Supplementary Information for: 'Adsorption Energies on Transition Metals Surfaces: Towards an Accurate and Balanced Description'

Araujo et al.

Supplementary Note 1

Optimized structure of C_6H_6/Pt(111)

C_6H_6_Pt111:
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Cluster structure (xyz format; Ångström)

Pt	12.53169669	8.81951902	7.11736263
Pt	13.90533434	11.21480254	7.15698980
Pt	12.48884767	12.07730979	9.38406973
Pt	13.92183100	6.42921244	7.13021967
Pt	16.66276914	6.43025807	7.12996328
Pt	15.29281937	8.83729397	7.16332612
Pt	18.05564930	8.82036605	7.11689501
Pt	16.68271269	11.21636789	7.15290701
Pt	12.49213394	7.18169737	9.38061056
Pt	15.30951171	7.25914956	9.52679642
Pt	18.12099113	7.17993712	9.37831653
Pt	13.82455157	9.64465876	9.49357908
Pt	16.79304075	9.64644165	9.48568560
Pt	15.30698514	12.02064527	9.55368308
Pt	18.12432374	12.08135360	9.38560696
H	13.17074983	10.84643478	11.87005820
H	15.32794246	7.20056959	12.12139794
C	15.31901108	11.13320334	11.51893416
C	16.55831547	10.33835534	11.54882127
C	16.56119858	8.90430019	11.53999538
C	15.32344827	8.10676746	11.50564540
C	14.08364606	8.90041487	11.54715233
C	14.08173859	10.33502836	11.55424410
H	15.32062262	12.03354610	12.14382602
H	17.47152519	10.85162781	11.85587481
H	17.47658637	8.39113017	11.84201429
H	13.17309622	8.38345289	11.85643229

C_6H_6/Pt111 structure with 5 Pt layers slab (POSCAR format):

Pt H C H
1.00000000000000
8.3367889501893959 0.0000000000000000 0.0000000000000000
4.1683944750946980 7.2198710168534168 0.0000000000000000
0.0000000000000000 0.0000000000000000 23.0759462316609181
Pt H C H
45 2 6 4
Selective dynamics
Direct

0.9144764033372326	0.1934946254310006	0.1216057653510703	F	F	F
0.2478097366705683	0.1934946254310006	0.1216057653510703	F	F	F
0.5811430700038969	0.1934946254310006	0.1216057653510703	F	F	F
0.9144764033372326	0.5268279587643363	0.1216057653510703	F	F	F
0.2478097366705683	0.5268279587643363	0.1216057653510703	F	F	F
0.5811430700038969	0.5268279587643363	0.1216057653510703	F	F	F
0.9144764033372326	0.8601612920976649	0.1216057653510703	F	F	F

0.2478097366705683	0.8601612920976649	0.1216057653510703	F	F	F
0.5811430700038969	0.8601612920976649	0.1216057653510703	F	F	F
0.0228962480068147	0.9672568285081866	0.2208079034827217	T	T	T
0.3564030041337661	0.9670467592941380	0.2217260400500299	T	T	T
0.6897077473349090	0.9672865947196773	0.2207528800914902	T	T	T
0.0232823780059122	0.3004443416119634	0.2218152080346320	T	T	T
0.3560017901433476	0.3004609108205153	0.2217626296846819	T	T	T
0.6896488441254860	0.3007070575317507	0.2204989418072976	T	T	T
0.0232100229237288	0.6334969212751145	0.2211491525635199	T	T	T
0.3562603166890955	0.6339913141480953	0.2213959205781182	T	T	T
0.6896910373013793	0.6340309989786285	0.2213788663045324	T	T	T
0.1335755840372012	0.0754435788724605	0.3194633476287911	T	T	T
0.4658490396786079	0.0755057604897510	0.3193302639088270	T	T	T
0.7993239947419004	0.0761248723715596	0.3181213836190628	T	T	T
0.1328642958801386	0.4094374597151204	0.3201006608035134	T	T	T
0.4660497524104241	0.4088929242849582	0.3185214420712605	T	T	T
0.7998939299607272	0.4089624806658726	0.3185566892168305	T	T	T
0.1329927675737651	0.7420022711322030	0.3188186527941850	T	T	T
0.4660768834184809	0.7427827363837227	0.3192504561186759	T	T	T
0.8002006499409668	0.7420417200174259	0.3188003591660344	T	T	T
0.9098617691803661	0.1863572020158298	0.4165724983149632	T	T	T
0.2413617081980177	0.1882414807578047	0.4188442027742766	T	T	T
0.5746517918925039	0.1863397227057857	0.4165681959965932	T	T	T
0.9096516781467692	0.5184437034026096	0.4182229628157428	T	T	T
0.2427636576310167	0.5183882719429856	0.4182748141244595	T	T	T
0.5760785602390700	0.5187880828498098	0.4154299011367478	T	T	T
0.9113455522701425	0.8485460708201221	0.4166726164442539	T	T	T
0.2430629395796729	0.8551764283514595	0.4172681376409536	T	T	T
0.5730377218137027	0.8550219674339747	0.4170866111690174	T	T	T
0.0161921385893373	0.9604492166706939	0.5157808743110761	T	T	T
0.3485898427854152	0.9714380079136012	0.5216827888284482	T	T	T
0.6912940920334667	0.9603795509209090	0.5157417224950097	T	T	T
0.0064078339673755	0.3006900171047454	0.5196954183802293	T	T	T
0.3610650440558852	0.3010712113190376	0.5199173332662670	T	T	T
0.6844181157622732	0.2993936998882984	0.5158182986299795	T	T	T
0.0188683353744711	0.6299341366198774	0.5218826673414257	T	T	T
0.3530066610442010	0.6385461048306298	0.5157330221229638	T	T	T
0.6763772835806754	0.6384858398523785	0.5157150961566314	T	T	T
0.8395146822196600	0.4695683082570775	0.6220789753843103	T	T	T
0.3508204728780940	0.9655128189218853	0.6344633987554946	T	T	T
0.0771352603942044	0.5105986634975663	0.6074356571429278	T	T	T
0.2809407558022748	0.4002112565609514	0.6090043370071562	T	T	T
0.3809713898559651	0.2014417934734795	0.6089059003754598	T	T	T
0.2884279708527792	0.0900613421197604	0.6073244244338383	T	T	T
0.0845460696807828	0.2005502049931713	0.6087416422353074	T	T	T
0.9847361361891532	0.3992903216311798	0.6088953142484919	T	T	T
0.0141850291296008	0.6355206448708007	0.6344128484162466	T	T	T
0.3548033029265241	0.4713746893485882	0.6223551410561577	T	T	T
0.5258555946027367	0.1312331850635386	0.6224112503937798	T	T	T
0.0104129972122613	0.1295052340347886	0.6219603404041454	T	T	T

Supplementary Table 1: Adsorption energies computed with PBC (blue), adsorption energies calculated with the finite size clusters (green), reference adsorption energies (orange), adsorption energies corrected with the additive scheme (black), errors of the corrected adsorption energies with respect to the experimental data (red).

Reaction	PW91-PBC	PBE-PBC	RPBE-PBC	SCAN-PBC	M06-Cluster	PW91-cluster	PBE-cluster	RPBE-cluster	SCAN-Cluster	Ref.	CORRECT-PW91	CORRECT-PBE	CORRECT-RPBE	CORRECT-SCAN	ERROR-PW91	ERROR-PBE	ERROR-RPBE	ERROR-SCAN
N/Ni100	-141.3	-146.7	-131.5	-149.0	-82.2	-115.3	-115.2	-102.4	-109.1	-100.4	-108.2	-113.7	-111.3	-122.1	-7.8	-13.3	-10.9	-21.6
CH/Pt111	-156.0	-153.9	-140.9	-177.3	-182.7	-173.4	-174.1	-164.1	-167.8	-163.1	-165.3	-162.5	-159.5	-192.3	-2.2	0.6	3.6	-29.2
CH_3/Pt111	-47.5	-47.1	-38.5	-64.2	-59.6	-57.0	-55.9	-49.0	-58.6	-50.9	-50.1	-50.8	-49.1	-65.2	0.8	0.1	1.8	-14.3
CO/Ni(111)	-42.5	-44.5	-33.6	-43.6	-15.7	-33.9	-33.3	-23.6	-26.1	-29.8	-24.3	-26.9	-25.7	-33.2	5.5	2.9	4.0	-3.4
CO/Pt(111)	-37.4	-38.9	-32.7	-44.9	-41.0	-49.2	-49.0	-41.3	-51.7	-29.8	-29.1	-30.9	-32.4	-34.2	0.6	-1.1	-2.7	-4.4
CO/Pd(111)	-44.9	-46.8	-36.6	-50.5	-28.8	-44.9	-44.6	-35.3	-46.1	-34.4	-28.8	-31.0	-30.1	-33.2	5.5	3.4	4.3	1.2
CO/Pd(100)	-43.3	-44.0	-36.9	-48.3	-28.6	-39.6	-39.2	-30.9	-38.7	-37.6	-32.2	-33.4	-34.6	-38.1	5.4	4.2	3.0	-0.5
CO/Rh(111)	-44.2	-43.7	-38.9	-47.0	-33.5	-43.0	-42.5	-35.7	-36.9	-33.9	-34.7	-34.8	-36.7	-43.7	-0.8	-0.8	-2.8	-9.7
CO/Ir(111)	-45.4	-45.5	-40.4	-47.0	-42.3	-47.8	-47.4	-40.6	-44.2	-39.2	-39.9	-40.4	-42.1	-45.1	-0.6	-1.2	-2.9	-5.9
CO/Cu(111)	-17.9	-17.3	-13.4	-21.0	2.0	-6.5	-5.8	1.0	-6.5	-13.6	-9.5	-9.5	-12.4	-12.5	4.1	4.1	1.2	1.1
CO/Ru(0001)	-44.0	-44.4	-38.7	-45.0	-28.8	-45.5	-45.1	-38.9	-40.3	-38.5	-27.3	-28.1	-28.7	-33.6	11.2	10.4	9.9	4.9
CO/Co(0001)	-38.7	-38.3	-32.7	-39.7	-17.2	-32.7	-31.9	-24.0	-36.1	-28.4	-23.2	-23.6	-25.9	-20.8	5.2	4.7	2.5	7.6
NO/Pt(111)	-42.3	-40.6	-35.3	-44.0	-12.7	-30.0	-29.5	-19.6	-27.6	-28.4	-24.9	-23.8	-28.4	-29.0	3.4	4.6	0.0	-0.7
NO/Pd(111)	-52.0	-54.0	-45.0	-54.8	-30.3	-44.9	-44.2	-33.5	-45.5	-43.6	-37.3	-40.0	-41.8	-39.5	6.3	3.6	1.8	4.1
NO/Pd(100)	-48.8	-51.0	-41.2	-50.5	-24.3	-39.6	-39.0	-28.3	-41.6	-39.0	-33.5	-36.3	-37.2	-33.2	5.5	2.7	1.8	5.7
O/Ni(111)	-125.9	-124.7	-113.5	-120.7	-90.7	-103.6	-102.9	-91.4	-111.4	-118.3	-113.0	-112.5	-112.8	-100.0	5.4	5.9	5.5	18.3
O/Ni(100)	-132.3	-132.5	-119.5	-131.7	-99.4	-116.1	-115.6	-103.4	-116.1	-123.6	-115.7	-116.4	-115.6	-115.1	8.0	7.3	8.0	8.6
O/Pt(111)	-97.7	-98.4	-85.7	-94.1	-48.5	-64.3	-64.3	-53.2	-56.8	-85.4	-81.9	-82.6	-80.9	-85.8	3.5	2.8	4.5	-0.4
O/Rh(100)	-121.9	-122.4	-109.1	-117.2	-65.9	-93.0	-92.3	-80.8	-85.2	-102.9	-94.8	-96.0	-94.2	-97.9	8.1	6.8	8.7	5.0
H/Pt(111)	-63.8	-62.2	-60.6	-67.5	-55.1	-58.0	-57.8	-54.3	-56.9	-63.4	-60.9	-59.6	-61.4	-65.7	2.5	3.9	2.0	-2.2
H/Ni(111)	-65.3	-65.0	-62.1	-69.5	-54.8	-56.9	-56.4	-52.6	-54.4	-66.7	-63.2	-63.3	-64.3	-69.9	3.5	3.4	2.4	-3.1
H/Ni(100)	-64.6	-64.0	-60.8	-69.6	-60.1	-59.8	-59.8	-55.5	-59.5	-65.1	-64.9	-64.3	-65.4	-70.3	0.2	0.8	-0.3	-5.2

