.2116040	2.9986100	18.6405310				
C	6.2087980	8.4882920	22.4792620				
C	12.1090970	11.8162390	6.0118400				
C	6.2568130	17.3215690	9.9038570				
C	13.9068420	3.9899000	9.9362970				
C	12.1319940	3.0032690	18.6397910				
C	4.4113900	16.3223900	18.5728590				
C	16.8669930	5.7306390	14.7535440				
C	1.4502690	14.5874620	13.7414360				
C	9.1386670	19.0102400	14.7168570				
C	1.4657010	5.7079580	14.7582420				
C	9.1700500	1.2725430	13.8203470				
C	16.8578580	14.6060130	13.7420230				
C	9.1603810	6.6923380	6.0535920				
C	9.1593330	13.6176540	22.4455550				
O	3.2893180	13.5537040	23.7278560				
O	15.0067220	6.7517740	4.7561230				
O	15.0366770	20.2448930	14.1574740				
O	3.2983470	0.0749510	14.3293690				
O	9.1176360	16.8980190	4.7197400				
O	9.1703810	3.4625010	23.8036320				
O	14.9793670	13.5435420	23.7688400				
O	3.3358480	6.7268280	4.7472890				
O	15.0221630	0.0803650	14.3222490				