H/Rh(111)	-65.9	-64.3	-62.8	-68.8	-56.3	-62.9	-62.9	-60.2	-61.7	-63.4	-59.3	-57.8	-58.9	-63.5	4.1	5.6	4.5	-0.1
H/Pd(111)	-66.3	-65.0	-63.2	-71.4	-60.7	-63.2	-62.9	-59.5	-63.8	-65.5	-63.8	-62.8	-64.4	-68.3	1.7	2.7	1.1	-2.8
I/Pt(111)	-57.9	-56.0	-49.9	-58.2	-49.6	-49.8	-49.0	-38.5	-48.7	-55.4	-57.6	-56.6	-61.0	-59.0	-2.3	-1.2	-5.6	-3.7
NH_3/Cu(100)	-10.0	-10.4	-8.6	-13.4	-4.9	-4.9	-4.0	1.7	-9.5	-14.3	-10.0	-11.3	-15.2	-8.8	4.3	3.0	-0.9	5.5
CH_3I/Pt(111)	-6.2	-5.4	-3.8	-9.0	-10.8	-8.9	-8.1	-0.8	-11.3	-20.1	-8.1	-8.2	-13.8	-8.5	11.9	11.9	6.3	11.6
CH_3OH/Pt(111)	-4.7	-4.5	-3.8	-16.8	-14.9	-8.4	-7.6	-1.1	-13.6	-13.1	-11.2	-11.8	-17.6	-18.1	1.9	1.4	-4.5	-4.9
CH_4/Pt(111)	-0.9	-1.0	-0.4	-2.0	-2.8	0.6	1.0	3.5	-0.7	-3.5	-4.3	-4.8	-6.7	-4.0	-0.9	-1.3	-3.2	-0.6
C_2H_6/Pt(111)	-1.2	-0.7	-0.8	-3.2	-2.9	-0.4	0.2	5.1	-2.5	-6.5	-3.6	-3.7	-8.8	-3.6	2.9	2.7	-2.3	2.9
C_3H_8/Pt(111)	-1.3	-1.1	-0.8	-4.5	-6.9	-1.6	-0.8	6.0	-4.1	-9.2	-6.7	-7.2	-13.8	-7.3	2.6	2.0	-4.6	1.9
C_4H_{10}/Pt(111)	0.1	1.0	0.8	-3.9	-13.2	-4.5	-3.5	6.0	-10.0	-9.2	-8.7	-8.7	-18.5	-7.1	0.6	0.5	-9.2	2.1
C_6H_6/Pt(111)	-21.8	-22.8	-2.7	-45.0	-36.9	-37.6	-37.6	-18.1	-49.1	-38.8	-21.0	-22.1	-21.4	-32.7	17.7	16.7	17.3	6.0
C_6H_6/Cu(111)	-6.4	-1.1	-4.7	-6.8	-9.9	-4.4	-3.5	6.1	-11.3	-15.7	-11.9	-7.5	-20.7	-5.4	3.8	8.2	-5.0	10.3
C_6H_6/Ag(111)	-1.4	-0.6	2.5	-6.1	-8.4	-1.5	-0.6	7.7	-8.8	-14.5	-8.3	-8.5	-13.7	-5.8	6.2	6.1	0.8	8.7
C_6H_6/Au(111)	4.0	-1.0	5.2	-8.9	-12.2	-6.3	-5.4	3.3	-14.2	-16.8	-1.9	-7.8	-10.3	-6.9	14.9	9.0	6.6	10.0
H_2O/Pt(111)	-5.0	-4.7	-1.1	-15.2	-10.0	-10.9	-10.3	-5.2	-13.9	-13.1	-4.2	-4.5	-5.9	-11.4	9.0	8.7	7.2	1.8
C_6H_{10}/Pt111	-17.7	-22.5	-5.5	-31.8	-30.4	-30.1	-29.4	-15.1	-42.0	-29.4	-18.0	-23.5	-20.8	-20.3	11.4	5.9	8.6	9.2

Supplementary Note 2.

Experimental uncertainties:

Experimental uncertainties were obtained as described below. Further, these values were averaged to compare to MAEs obtained theoretically.

CO/Ni(111):

Ref. (1), estimated from Figure 9 of the reference.

Ref. (2), estimated from Figure 8 of the reference.

Ref. (3), explicitly reported for a coverage close to 0. We assume a similar value for ¼ ML coverage.

CO/Pt(111):

Ref (1), estimated from Figure 11 of the reference.

Ref(4), explicitly reported for a coverage close to 0 ML – We assumed to be similar for ¼ ML coverage.

CO/Pd(111):

Ref(5), estimated from Figure 4 of the reference.

CO/Pd(100):

Ref.(6), estimated from Figure 11.

Ref.(7), explicitly shown in the reference text.

CO/Rh(111):

Ref.(8), explicitly shown in Table 1 of the reference. Since, two methods are employed, we used the average of them.

Ref. (9), Explicitly shown in the reference text for low coverage of CO on Rh(111). We, hence, assumed a similar error.

CO/Cu(111):

Ref. (10), estimated from Figure 2 in the reference.

CO/Co(0001):

Ref.(11), explicitly shown in the reference's text.

NO/Pd(111):

Ref.(12), estimated from Figure 2 of the reference by considering low NO exposure.

O/Ni(100):

Ref. (1), estimated from Figure 18 in the reference. Low coverage was assumed and the error was divided by 2 since, in the reference, the adsorption is given per O2.

O/Pt(111):

Ref. (13), Explicitly showed in Tab. 1 of the Ref.

I/Pt(111):

Ref. (14), Extracted from Fig. 5 of the reference.

NH_3/Cu(100):

Ref. (15), Explicitly given in the reference's text.

CH_3I/Pt(111):

Ref.(16), Explicitly showed in the reference for low coverages. We assume a similar uncertainty.

CH_3OH/Pt(111):

Ref. (17), Explicitly showed in the reference text for low coverages. We assumed a similar error for 0.25 ML (used coverage for our calculations).

C_6H_6/Pt(111):

Ref. (18), Computed as 1.4% of the measured data (this percentage is estimated in the reference text).

C_6H_6/Cu(111):

Ref. (19), Uncertainty estimated from Figure 8 of the reference.

D_2O/Pt(111):

Ref. (20), Explicitly written in the reference text.

CH_3/Pt111:

Ref. (21), Explicitly written in the reference text.

Supplementary Table 2: MAE and RMSE calculated using RPBE, BEEF-vdW and PBE+D3/M06. All energies in kcal mol^{-1}. Here, MAEs and RMSEs are computed by removing the reactions involving water adsorption, C_6H_6 adsorption on Pt(111), CH adsorption on Pt(111), CH_3 adsorption on (Pt111) and C_6H_{10} adsorption on Pt(111).

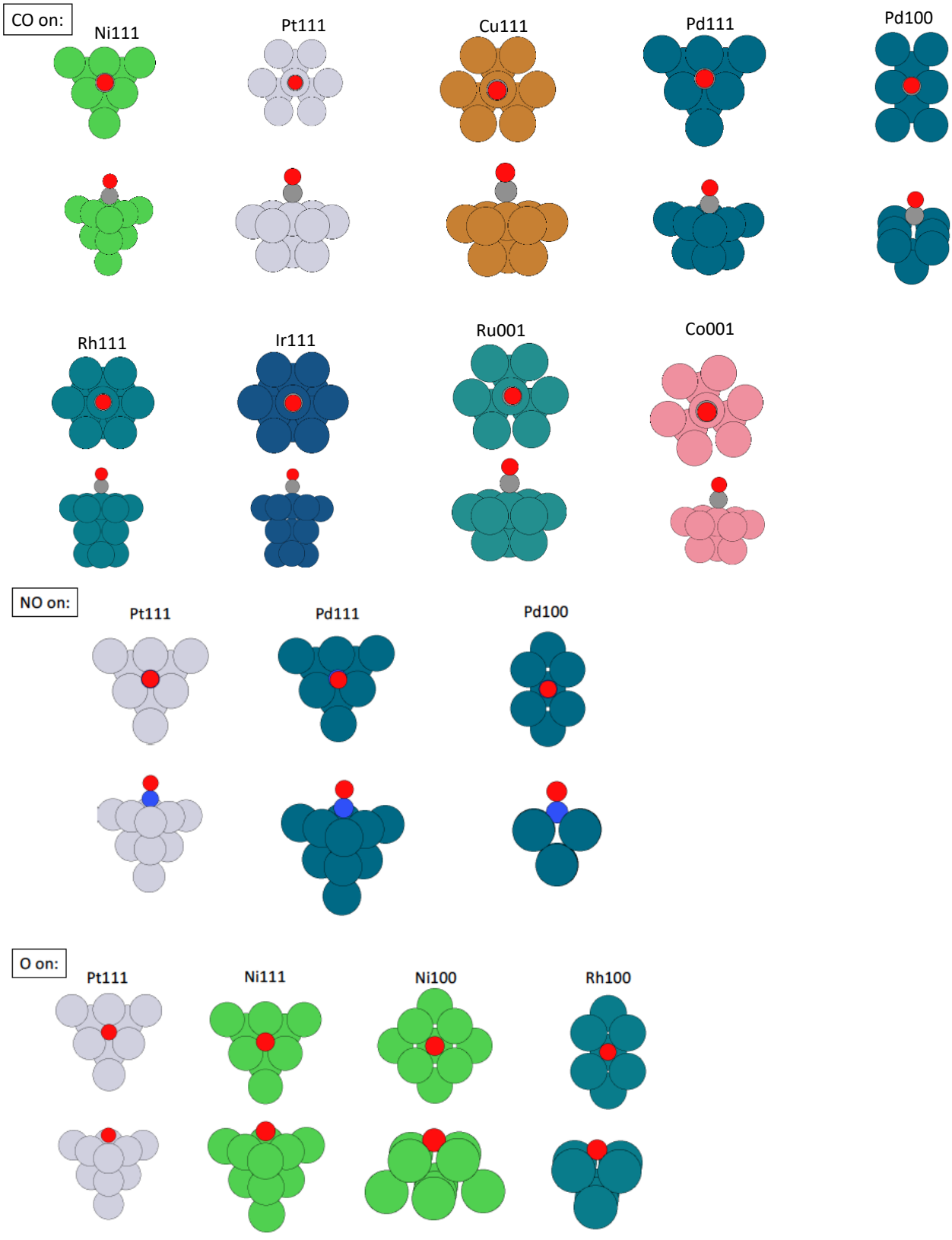
	RPBE[a]	BEEF-vdW[a]	PBE+D3/M06[b]
MAE-Chem.	4.2	3.7	2.2
MAE-Phys.	10.9	5.4	2.5
MAE-Tot.	6.2	4.2	2.3
RMSE-Chem.	7.4	5.9	2.5
RMSE-Phys.	12.2	6.8	3.4
RMSE-Tot.	9.1	6.2	2.8

[a] From ref. [4]
[b] Present work

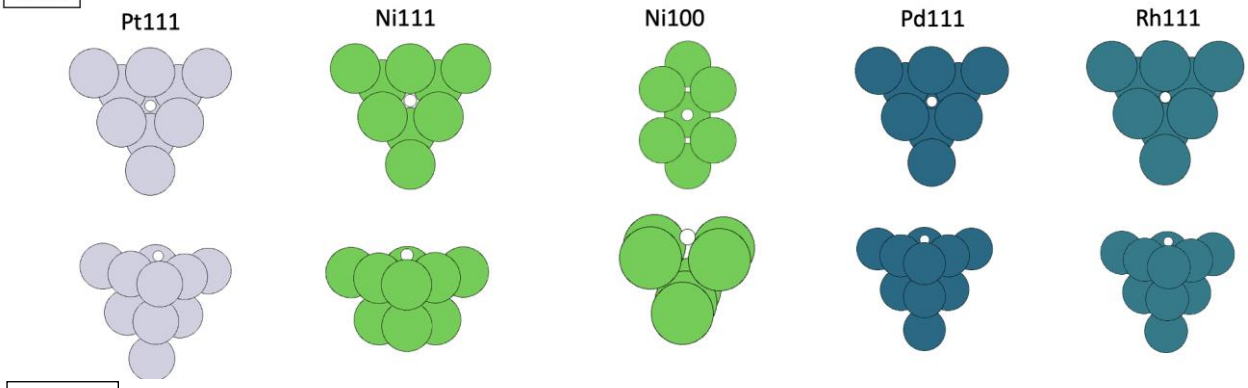
Supplementary Table 3: Experimental transition barriers, barrier heights using PBE+D3 and PBC (PBE+D3-PBC), corrected barriers with the M06 hybrid (PBE+D3/M06), barriers on the finite-size cluster using PBE+D3 and M06(PBE+D3-cluster, M06-cluster), multiplicities found as the energy ground state for the cluster calculations.

Reaction	EXP.	PBE+D3-PBC	PBE+D3/M06	PBE-D3 cluster	M06 Cluster	Mult. PBE GS	Mult. PBE TS
H_2 + Cu(111) → H_2/Cu(111)	14.53	3.52	15.07	21.37	32.88	3	3
H_2 + Cu(100) →H_2/Cu(100)	17.07	6.88	17.24	8.10	18.44	1	1
H_2 + Pt(111) → H_2/Pt(111)	0.00	0.00	0.00	-6.64	-8.77	13	13
CH_4 + Ni(100) →CH_4/ Ni(100)	17.53	5.78	20.54	12.65	27.37	11	11
CH_4 + Ni(111) →CH_4/ Ni(111)	23.29	9.43	25.11	25.07	40.71	9	9

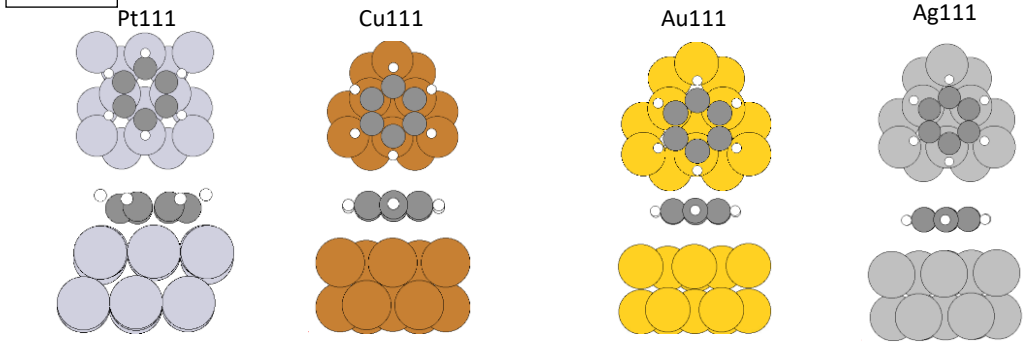
Supplementary Figure 1: Finite-size clusters used in our investigation.



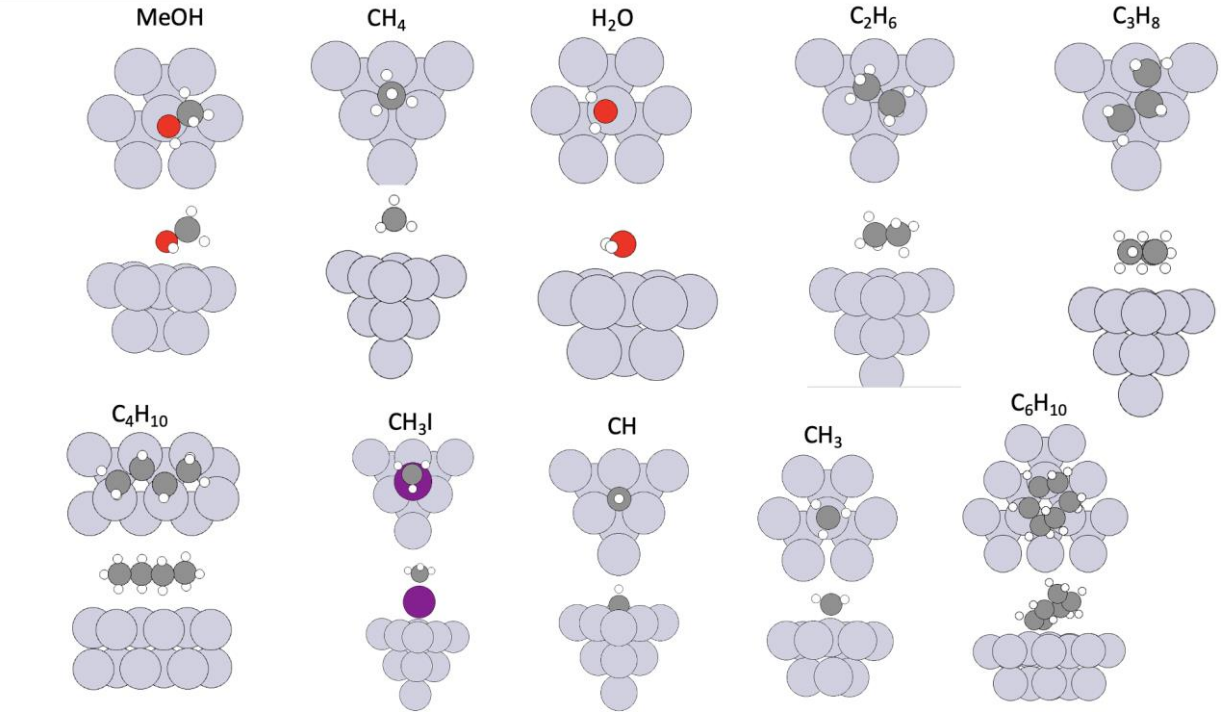
H on:



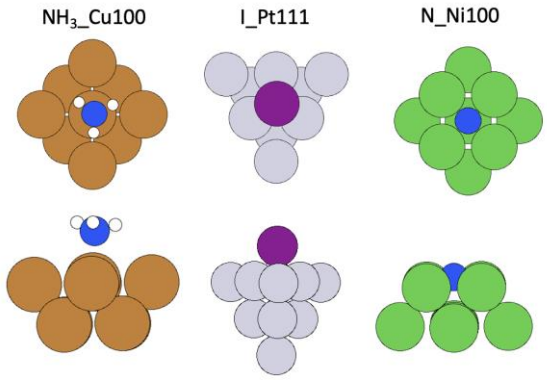
C_6H_6 on:



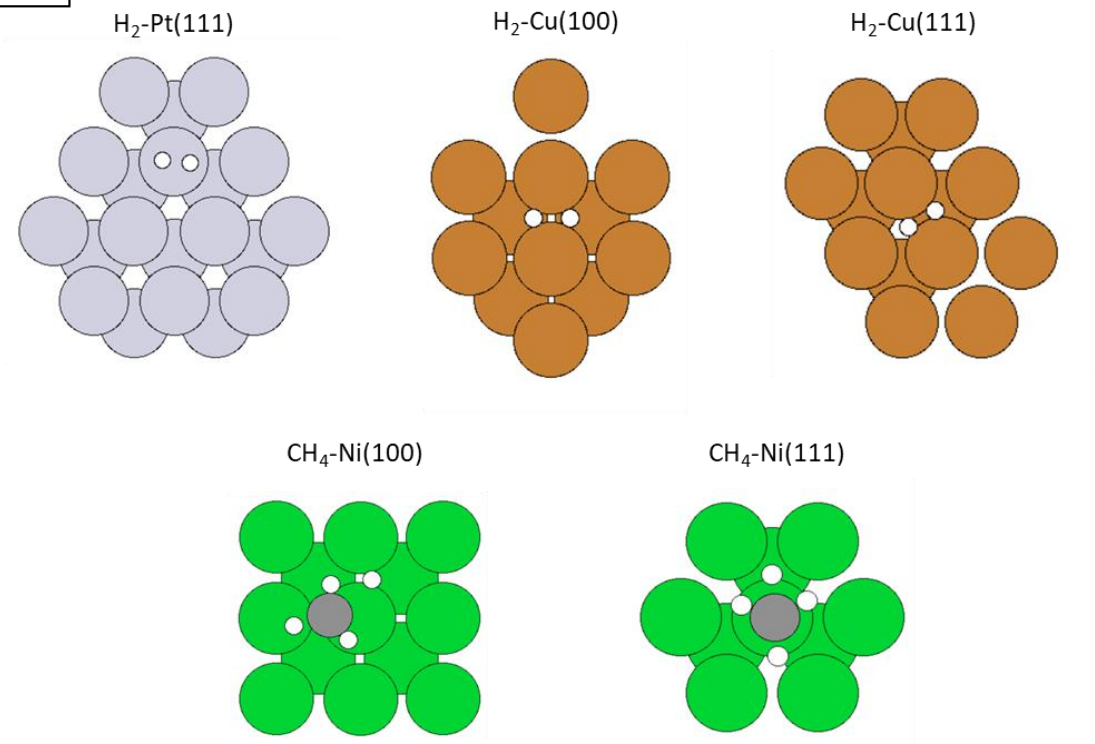
Mol on Pt(111):



Other cases:

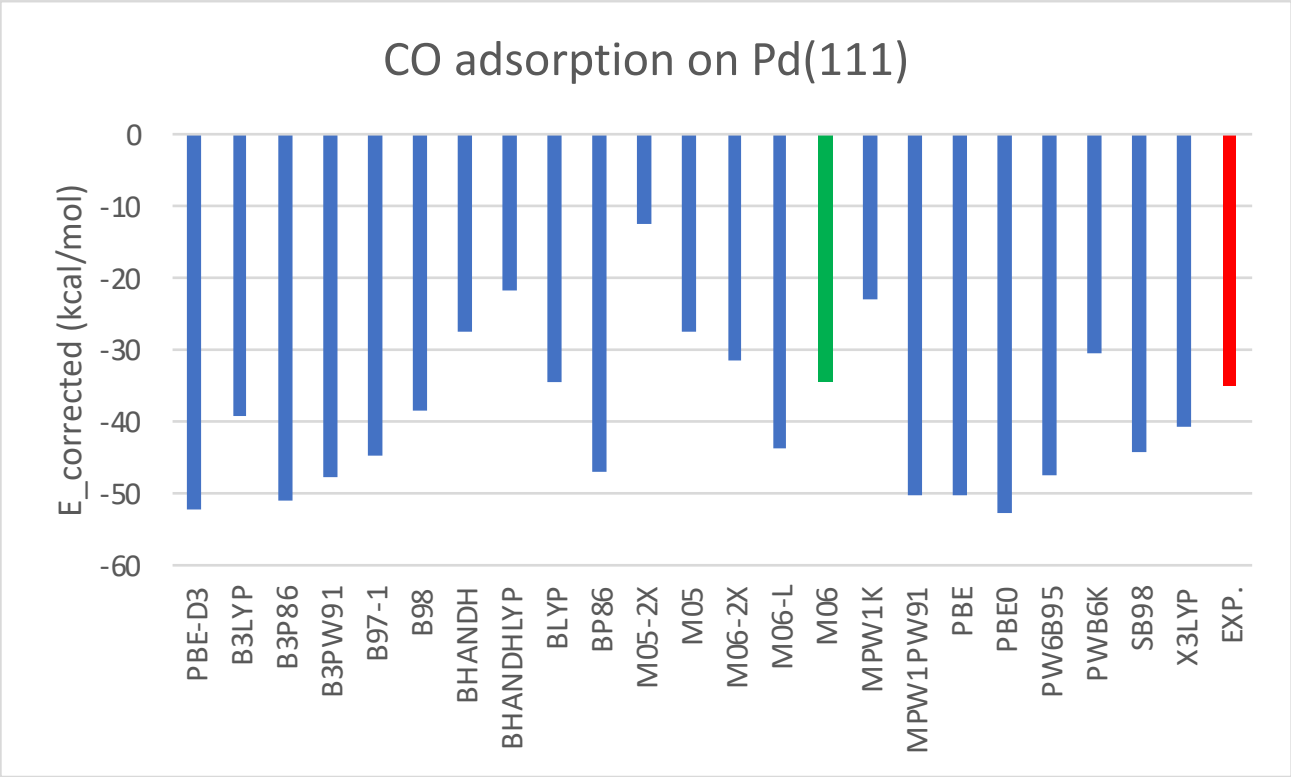


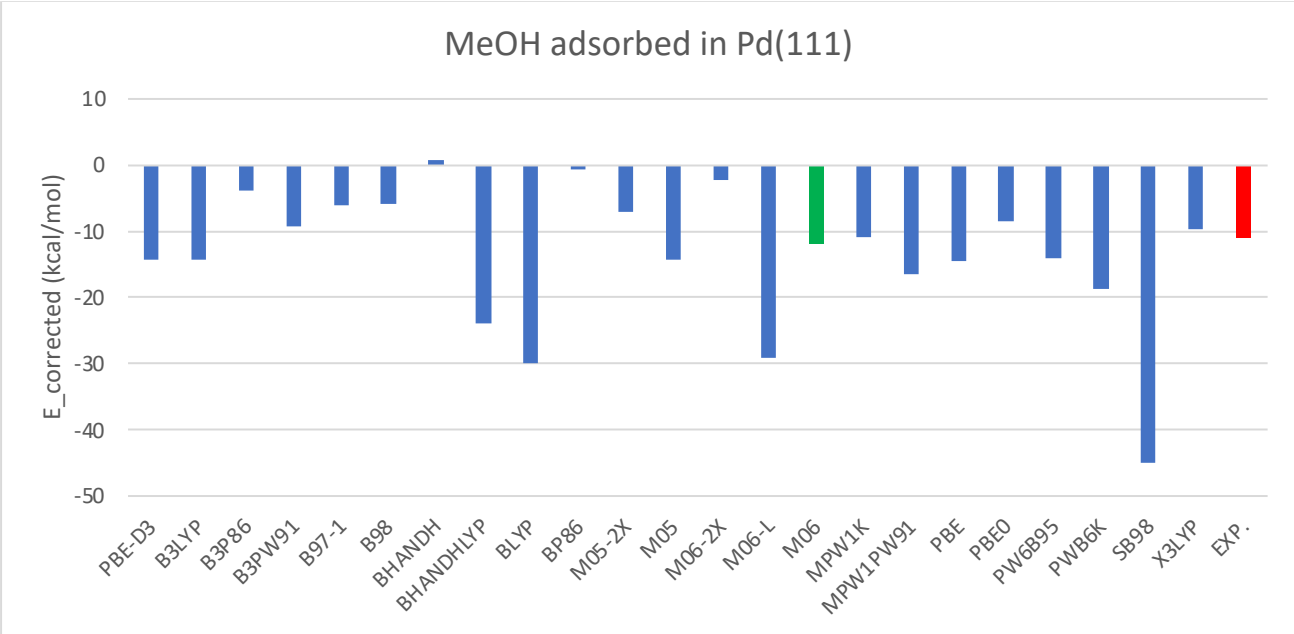
Transition States:



Supplementary Table 4: Optimized lattice parameters (Å). Optimization of bulk structures were performed using a *k*-point mesh of 15x15x15 for the FCC structures and 15x15x13 for the HCP structures together with a cutoff energy of 500 eV.

Metal	PBE+D3		RPBE	
	a (Å)	c (Å)	a (Å)	c (Å)
Ni	3.48		3.55	
Pt	3.93		3.99	
Pd	3.89		3.98	
Rh	3.79		3.85	
Ir	3.84		3.89	
Cu	3.57		3.67	
Ag	4.07		4.21	
Au	4.10		4.20	
Co	2.46	3.98	2.51	4.07
Ru	2.70	4.24	2.73	4.28





Supplementary Figure 2: (Top) Corrected CO adsorption energy and (bottom) corrected MeOH adsorption energy. Adsorption energies were calculated as $\boldsymbol{E_{ads} = E_{PBE+D3}^{Ads,PBC} + E_{X}^{Ads,Cluster} - E_{PBE+D3}^{Ads,Cluster}}$. Here, $\boldsymbol{E_{ads}}$ is the corrected adsorption energy, $\boldsymbol{E_{PBE+D3}^{PBC}}$ is the adsorption energy calculated with the PBC and using PBE+D3, $\boldsymbol{E_{X}^{Cluster}}$ is the adsorption energy calculated with the finite-size cluster with the distinct functionals (X here assumes the functionals shown in the figure), $\boldsymbol{E_{PBE+D3}^{Cluster}}$ is the finite-size adsorption energy computed using PBD+D3. Source data are provided as Source Data file.

Supplementary Table 5: Basis set superposition error, in kcal mol^{-1}, for randomly selected reactions.

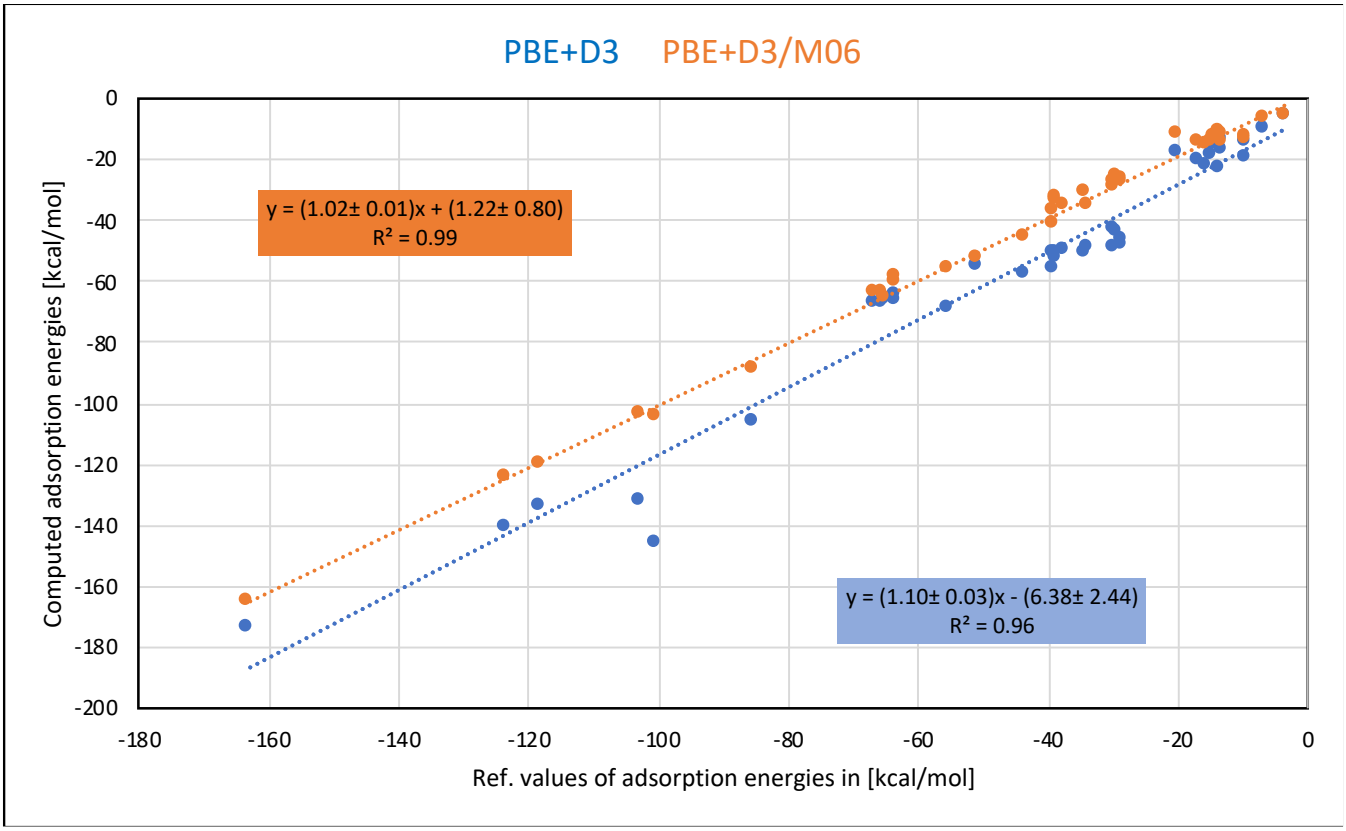
Reaction	PBE+D3-BSSE	M06-BSSE	BSSE(PBE+D3-M06)
C_6H_6/Pt(111)	-5.54	-6.00	0.46
C_6H_6/Cu(111)	-2.08	-2.08	0.00
C_6H_6/Ag(111)	-1.22	-1.31	0.09
C_6H_6/Au(111)	-3.46	-3.23	-0.23
NO/Pt111	-1.38	-0.92	-0.46
CO/Pt(111)	-2.08	-1.85	-0.23
CO/Cu(111)	-1.61	-1.38	-0.23
CO/Ni(111)	-1.15	-0.46	-0.69
CO/Ru(0001)	-1.85	-1.85	0.00
O/Pt(111)	-1.15	-0.92	-0.23

Supplementary Table 6: Experimental adsorption energies (EXP.) from which zero-point energies were removed, PBE+D3 level adsorption energies using PBC (PBE+D3-PBC), adsorption energies for the finite size cluster using PBE+D3 and M06(PBE+D3-cluster, M06-cluster), corrected adsorption energies with the M06 hybrid (PBE+D3/M06), multiplicities found as the energy ground state for the cluster calculations (Mult. PBE+D3 cluster, Mult. PBE+D3 cluster-mol), and the position of the adsorbates (site).

Reaction	Exp.	PBE+D3-PBC	PBE+D3 cluster	M06 cluster	PBE+D3/M06	error	MULT. PBE+D3 cluster	MULT. PBE+D3 cluster+mol	Site
N/Ni100	-100.4	-146.7	-124.5	-82.2	-104.4	-3.9	9	4	fcc
CH/Pt111	-163.2	-173.7	-174.6	-166.3	-165.4	-2.2	9	6	fcc
CH_3/Pt111	-50.9	-55.0	-61.7	-59.6	-52.9	-2.0	7	6	top
CO/Ni(111)	-29.8	-49.4	-37.1	-15.7	-28.0	1.6	9	7	fcc
CO/Pt(111)	-29.8	-42.9	-54.7	-41.0	-29.3	0.2	5	5	top
CO/Pd(111)	-34.4	-51.2	-49.1	-28.8	-30.9	3.5	7	7	fcc
CO/Pd(100)	-37.6	-50.3	-43.7	-28.6	-35.1	2.5	5	3	br
CO/Rh(111)	-33.9	-49.5	-47.2	-33.5	-35.8	-1.8	20	18	top
CO/Ir(111)	-39.2	-51.2	-52.4	-42.3	-41.1	-2.1	22	20	top
CO/Cu(111)	-13.6	-23.0	-10.1	2.0	-10.9	2.8	3	3	top
CO/Ru(0001)	-38.5	-50.8	-45.9	-28.9	-33.7	4.8	21	21	top
CO/Co(0001)	-28.4	-46.6	-36.2	-17.2	-27.6	0.7	21	21	top
NO/Pt(111)	-28.4	-48.1	-34.3	-12.7	-26.6	1.8	9	8	fcc
NO/Pd(111)	-43.6	-58.1	-42.9	-30.3	-45.5	-2.1	9	8	fcc
NO/Pd(100)	-39.0	-56.1	-43.4	-24.3	-37.0	2.1	5	4	hl
O/Ni(111)	-118.3	-134.3	-104.7	-90.7	-120.2	-1.6	9	11	fcc
O/Ni(100)	-123.6	-140.7	-115.8	-99.5	-124.4	-0.7	9	9	hl
O/Pt(111)	-85.4	-106.0	-65.5	-48.5	-89.0	-3.7	9	7	fcc
O/Rh(100)	-102.9	-132.2	-94.1	-65.9	-104.0	-1.2	12	12	hl
H/Pt(111)	-63.4	-64.8	-59.5	-55.1	-60.4	3.0	9	8	top
H/Ni(111)	-66.7	-67.1	-57.9	-54.8	-64.0	2.5	9	8	fcc
H/Ni(100)	-65.1	-66.5	-61.1	-60.1	-65.6	-0.5	9	8	hl
H/Rh(111)	-63.4	-66.4	-64.1	-56.4	-58.7	4.7	15	16	fcc
H/Pd(111)	-65.5	-67.6	-64.6	-60.7	-63.7	1.8	9	8	fcc
I/Pt(111)	-55.4	-69.0	-62.7	-49.6	-55.8	-0.2	9	8	fcc
NH_3/Cu(100)	-14.3	-15.7	-7.8	-4.9	-12.7	1.6	2	2	top
CH_3I/Pt(111)	-20.1	-18.5	-16.8	-10.8	-12.5	7.4	13	13	top
CH_3OH/Pt(111)	-13.1	-14.1	-14.1	-14.9	-14.9	-1.8	7	5	top
CH_4/Pt(111)	-3.5	-6.0	-2.8	-2.8	-6.1	-2.5	9	9	fcc
C_2H_6/Pt(111)	-6.5	-10.4	-6.1	-2.9	-7.2	-0.7	9	9	fcc
C_3H_8/Pt(111)	-9.2	-15.0	-9.2	-6.9	-12.7	-3.5	9	9	top
C_4H_{10}/Pt(111)	-9.2	-20.1	-19.1	-13.2	-14.1	-4.8	15	15	top
C_6H_6/Pt(111)	-38.8	-52.4	-56.1	-36.9	-33.2	4.8	11	9	br
C_6H_6/Cu(111)	-15.7	-22.4	-16.4	-9.9	-15.9	0.0	2	2	fcc
C_6H_6/Ag(111)	-14.5	-19.4	-12.9	-8.4	-14.9	-0.5	2	2	fcc
C_6H_6/Au(111)	-16.8	-20.5	-18.2	-12.2	-14.5	2.3	2	2	fcc
H_2O/Pt(111)	-13.1	-16.8	-14.5	-10.0	-12.3	0.7	5	5	surface
C_6H_{10}/Pt111	-29.4	-43.7	-48.6	-30.4	-25.5	3.9	7	7	surface

Supplementary Note 3

Linear regression fits were performed to obtain the correlation between the reference data and the calculated adsorption energies with PBE+D3 and PBE+D3/M06 (Supplementary Figure 3). This shows that the R^2 (goodness of the linear fitting) for the PBE+D3/M06 is 0.99 confirming the good correlation between the computed and reference data, while for PBE+D3 the value is 0.96 – still correlating with the reference data, but not as well as the PBE+D3/M06. Interestingly, the different slopes revealed that, for strongly bonded adsorbates, the correction acts more intensively resulting in larger shifts while, for lower adsorption energies, smaller shifts are obtained. This confirms that our correction acts differently depending on the nature of the adsorbate interaction with the metal surface.



Supplementary Figure 3: Linear regression showing the correlation between the reference adsorption energies (reference data) and the values obtained with PBE+D3 (blue) and PBE+D3/M06 (orange). Source data are provided as Source Data file.

Supplementary Note 4

Structure of the employed clusters as shown in Supplementary Figure 1 (.xyz format).

C_2H_6_Pt111:
18
cluster

Pt	12.48374422	7.21008906	9.40168272
Pt	12.49993470	8.82268617	7.11773511
Pt	13.87952243	9.62688996	9.40942089
Pt	11.10174691	9.62095761	9.41450854
H	13.13636140	8.78995529	13.56234874
H	13.62627147	9.27225568	11.92590218
H	12.65549532	7.80901752	12.15918331
Pt	13.89105403	6.41483707	7.12188548
Pt	15.27321383	7.21003084	9.41988152
Pt	13.88138145	4.80437257	9.41904383
H	15.06617264	7.17812915	11.73038696
H	14.62259853	6.71423538	13.38059569
Pt	13.89464825	8.02207891	4.86898656
Pt	15.27938379	8.82100378	7.12374618
Pt	16.66262602	9.62230255	9.41825043
C	14.75362317	7.58234899	12.72061575
C	13.47868854	8.40103596	12.59236036
H	15.59605340	8.18052106	13.09329159

C_3H_8_Pt111:
21
cluster
Pt 12.50675418 8.83676071 7.12212079
Pt 12.50249780 7.24759233 9.41691996
Pt 13.89518358 9.66460530 9.40985748
Pt 11.11533582 9.65839887 9.41961470
H 13.88053287 9.72139346 11.70377568
H 13.87343398 9.82682733 13.47334775
H 12.54401229 7.53926789 13.53979375
H 12.60812748 7.44677168 11.76923648
Pt 13.89689515 6.43128998 7.12430550
Pt 13.89927219 4.84049869 9.41781672
C 13.16979791 7.20278147 12.69935544
H 13.26050362 6.10927471 12.74034562
Pt 13.89464825 8.02207891 4.86898656
Pt 15.28631266 8.83718597 7.12250834
Pt 15.29687189 7.24588078 9.41588481
Pt 16.68322183 9.65883645 9.41276805
C 14.52736420 7.89112325 12.69064977
C 14.43345693 9.40902981 12.62236995
H 15.11115534 7.58915271 13.57623640
H 15.11145642 7.52725625 11.81182438
H 15.42102002 9.88862261 12.57680371

C_4H_{10}_Pt111:
38
cluster
Pt 11.10454414 6.42514596 7.11620693
Pt 11.08550981 4.83370194 9.42111551
Pt 12.49392185 8.83276341 7.12265210
Pt 9.71348407 8.83183940 7.12028316
Pt 13.88316107 11.24006669 7.11990071
Pt 11.10401429 11.23968730 7.12294001
Pt 12.47140808 7.23100697 9.41560737
Pt 9.69832257 7.23667674 9.41258680
Pt 13.86562727 9.65768124 9.41417028
Pt 11.08418790 9.64561869 9.41483391
Pt 15.25390428 12.05357296 9.42111551
Pt 12.47402606 12.05079368 9.42208109
C 12.63848768 8.11824103 12.67376479
H 11.76387034 8.78060171 12.61446892
H 12.57958712 7.43000987 11.80181950
H 12.54821394 7.49704845 13.57784499
Pt 13.88274375 6.42518817 7.12117327
Pt 16.66035789 6.42547780 7.12095664
Pt 13.86454332 4.82749244 9.42329988
Pt 16.64242053 4.83092266 9.42208109
Pt 15.27049529 8.83191127 7.12615124
Pt 18.05027302 8.83183940 7.12028316
Pt 16.66163856 11.23911515 7.12243772
Pt 15.25504021 7.22770248 9.41719349
Pt 18.03511152 7.23667674 9.41258680
Pt 16.65027583 9.65059592 9.41663491
Pt 19.42097685 9.64561869 9.41483391
Pt 18.03293780 12.04736346 9.42329988
C 13.94535277 8.89726966 12.65118042
C 15.19201342 8.01943512 12.64918859
C 16.49860917 8.79626617 12.72612378
H 13.98510837 9.60411691 13.49823820
H 13.96999653 9.54366229 11.73664516
H 15.18846649 7.40860015 11.70876087
H 15.13449815 7.28098454 13.46756528
H 17.37353056 8.13292939 12.67169018
H 16.58099676 9.50823737 11.87729405
H 16.56405179 9.38742984 13.65280629

C_6H_6_Ag111:
25
cluster
Ag 10.08369770 4.15323033 7.49500286
Ag 11.52322801 6.64662692 7.49529121
Ag 11.51771702 4.98801299 9.84693778
Ag 11.52270380 1.66004148 7.49403569
Ag 14.40205642 1.65970685 7.49535511
Ag 12.96231410 4.15317799 7.50393501

Ag	15.84231110	4.15312758	7.49560784
Ag	14.40237726	6.64672181	7.49426410
Ag	10.07805634	2.48806951	9.85476295
Ag	12.96318889	2.47669526	9.84593819
Ag	15.84977187	2.48650678	9.85102400
Ag	14.41605474	4.99168482	9.84482284
Ag	12.96267391	7.48457247	9.85303696
H	10.93646741	5.34926916	12.86156350
C	13.09460183	5.50320147	12.85437275
C	14.30806487	4.80430160	12.84268792
C	14.30718870	3.40387927	12.84319099
C	13.09504825	2.70260004	12.84702887
C	11.88275322	3.40361527	12.85826649
C	11.88163033	4.80379409	12.86052728
H	13.09469020	6.59458072	12.83670268
H	15.25290114	5.34967778	12.82864271
H	15.25256056	2.85843452	12.81812214
H	13.09568991	1.61151290	12.83629374
H	10.93800118	2.85747000	12.84387869

C_6H_6_Au111:
25
cluster

Au	10.15002349	4.17605360	7.22742009
Au	11.60189771	6.68807151	7.22711592
Au	11.59876483	1.66369356	7.22677150
Au	14.50162416	1.66331528	7.22642591
Au	13.05157885	4.17579112	7.23982056
Au	15.95278619	4.17699734	7.22745659
Au	14.50196770	6.68930091	7.22717102
Au	10.14834627	2.49609626	9.63185471
Au	13.05264932	2.47636359	9.61060587
Au	15.95690461	2.49506927	9.62845443
Au	11.59336641	5.01613038	9.61674029
Au	14.51669277	5.01661747	9.61366417
Au	13.05504342	7.52529803	9.63402218
H	10.95759287	5.32187206	12.67974921
C	13.11614728	5.47469702	12.68354355
C	14.32944466	4.77535504	12.66912079
C	14.32776483	3.37490834	12.66526565
C	13.11539405	2.67397109	12.65755341
C	11.90375150	3.37601953	12.67266284
C	11.90281645	4.77615056	12.67798468
H	13.11662210	6.56501619	12.67314729
H	15.27470864	5.32019848	12.66446752
H	15.27234954	2.82902323	12.64103500
H	13.11502324	1.58302807	12.64396562
H	10.95859995	2.83055610	12.65417498

C_6H_6_Cu111:
25
cluster

Cu	7.57170004	1.45859568	6.51615833
Cu	5.05071188	1.45924472	6.51504041
Cu	8.83343916	3.64339317	6.51495284
Cu	3.78997912	3.64325290	6.51526395
Cu	6.31193215	3.64306545	6.54605923
Cu	5.04994454	5.82644466	6.51621937
Cu	7.57260587	5.82696626	6.51481551
Cu	3.78009739	2.18093212	8.56844093
Cu	6.31169573	2.16657485	8.58411055
Cu	5.03362679	4.38051312	8.58458057
Cu	7.59150689	4.38148417	8.58277098
Cu	6.31180445	6.56578696	8.56890291
Cu	8.84344405	2.18088894	8.56868246
C	6.34097246	5.05077191	11.34898468
C	7.55605855	4.35065495	11.34499064
C	7.55373195	2.94787789	11.34794377
C	6.33949206	2.24616142	11.34870489
C	5.12653167	2.94961373	11.35184390
C	5.12564335	4.35162924	11.35061437
H	6.34188375	6.14240468	11.34084805
H	8.50123622	4.89501926	11.34388177
H	8.49884794	2.40117943	11.34097872
H	6.33877276	1.15567972	11.35152148
H	4.18137725	2.40428052	11.34744582
H	4.18143533	4.89737290	11.35387275

C_6H_6_Pt111:
27
cluster
Pt 12.53169669 8.81951902 7.11736263
Pt 13.90533434 11.21480254 7.15698980
Pt 12.48884767 12.07730979 9.38406973
Pt 13.92183100 6.42921244 7.13021967
Pt 16.66276914 6.43025807 7.12996328
Pt 15.29281937 8.83729397 7.16332612
Pt 18.05564930 8.82036605 7.11689501
Pt 16.68271269 11.21636789 7.15290701
Pt 12.49213394 7.18169737 9.38061056
Pt 15.30951171 7.25914956 9.52679642
Pt 18.12099113 7.17993712 9.37831653
Pt 13.82455157 9.64465876 9.49357908
Pt 16.79304075 9.64644165 9.48568560
Pt 15.30698514 12.02064527 9.55368308
Pt 18.12432374 12.08135360 9.38560696
H 13.17074983 10.84643478 11.87005820
H 15.32794246 7.20056959 12.12139794
C 15.31901108 11.13320334 11.51893416
C 16.55831547 10.33835534 11.54882127
C 16.56119858 8.90430019 11.53999538
C 15.32344827 8.10676746 11.50564540
C 14.08364606 8.90041487 11.54715233
C 14.08173859 10.33502836 11.55424410
H 15.32062262 12.03354610 12.14382602
H 17.47152519 10.85162781 11.85587481
H 17.47658637 8.39113017 11.84201429
H 13.17309622 8.38345289 11.85643229

CH_3I_Pt111:
22
cluster
Pt 6.92943330 3.98772978 6.93367869
Pt 8.30107510 4.77650432 9.24106745
Pt 5.55712647 4.77606254 9.24039051
Pt 8.31854403 6.39058298 6.92550886
Pt 6.92900115 7.18724905 9.21506713
H 8.72158844 6.64818489 14.22688174
Pt 11.09040261 1.58958309 6.92550886
Pt 8.31077133 1.58937460 6.92662553
Pt 12.47315046 3.98772978 6.93367869
Pt 9.70067832 3.99658750 6.92905732
Pt 13.84479226 4.77650432 9.24106745
Pt 11.10084363 4.77606254 9.24039051
Pt 6.92928725 2.39629815 9.25967388
Pt 9.70085973 2.38624915 9.21506713
Pt 11.08262991 6.39037450 6.92662553
Pt 9.70114584 7.19729805 9.25967388
Pt 12.47271831 7.18724905 9.21506713
C 9.65247138 6.10514913 14.04569704
H 9.67965454 5.14778657 14.57357626
H 10.53376135 6.71617590 14.25643118
I 9.70684792 5.62444055 11.86205804
Pt 12.47300442 2.39629815 9.25967388

CH_3OH_Pt111:
16
cluster
Pt 13.85302543 6.41808348 6.92799076
Pt 11.08786518 6.42077998 6.92077573
Pt 12.46678239 8.81134677 6.92967118
Pt 11.07485987 4.84643030 9.22286048
Pt 9.69221556 7.24812983 9.21457620
Pt 12.45612902 7.26181514 9.25140666
C 13.74080144 7.51401265 12.35636623
O 12.64587929 6.83523472 11.71054465
H 14.67006434 7.43318779 11.76130892
H 12.96069016 5.95014803 11.40730899
H 13.45979412 8.57107454 12.42813410
H 13.90242613 7.09489905 13.36213521
Pt 11.07456760 9.64406247 9.23906159
Pt 13.84671845 9.64743019 9.22286048
Pt 13.84642618 4.84306258 9.23906159
Pt 15.23593273 7.24812983 9.21457620

CH_4_Pt111:
15
cluster
Pt 8.31127085 6.40147512 6.92844491
Pt 8.30321046 4.80038015 9.23609008
Pt 6.91952762 7.20286231 9.24022630
H 9.42053360 6.74876582 12.09240950
Pt 9.69730440 4.00118742 6.93001033
Pt 9.69138620 2.40186242 9.24022630
Pt 9.70150504 5.60116655 4.66321306
Pt 11.08307500 6.40204326 6.92913631
Pt 11.07739895 4.80267430 9.23664994
Pt 9.68991772 7.20507304 9.23459744
Pt 12.46324479 7.20286231 9.24022630
C 9.66600104 5.77045809 12.52900428
H 10.65664586 5.45446640 12.17835727
H 8.92001932 5.03528360 12.20253234
H 9.66563086 5.84752411 13.62347571

CO_Co001:
12
cluster
Co 4.92377685 5.69177440 27.11318984
Co 6.14913510 3.55109016 27.12549101
Co 8.62530043 3.55120927 27.12523221
Co 9.84977685 5.69177440 27.11318984
Co 7.38695601 5.68432721 27.02177856
Co 6.14913510 7.81713130 27.12549101
Co 8.62530043 7.81725041 27.12523221
Co 7.38726701 4.26873810 29.07003288
Co 6.15790452 6.39338626 29.05118476
Co 8.61676347 6.39324225 29.05101031
C 7.38117516 5.78275254 25.28760726
O 7.37808508 5.86255939 24.12289398

CO_Cu111:
12
cluster
Cu 5.03462013 1.46349251 6.21948262
Cu 2.53464325 1.46316604 6.21791562
Cu 3.78496205 3.62771905 6.22029783
Cu 2.52406054 -0.00321329 8.24806447
Cu 1.25957416 2.18806106 8.24776863
Cu 3.78439153 2.18483059 8.36015032
Cu 2.52200660 4.37059927 8.24818176
Cu 5.04843175 4.36912590 8.24806447
Cu 5.04637781 -0.00173992 8.24818176
Cu 6.30831658 2.18806106 8.24776863
C 3.74376599 2.13942999 10.20225189
O 3.72068414 2.11228427 11.35951369

CO_Ir111:
15
cluster
Ir 10.85471934 9.39994915 8.68535774
Ir 13.57000938 4.69692885 8.68535774
Ir 12.21880518 5.48685702 4.31702503
Ir 10.86116016 7.83836718 4.31702503
Ir 13.57645020 7.83836718 4.31702503
Ir 13.57122118 6.27356238 6.51405183
Ir 10.86651278 6.27343213 6.51398772
Ir 12.21875752 8.61583216 6.51379716
Ir 10.86805026 4.69700147 8.68517231
Ir 9.50404140 7.06275498 8.68567736
Ir 12.21925725 7.05230723 8.90590832
Ir 13.58334030 9.40002177 8.68517231
Ir 14.93462148 7.06275498 8.68567736
C 12.22143130 7.03387929 10.75490411
O 12.22357123 7.01710872 11.91847315
CO_Ni111:
12
cluster
Ni 9.83726957 2.83977511 3.60802424
Ni 9.84197817 1.42312592 5.60705587
Ni 11.07142539 3.55082962 5.60420218
Ni 8.61445027 3.55020900 5.60744709

Ni 8.61967684 2.13331427 7.67724373
Ni 7.39165638 4.26428660 7.58945527
Ni 9.85060301 4.26802295 7.66821531
Ni 9.85097378 0.00462391 7.58945527
Ni 11.08419999 2.13169863 7.66506220
Ni 12.31029118 4.26428660 7.58945527
C 9.86637993 2.84982308 8.99711331
O 9.88945322 2.85708680 10.18684731

CO_Pd100:
10
cluster
Pd 6.87294445 6.87760142 6.29147945
Pd 6.87336215 9.63279604 6.29235930
Pd 5.49637774 5.51021257 8.26173682
Pd 8.24681335 5.51007879 8.26171582
Pd 5.48588536 8.26038737 8.32514484
Pd 8.23838790 8.26144452 8.33485139
Pd 5.49637774 11.01150332 8.26173682
Pd 8.24681335 11.01136955 8.26171582
C 6.85618505 8.33845818 9.75869963
O 6.85024942 8.39496113 10.93493394

CO_Pd111:
11
cluster
Pd 8.25324455 6.35227522 6.78811119
Pd 9.62818241 8.73366836 6.78817587
Pd 6.88030468 8.73258693 6.78882030
Pd 5.50535103 9.52613962 9.04189958
Pd 6.87336986 7.13969314 9.12556848
Pd 8.25615161 9.53509085 9.12546511
Pd 8.25599641 4.76188207 9.04189958
Pd 11.00664179 9.52613962 9.04189958
Pd 9.63876994 7.13975023 9.12185650
C 8.26076412 7.93578949 10.43894557
O 8.26376835 7.93427988 11.62760827

CO_Pt111:
12
cluster
Pt 5.52889351 1.60928810 6.94006791
Pt 2.78718046 1.60921297 6.94054149
Pt 4.15808040 3.98343901 6.94020997
Pt 2.76992817 0.00168932 9.19080887
Pt 1.38626726 2.39824377 9.19084668
Pt 4.15765076 2.40084959 9.39868752
Pt 2.77424284 4.80267617 9.19081793
Pt 5.54178675 4.80268922 9.19080887
Pt 5.54610142 0.00167627 9.19081793
Pt 6.92998442 2.39824377 9.19084668
C 4.16682362 2.40414988 11.23747497
O 4.17306219 2.40643617 12.39570154

CO_Rh111:
15
cluster
Rh 10.68927721 9.26091401 8.80178886
Rh 12.02788635 5.40112488 4.48238402
Rh 10.69145453 7.71589269 4.48238402
Rh 13.36431816 7.71589269 4.48238402
Rh 13.36461816 6.17467136 6.65331218
Rh 10.69219042 6.17479363 6.65382476
Rh 12.02844158 8.48977906 6.65176999
Rh 13.36214084 4.63137840 8.80178886
Rh 10.69537532 4.63162328 8.80181224
Rh 9.35597484 6.94976758 8.80113945
Rh 12.02868459 6.94743341 8.99228886
Rh 13.36823895 9.26115889 8.80181224
Rh 14.70170211 6.94976758 8.80113945
C 12.03795213 6.99123423 10.81779994
O 12.04412671 7.02192630 11.98145547

CO_Ru100:
12
cluster
Ru 5.09864852 1.11152893 21.25916311

Ru 3.77468054 3.45666080 21.25862305
Ru 5.11564767 4.23468330 23.30929466
Ru 5.09864852 5.78460201 21.25916311
Ru 7.84172344 1.10922272 21.25900042
Ru 6.47277792 3.44199246 21.12616763
Ru 9.17068054 3.45666080 21.25862305
Ru 7.81994702 4.23486624 23.30923017
Ru 6.46721421 1.88052035 23.33136756
Ru 7.84172344 5.78229579 21.25900042
C 6.52063798 3.41944075 19.24483422
O 6.55697498 3.40895685 18.07838639

H_Ni100:
8
cluster
Ni 6.14622995 3.69351428 7.49751729
Ni 6.14574795 6.15337507 7.47696287
Ni 6.14622995 8.61214905 7.49751729
Ni 4.91951016 4.93188246 9.23389000
Ni 7.37234274 4.92882592 9.23444272
Ni 4.91506602 7.38600143 9.23583026
Ni 7.36828141 7.38137396 9.23494095
H 6.14010681 6.16495236 9.81808587

H_Ni111:
10
cluster
Ni 7.38381283 5.68312716 5.60721577
Ni 6.15976809 6.39828949 7.60204870
Ni 8.61244599 3.55502200 5.60660215
Ni 8.61908549 2.13862680 7.60204870
Ni 9.84238773 5.68391876 5.60798454
Ni 7.37796631 4.26169949 7.63751607
Ni 9.85676407 4.26296153 7.63823602
Ni 8.61769288 6.40825896 7.63854326
Ni 11.07840289 6.39828949 7.60204870
H 8.61525439 4.97625919 8.55271530

H_Pd111:
11
cluster
Pd 13.75614395 6.36116818 6.78913198
Pd 12.38012256 7.15829396 9.05627867
Pd 15.12975826 3.98020469 6.78801776
Pd 15.13076794 2.39403641 9.05627867
Pd 15.12854958 5.55830047 4.54589255
Pd 16.50428585 6.36143315 6.78920298
Pd 13.73884898 4.76575545 9.08466647
Pd 16.52143608 4.76632910 9.08408277
Pd 15.12978109 7.17851247 9.08456322
Pd 17.88141332 7.15829396 9.05627867
H 15.13079167 5.56818699 9.90653643

H_Pt111:
11
cluster
Pt 13.83723166 4.78142046 9.26959566
Pt 13.86454218 6.39799243 6.93137809
Pt 12.47661319 7.19685582 9.20797407
Pt 15.24585819 4.00375300 6.93020390
Pt 16.65927916 4.78231219 9.26971117
Pt 15.24847177 2.39585592 9.20797407
Pt 15.24522220 5.60116655 4.66321306
Pt 16.62834945 6.39860079 6.93002693
Pt 15.24967819 7.22689978 9.26982772
Pt 18.02033035 7.19685582 9.20797407
H 15.24959802 5.58914228 10.16425973

H_Rh111:
11
cluster
Rh 8.02016156 6.18221292 6.63805764
Rh 8.00130747 4.63626407 8.82135544
Rh 6.68814444 6.96362689 8.80677722
Rh 9.35756957 3.86508423 6.63670298
Rh 9.36100807 2.33409127 8.80677722
Rh 9.35502272 5.40112488 4.48238402

Rh 10.69484388 6.18205497 6.63839809
Rh 10.72052579 4.63439954 8.82063660
Rh 9.36109973 6.99088573 8.82157704
Rh 12.03387170 6.96362689 8.80677722
H 9.37022030 5.42279899 9.78952550

H_2O_Pt111:
13
cluster
Pt 6.96836618 4.00325525 6.92504550
Pt 8.35455752 6.40278168 6.92742865
Pt 5.63343295 4.80926117 9.22678926
Pt 7.01835158 7.20822426 9.23325817
Pt 9.73487271 4.00957904 6.92694572
Pt 7.02045853 2.40585823 9.23382403
Pt 9.79021016 2.40722437 9.23325817
Pt 8.42362846 4.80757318 9.24384518
Pt 11.17715012 4.80926117 9.22678926
Pt 9.79231712 7.20685812 9.23382403
H 7.42716613 5.47417891 11.63353300
H 7.60763196 3.93843104 11.61412808
O 8.11308383 4.77554579 11.70524621

I_Pt111:
11
cluster
Pt 13.82882845 4.78083429 9.24999405
Pt 13.86658619 6.39719385 6.90968685
Pt 12.47455061 7.20022797 9.15514429
Pt 15.24536592 4.00888326 6.90947581
Pt 16.66535313 4.78072275 9.24881578
Pt 15.24640919 2.39922808 9.15514429
Pt 15.24522220 5.60116655 4.66321306
Pt 16.62408310 6.39702165 6.90960631
Pt 15.24651659 7.23650927 9.25068382
Pt 18.01826777 7.20022797 9.15514429
I 15.25298881 5.59262132 11.42538883

NH_3_Cu001:
13
cluster
Cu 1.27481431 1.26948832 5.90147840
Cu 3.78184473 1.26929264 5.90315678
Cu 1.27495335 3.77689153 5.90152952
Cu 3.78172216 3.77714709 5.90304952
Cu 2.52592656 -0.00251336 7.64831081
Cu 0.01275388 2.52269160 7.64664940
Cu 2.52867637 2.51753308 7.78710196
Cu 2.52592656 5.04622905 7.64831081
Cu 5.06149630 2.52269160 7.64664940
N 2.64525931 2.56191655 9.89322148
H 2.59950145 1.61620159 10.28213491
H 3.54152815 2.98846596 10.14631218
H 1.88306263 3.12713926 10.27723314

NO_Pd100:
9
cluster
Pd 6.87930938 4.12807388 6.29591723
Pd 6.87783073 6.87896290 6.26348737
Pd 6.87930938 9.62936464 6.29591723
Pd 5.52057178 5.52071228 8.31802108
Pd 8.23845230 5.52275056 8.31937999
Pd 5.52031872 8.24002705 8.32049363
Pd 8.24200440 8.24396997 8.31781288
N 6.88960819 6.89241795 9.35139034
O 6.89578353 6.89879709 10.57230225

NO_Pd111:
12
cluster
Pd 13.75322689 7.94042925 4.54589255
Pd 13.75575217 6.35259579 6.78487769
Pd 15.12982622 8.73241349 6.78496489
Pd 12.38196247 8.73221889 6.78443069
Pd 11.00552835 9.52686002 9.01655156
Pd 12.36217685 7.13409567 9.12951946

Pd 13.75634108 9.54855968 9.12920803
Pd 13.75617373 4.76260247 9.01655156
Pd 16.50681911 9.52686002 9.01655156
Pd 15.15084425 7.13375759 9.12832417
N 13.75846183 7.93782068 10.36286201
O 13.76127778 7.93640337 11.57179759

NO_Pt111:
12
cluster
Pt 6.92122606 4.01231119 6.92499392
Pt 5.51141485 4.83326373 9.16179610
Pt 8.31557575 3.20066660 4.66321306
Pt 8.29974785 1.62481167 6.92248341
Pt 9.67874885 4.01300002 6.92199045
Pt 8.28327343 0.03226383 9.16179610
Pt 6.86319291 2.41116649 9.31684151
Pt 9.69924977 2.41563540 9.31588029
Pt 8.28178799 4.87178134 9.31812713
Pt 11.05513201 4.83326373 9.16179610
N 8.27628810 3.23774828 10.59269260
O 8.27554135 3.23935902 11.80539685

O_Ni100:
10
cluster
Ni 3.68635694 6.15432145 7.50126510
Ni 6.14570962 3.69468715 7.50143119
Ni 6.14559966 6.15428832 7.43625248
Ni 8.60499171 6.15432145 7.50126510
Ni 6.14570962 8.61332192 7.50143119
Ni 4.91520357 4.92397300 9.27075557
Ni 7.37561222 4.92454653 9.27171733
Ni 4.91493119 7.38426800 9.27181113
Ni 7.37550822 7.38498715 9.27038584
O 6.14576246 6.15316226 10.13339731

O_Ni111:
11
cluster
Ni 9.84329618 9.94219077 5.60810200
Ni 8.62037690 10.65920749 7.57337492
Ni 11.07161552 7.81470721 5.60806949
Ni 11.07969430 6.39954480 7.57337492
Ni 11.06692829 9.22926915 3.60802424
Ni 12.29909396 9.94148211 5.60600184
Ni 9.82440451 8.51466353 7.68408161
Ni 12.33382255 8.51523074 7.68245588
Ni 11.07956852 10.68837147 7.68223456
Ni 13.53901170 10.65920749 7.57337492
O 11.07961087 9.23926167 8.80878205

O_Pt111:
11
cluster
Pt 5.55785930 3.20883156 4.86898656
Pt 5.55773842 1.61048720 7.12957538
Pt 4.17355948 4.00787271 7.12960104
Pt 6.94180111 4.00781988 7.12965687
Pt 5.55755744 -0.01697148 9.38884839
Pt 4.07389980 2.35190524 9.47139205
Pt 7.04128388 2.35205806 9.47138893
Pt 2.76414575 4.82120748 9.38897237
Pt 5.55755115 4.92166311 9.47149813
Pt 8.35121013 4.82144587 9.38917186
O 5.55776541 3.20866965 10.58066404

O_Rh111:
8
cluster
Rh 6.72034778 4.02942595 6.76566505
Rh 6.72077898 6.71673819 6.73636120
Rh 6.72034778 9.40343749 6.76566505
Rh 5.38562284 5.37932355 8.66490009
Rh 8.06067256 5.37709096 8.66441574
Rh 5.38401322 8.05330926 8.66405018
Rh 8.05768778 8.05136581 8.66517382

O 6.72476541 6.71230279 9.64723375

N_Ni100
10
test
Ni 3.68753990 6.15183821 7.48049009
Ni 6.14644624 3.69102148 7.47997127
Ni 6.14764684 6.14918701 7.47265805
Ni 8.60617467 6.15183821 7.48049009
Ni 6.14644624 8.60965625 7.47997127
Ni 4.89209096 4.90039446 9.29676122
Ni 7.39903514 4.89968286 9.29693297
Ni 4.89316450 7.40574091 9.29815936
Ni 7.39917108 7.40541580 9.29715400
N 6.14613417 6.15223449 9.72555914

CH_Pt111
12
test
Pt 8.30567751 6.38003108 6.94063881
Pt 6.90580301 7.17087491 9.19921236
Pt 9.68732388 3.98868906 6.94136990
Pt 9.67766160 2.36987502 9.19921236
Pt 9.70150504 5.60116655 4.66321306
Pt 11.06986902 6.38053734 6.93946860
Pt 8.25643292 4.75060901 9.34345527
Pt 11.09576450 4.75127494 9.33671040
Pt 9.67852234 7.20475662 9.33174283
Pt 12.44952018 7.17087491 9.19921236
C 9.67749754 5.56867464 10.47939396
H 9.67517322 5.56412195 11.57631774

C_6H_{10}_Pt111
34
test
Pt 11.10558976 4.83159364 9.36694215
Pt 16.69143632 1.60208552 7.10022384
Pt 11.14554627 1.61615586 7.15665292
Pt 13.88764459 1.61881253 7.14608011
Pt 12.51583019 4.01026265 7.13814680
Pt 15.27889626 4.01937867 7.13905812
Pt 13.90969962 6.39803416 7.15092643
Pt 11.13960759 0.00592376 9.41973859
Pt 13.91257037 0.00168698 9.40258102
Pt 9.75013020 2.40663612 9.41332560
Pt 12.53086540 2.44196363 9.59102062
Pt 15.33907969 2.39257577 9.37804288
Pt 13.90282082 4.79346308 9.55639170
Pt 16.69249752 4.82056855 9.40006539
C 14.53796877 2.35333356 13.45512216
C 15.49586701 3.39919647 12.89056905
C 13.60323257 1.85936806 12.34438626
C 14.72119512 4.64190184 12.46927875
C 12.86923458 2.99250046 11.62709498
C 13.49706154 4.35759167 11.59621811
H 15.08535959 1.49475763 13.87250940
H 13.95279129 2.79532401 14.28153641
H 16.26860861 3.67704365 13.62318160
H 16.02693600 2.97639361 12.01507255
H 14.23207411 1.29594075 11.62701076
H 12.86267106 1.13540148 12.71401521
H 14.34561879 5.15369046 13.37617110
H 15.38135260 5.37067836 11.97366304
H 11.81530990 3.06514819 11.93465177
H 12.72585580 5.12710323 11.74339726
Pt 12.53132154 7.22237252 9.40369878
Pt 15.30800206 7.22579478 9.41973859
Pt 16.69971601 0.00250150 9.40369878
Pt 18.08691915 2.40663612 9.41332560

CH_3_Pt111
14
cluster
Pt 5.53715368 1.61168495 6.94155256
Pt 2.78688683 1.61083524 6.94208469

Pt 4.16200503 3.99329205 6.94149763
Pt 2.78012750 0.01615641 9.20355317
Pt 1.39645192 2.41028638 9.20427125
Pt 4.16901071 2.41655047 9.40431102
Pt 2.78235422 4.81569174 9.20400762
Pt 5.55198608 4.81715631 9.20355317
Pt 5.55421281 0.01469185 9.20400762
Pt 6.94016908 2.41028638 9.20427125
C 4.20317611 2.46065314 11.47087154
H 5.22221945 2.71294650 11.78965043
H 3.49147495 3.22498207 11.80653368
H 3.91391124 1.46639300 11.82871089

Pt111 (2x2x1 supercell)

Pt
1.00000000000000
5.5437171645025325 0.0000000000000000 0.0000000000000000
2.7718585822512662 4.8009998958550284 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.7896391656699997
Pt
16
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0895868729383835 F F F
0.5000000000000000 0.0000000000000000 0.0895868729383835 F F F
0.0000000000000005 0.5000000000000002 0.0895868729383835 F F F
0.4999999999999999 0.5000000000000002 0.0895868729383835 F F F
0.1666666666666641 0.1666666666666648 0.1740677814428793 F F F
0.6666666666666649 0.1666666666666648 0.1740677814428793 F F F
0.1666666666666637 0.6666666666666662 0.1740677814428793 F F F
0.6666666666666641 0.6666666666666662 0.1740677814428793 F F F
0.8333340069926380 0.3333338726708500 0.2585297093494143 T T T
0.3333326223805705 0.3333332933412504 0.2585299340394671 T T T
0.8333333434590441 0.8333326644556263 0.2585300433509711 T T T
0.3333336527823206 0.8333337629046895 0.2585295821347396 T T T
-0.0000000210450377 -0.0000000499522746 0.3445157136434697 T T T
0.5000002940609619 -0.0000000445545241 0.3445158048506652 T T T
0.0000000286842452 0.5000002714609068 0.3445160339986025 T T T
0.5000000121744990 0.5000000965673168 0.3445156525588364 T T T

Pt111 (3x3x1 supercell)

Pt
1.00000000000000
8.3367889501893959 0.0000000000000000 0.0000000000000000
4.1683944750946980 7.2198710168534168 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.8069596737456877
Pt
36
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0969897381740878 F F F
0.3333333333333357 0.0000000000000000 0.0969897381740878 F F F
0.6666666666666643 0.0000000000000000 0.0969897381740878 F F F

0.0000000000000000 0.3333333333333357 0.0969897381740878 F F F
0.3333333333333357 0.3333333333333357 0.0969897381740878 F F F
0.6666666666666643 0.3333333333333357 0.0969897381740878 F F F
0.0000000000000000 0.6666666666666643 0.0969897381740878 F F F
0.3333333333333357 0.6666666666666643 0.0969897381740878 F F F
0.6666666666666643 0.6666666666666643 0.0969897381740878 F F F
0.1111111111111143 0.1111111111111143 0.1816314351636024 F F F
0.4444444444444429 0.1111111111111143 0.1816314351636024 F F F
0.7777777777777786 0.1111111111111143 0.1816314351636024 F F F
0.1111111111111143 0.4444444444444429 0.1816314351636024 F F F
0.4444444444444429 0.4444444444444429 0.1816314351636024 F F F
0.7777777777777786 0.4444444444444429 0.1816314351636024 F F F
0.1111111111111143 0.7777777777777786 0.1816314351636024 F F F
0.4444444444444429 0.7777777777777786 0.1816314351636024 F F F
0.7777777777777786 0.7777777777777786 0.1816314351636024 F F F
0.8888890127519341 0.2222222269445771 0.2657372577890565 T T T
0.2222218816651465 0.2222228417991479 0.2657370201733298 T T T
0.5555552861251661 0.2222225573689326 0.2657371559939429 T T T
0.8888894457456541 0.5555554038043884 0.2657371609688066 T T T
0.2222220487673936 0.5555557135098972 0.2657371083946404 T T T
0.5555551988293859 0.5555555182767979 0.2657373123685480 T T T
0.8888893700380062 0.8888884505426345 0.2657372228834760 T T T
0.2222220117660632 0.8888884817776871 0.2657372482952844 T T T
0.5555557475453665 0.8888888133851119 0.2657371999500746 T T T
0.0000004759649399 -0.0000005228963283 0.3512615566675056 T T T
0.3333327064827917 -0.0000000683193930 0.3512614395061254 T T T
0.6666672125309349 -0.0000001814741417 0.3512617915718652 T T T
-0.0000000750959787 0.3333336970037389 0.3512610855082949 T T T
0.3333326310824495 0.3333344680702237 0.3512612761610956 T T T
0.6666665215500053 0.3333337238109174 0.3512618121721231 T T T
0.0000007206509594 0.6666662864920799 0.3512610734764204 T T T
0.3333327762314443 0.6666665690862045 0.3512609140923444 T T T
0.6666670715322063 0.6666660735684334 0.3512613764164751 T T T

Rh(100) (2x2x1 supercell)

Rh
1.00000000000000
5.3740115370177612 0.0000000000000000 0.0000000000000000
0.0000000000000000 5.3740115370177612 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.6999999999999993
Rh
16
Selective dynamics
Direct
0.2500000000000000 0.2500000000000000 0.1167315175097272 F F F
0.7500000000000000 0.2500000000000000 0.1167315175097272 F F F
0.2500000000000000 0.7500000000000000 0.1167315175097272 F F F
0.7500000000000000 0.7500000000000000 0.1167315175097272 F F F
0.0000000000000000 0.0000000000000000 0.1906614785992247 F F F
0.5000000000000000 0.0000000000000000 0.1906614785992247 F F F

0.0000000000000000 0.5000000000000000 0.1906614785992247 F F F
0.5000000000000000 0.5000000000000000 0.1906614785992247 F F F
0.2499970670278453 0.2500042972389692 0.2642456701054445 T T T
0.7500029323735170 0.2500042746375212 0.2642454338421469 T T T
0.2499970801520135 0.7499956939426405 0.2642457853936055 T T T
0.7500029187124853 0.7499957334065528 0.2642459399056453 T T T
-0.0000001247046301 0.0000012938291801 0.3356567255106531 T T T
0.5000000758375223 0.0000012441933546 0.3356567449585329 T T T
-0.0000000648602555 0.4999987535321702 0.3356594289893680 T T T
0.5000001129703053 0.4999987136853782 0.3356573371091065 T T T

Rh(111) (2x2x1 supercell)

Rh
1.00000000000000
5.3457272657702992 0.0000000000000000 0.0000000000000000
2.6728636328851496 4.6295356138602060 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.5471520526103575
Rh
16
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0866382953411318 F F F
0.5000000000000001 0.0000000000000000 0.0866382953411318 F F F
0.0000000000000002 0.5000000000000003 0.0866382953411318 F F F
0.5000000000000003 0.5000000000000003 0.0866382953411318 F F F
0.1666666666666645 0.1666666666666646 0.1688461349320534 F F F
0.6666666666666647 0.1666666666666646 0.1688461349320534 F F F
0.1666666666666642 0.6666666666666654 0.1688461349320534 F F F
0.6666666666666653 0.6666666666666654 0.1688461349320534 F F F
0.8333230516337994 0.3333406107762537 0.2499703275640218 T T T
0.3333313242273475 0.3333389215226080 0.2499704467606713 T T T
0.8333295381365132 0.8333328268765028 0.2499673554897362 T T T
0.3333339084307911 0.8333284533198703 0.2499675610309310 T T T
-0.0000514267889501 0.0000185858453438 0.3317004551080254 T T T
0.5000563533788362 -0.0000142453039552 0.3317018464391515 T T T
-0.0000085658086618 0.5000025189806266 0.3316817654853931 T T T
0.5000565074991359 0.4999706982994521 0.3316862514267272 T T T

Pd111 (2x2x1 supercell)

Pd
1.00000000000000
5.5012907576313399 0.0000000000000000 0.0000000000000000
2.7506453788156700 4.7642575497132809 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.7376776414429358
Pd
16
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0860209338613274 F F F
0.4999999999999999 0.0000000000000000 0.0860209338613274 F F F

0.0000000000000002 0.4999999999999992 0.0860209338613274 F F F
0.5000000000000001 0.4999999999999992 0.0860209338613274 F F F
0.1666666666666643 0.1666666666666642 0.1700182270169037 F F F
0.6666666666666642 0.1666666666666642 0.1700182270169037 F F F
0.1666666666666647 0.6666666666666633 0.1700182270169037 F F F
0.6666666666666641 0.6666666666666633 0.1700182270169037 F F F
0.8333333457958625 0.3333334756716129 0.2535242171355883 T T T
0.3333332901871255 0.3333333137939591 0.2535242599488715 T T T
0.8333332533682236 0.8333332640695104 0.2535242498715624 T T T
0.3333334662358985 0.8333333547853732 0.2535242223323442 T T T
-0.0000000076487719 -0.0000000288590316 0.3384668089787924 T T T
0.5000000232380537 0.0000000980640834 0.3384668590585695 T T T
0.0000000992940489 0.5000000110020998 0.3384668657885029 T T T
0.4999999525034253 0.4999999600183490 0.3384666735230565 T T T

Pd(100) (2x2x1 supercell)

Pd

1.00000000000000

5.5012907576313399 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.5012907576313399 0.0000000000000000

0.0000000000000000 0.0000000000000000 25.8350000000000009

Pd

16

Selective dynamics

Direct

0.2500000000000000 0.2500000000000000 0.0928972324366200 F F F
0.7500000000000001 0.2500000000000000 0.0928972324366200 F F F
0.2500000000000000 0.7500000000000001 0.0928972324366200 F F F
0.7500000000000001 0.7500000000000001 0.0928972324366200 F F F
0.0000000000000000 0.0000000000000000 0.1681826978904582 F F F
0.5000000000000000 0.0000000000000000 0.1681826978904582 F F F
0.0000000000000000 0.5000000000000000 0.1681826978904582 F F F
0.5000000000000000 0.5000000000000000 0.1681826978904582 F F F
0.2500000942472548 0.2499998867895026 0.2434721742191240 T T T
0.7499998995094297 0.2499998814148580 0.2434721702878453 T T T
0.2500000918990114 0.7500001245409789 0.2434721861013840 T T T
0.7499999101231194 0.7500001172761029 0.2434721823963721 T T T
0.0000000063098411 0.0000000076093677 0.3187796361574931 T T T
0.4999999963839423 0.0000000122798470 0.3187795785730169 T T T
0.0000000084500169 0.4999999819925317 0.3187796549181975 T T T
0.4999999922514839 0.4999999896234494 0.3187796098185537 T T T

Ni111 (2x2x1 supercell)

Ni

1.00000000000000

4.9186348000000004 0.0000000000000000 0.0000000000000000

2.4593174000000002 4.2596626887381914 0.0000000000000000

0.0000000000000000 0.0000000000000000 25.0240727000000014

Ni

16

Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0639384331711952 F F F
0.4999999969436288 0.0000000000000000 0.0639384331711952 F F F
0.0000000000000000 0.4999999969436288 0.0639384331711952 F F F
0.4999999969436288 0.4999999969436288 0.0639384331711952 F F F
0.1666666656478739 0.1666666656478739 0.1441821353181041 F F F
0.6666666625915028 0.1666666656478739 0.1441821353181041 F F F
0.1666666656478739 0.6666666625915028 0.1441821353181041 F F F
0.6666666625915028 0.6666666625915028 0.1441821353181041 F F F
0.8333333343521261 0.3333333312957478 0.2244258374650201 T T T
0.3333333312957478 0.3333333312957478 0.2244258374650201 T T T
0.8333333343521261 0.8333333282393767 0.2244258374650201 T T T
0.3333333312957478 0.8333333282393767 0.2244258374650201 T T T
0.0000000000000000 0.0000000000000000 0.3046695396119290 T T T
0.4999999969436288 0.0000000000000000 0.3046695396119290 T T T
0.0000000000000000 0.4999999969436288 0.3046695396119290 T T T
0.4999999969436288 0.4999999969436288 0.3046695396119290 T T T

Ni100 (2x2x1 supercell)

Ni
1.00000000000000
4.9186347699336253 0.0000000000000000 0.0000000000000000
0.0000000000000000 4.9186347699336253 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.2169999999999987
Ni
16
Selective dynamics
Direct
0.2500000000000000 0.2500000000000000 0.1586231510488926 F F F
0.7500000000000000 0.2500000000000000 0.1586231510488926 F F F
0.2500000000000000 0.7500000000000000 0.1586231510488926 F F F
0.7500000000000000 0.7500000000000000 0.1586231510488926 F F F
0.0000000000000000 0.0000000000000000 0.2275845659674042 F F F
0.5000000000000000 0.0000000000000000 0.2275845659674042 F F F
0.0000000000000000 0.5000000000000000 0.2275845659674042 F F F
0.5000000000000000 0.5000000000000000 0.2275845659674042 F F F
0.2499972418774926 0.2499978387553272 0.2976164466529927 T T T
0.7500027321396995 0.2499978777901851 0.2976177335537874 T T T
0.2499972868433138 0.7500021934983504 0.2976181782045113 T T T
0.7500027670063548 0.7500021886834187 0.2976161373281354 T T T
0.0000003540775612 -0.0000000911168804 0.3656279130677312 T T T
0.4999996619011077 -0.0000000942104551 0.3656248764911313 T T T
0.0000003427523623 0.5000001020034130 0.3656257030276616 T T T
0.4999996534699727 0.5000000966731378 0.3656230221101746 T T T

Ir111 (2x2x1 supercell)

Ir

1.00000000000000
5.4305800795126853 0.0000000000000000 0.0000000000000000
2.7152900397563426 4.7030203061437010 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.6510751010644888
Ir
16
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0787960707790063 F F F
0.5000000000000000 0.0000000000000000 0.0787960707790063 F F F
0.0000000000000003 0.5000000000000000 0.0787960707790063 F F F
0.5000000000000000 0.5000000000000000 0.0787960707790063 F F F
0.1666666666666644 0.1666666666666643 0.1619831476710587 F F F
0.6666666666666644 0.1666666666666643 0.1619831476710587 F F F
0.1666666666666643 0.6666666666666643 0.1619831476710587 F F F
0.6666666666666643 0.6666666666666643 0.1619831476710587 F F F
0.8333310831596678 0.3333334536144148 0.2441236808616243 T T T
0.3333336985974243 0.3333375547282915 0.2441219422996846 T T T
0.8333371080254190 0.8333323390909156 0.2441212108412593 T T T
0.3333323302357448 0.8333292583826618 0.2441224966304276 T T T
-0.0000004286931938 -0.0000027588085721 0.3263411947726383 T T T
0.5000015411667580 0.0000000260692540 0.3263430430857564 T T T
0.0000006680352649 0.5000028064661819 0.3263417003060597 T T T
0.4999976646082094 0.5000004285366602 0.3263403955064122 T T T

Cu111 (2x2x1 supercell)

Cu
1.00000000000000
5.0487424176719493 0.0000000000000000 0.0000000000000000
2.5243712088359747 4.3723391908679723 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.1834213830208924
Cu
16
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0802034222067647 F F F
0.5000000000000000 0.0000000000000000 0.0802034222067647 F F F
0.0000000000000000 0.5000000000000000 0.0802034222067647 F F F
0.5000000000000000 0.5000000000000000 0.0802034222067647 F F F
0.1666666666666642 0.1666666666666644 0.1589227167884672 F F F
0.6666666666666643 0.1666666666666644 0.1589227167884672 F F F
0.1666666666666641 0.6666666666666646 0.1589227167884672 F F F
0.6666666666666642 0.6666666666666646 0.1589227167884672 F F F
0.8333331176655858 0.3333331209366991 0.2375655716641815 T T T
0.3333331037116481 0.3333330955763999 0.2375655915542818 T T T
0.8333330698173287 0.8333331268680317 0.2375655779609254 T T T
0.3333331192599565 0.8333331261027411 0.2375655801916680 T T T
0.0000000328022348 0.0000000936740210 0.3163401961246302 T T T
0.5000000535403289 0.0000001123265679 0.3163402594893535 T T T
0.0000000891453730 0.5000000346958073 0.3163401800932025 T T T

0.5000000716556622 0.5000000170874668 0.3163402064769956 T T T

Cu100 (3x3x1 supercell)

Cu
1.00000000000000
5.0487424176719493 0.0000000000000000 0.0000000000000000
0.0000000000000000 5.0487424176719493 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.3550000000000004
Cu
16
Selective dynamics
Direct
0.2500000000000000 0.2500000000000000 0.0907118911457303 F F F
0.7500000000000000 0.2500000000000000 0.0907118911457303 F F F
0.2500000000000000 0.7500000000000000 0.0907118911457303 F F F
0.7500000000000000 0.7500000000000000 0.0907118911457303 F F F
0.0000000000000000 0.0000000000000000 0.1611122066653508 F F F
0.5000000000000000 0.0000000000000000 0.1611122066653508 F F F
0.0000000000000000 0.5000000000000000 0.1611122066653508 F F F
0.5000000000000000 0.5000000000000000 0.1611122066653508 F F F
0.2499998935473775 0.2499995446668574 0.2325656101994300 T T T
0.7500000213604063 0.2499999978659114 0.2325657184118313 T T T
0.2499996404513687 0.7499998633728657 0.2325656869095045 T T T
0.7500001069257126 0.7499999405162877 0.2325655613210251 T T T
-0.0000002430745693 -0.0000001828257389 0.3025281032004022 T T T
0.5000000209109416 0.0000001692174809 0.3025280615530543 T T T
0.0000000880902709 0.4999999979772046 0.3025281546410095 T T T
0.5000002769019379 0.5000002203140921 0.3025281483420720 T T T

Cu111 (3x3x1 supercell)

Cu
1.0000000000000000
7.5731136265079240 0.0000000000000000 0.0000000000000000
3.7865568132539620 6.5585087863019584 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.1834213830208924
36
Selective dynamics
Cartesian
0.0000000000000000 -0.0000000000000005 2.4000000000000199 F F F
2.5243712088359747 -0.0000000000000005 2.4000000000000199 F F F
5.0487424176719493 -0.0000000000000005 2.4000000000000199 F F F
1.2621856044179873 2.1861695954339861 2.4000000000000199 F F F
3.7865568132539620 2.1861695954339861 2.4000000000000199 F F F
6.3109280220899366 2.1861695954339861 2.4000000000000199 F F F
2.5243712088359747 4.3723391908679723 2.4000000000000199 F F F
5.0487424176719493 4.3723391908679723 2.4000000000000199 F F F
7.5731136265079240 4.3723391908679723 2.4000000000000199 F F F
1.2621856044179873 0.7287231984779954 4.4611404610069911 F F F
3.7865568132539620 0.7287231984779954 4.4611404610069911 F F F
6.3109280220899366 0.7287231984779954 4.4611404610069911 F F F

2.5243712088359747 2.9148927939119815 4.4611404610069911 F F F
5.0487424176719493 2.9148927939119815 4.4611404610069911 F F F
7.5731136265079240 2.9148927939119815 4.4611404610069911 F F F
3.7865568132539620 5.1010623893459677 4.4611404610069911 F F F
6.3109280220899366 5.1010623893459677 4.4611404610069911 F F F
8.8352992309259122 5.1010623893459677 4.4611404610069911 F F F
0.0000000000000000 1.4574463969559908 6.5222809220139553 T T T
2.5243712088359747 1.4574463969559908 6.5222809220139553 T T T
5.0487424176719502 1.4574463969559908 6.5222809220139553 T T T
1.2621856044179873 3.6436159923899765 6.5222809220139553 T T T
3.7865568132539620 3.6436159923899765 6.5222809220139553 T T T
6.3109280220899375 3.6436159923899765 6.5222809220139553 T T T
2.5243712088359747 5.8297855878239631 6.5222809220139553 T T T
5.0487424176719493 5.8297855878239631 6.5222809220139553 T T T
7.5731136265079240 5.8297855878239631 6.5222809220139553 T T T
0.0000000000000000 -0.0000000000000005 8.5834213830209176 T T T
2.5243712088359747 -0.0000000000000005 8.5834213830209176 T T T
5.0487424176719493 -0.0000000000000005 8.5834213830209176 T T T
1.2621856044179873 2.1861695954339861 8.5834213830209176 T T T
3.7865568132539620 2.1861695954339861 8.5834213830209176 T T T
6.3109280220899366 2.1861695954339861 8.5834213830209176 T T T
2.5243712088359747 4.3723391908679723 8.5834213830209176 T T T
5.0487424176719493 4.3723391908679723 8.5834213830209176 T T T
7.5731136265079240 4.3723391908679723 8.5834213830209176 T T T

Au111 (2x2x1 supercell)

Au
1.00000000000000
5.7982756057296898 0.0000000000000000 0.0000000000000000
2.8991378028648449 5.0214539727055145 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.1014083110323973
Au
16
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0811765932881201 F F F
0.5000000000000000 0.0000000000000000 0.0811765932881201 F F F
0.0000000000000000 0.5000000000000000 0.0811765932881201 F F F
0.5000000000000001 0.5000000000000000 0.0811765932881201 F F F
0.1666666666666643 0.1666666666666643 0.1685202499907845 F F F
0.6666666666666644 0.1666666666666643 0.1685202499907845 F F F
0.1666666666666644 0.6666666666666643 0.1685202499907845 F F F
0.6666666666666645 0.6666666666666643 0.1685202499907845 F F F
0.8333333084065306 0.3333333125703085 0.2554606123748515 T T T
0.3333333027980924 0.3333333164461311 0.2554606141130945 T T T
0.8333333167520310 0.8333333009899736 0.2554606137444545 T T T
0.3333333093657330 0.8333333072889002 0.2554606127756900 T T T
-0.0000000110373802 -0.0000000080477693 0.3442307110993361 T T T
0.4999999940252081 -0.0000000095310658 0.3442307100591347 T T T
-0.0000000060804608 0.4999999911802346 0.3442307118656107 T T T

0.4999999905662276 0.4999999905515556 0.3442307107199422 T T T

Au111 (3x3x1 supercell)

Au
1.00000000000000
8.6974134085945352 0.0000000000000000 0.0000000000000000
4.3487067042972676 7.5321809590582713 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.1014083110323973
Au
36
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0922461287365056 F F F
0.3333333333333360 0.0000000000000000 0.0922461287365056 F F F
0.6666666666666644 0.0000000000000000 0.0922461287365056 F F F
0.0000000000000008 0.3333333333333350 0.0922461287365056 F F F
0.3333333333333373 0.3333333333333350 0.0922461287365056 F F F
0.6666666666666663 0.3333333333333350 0.0922461287365056 F F F
0.0000000000000011 0.6666666666666643 0.0922461287365056 F F F
0.3333333333333358 0.6666666666666643 0.0922461287365056 F F F
0.6666666666666649 0.6666666666666643 0.0922461287365056 F F F
0.1111111111111148 0.1111111111111143 0.1795897854391633 F F F
0.4444444444444429 0.1111111111111143 0.1795897854391633 F F F
0.7777777777777793 0.1111111111111143 0.1795897854391633 F F F
0.1111111111111144 0.4444444444444428 0.1795897854391633 F F F
0.4444444444444434 0.4444444444444428 0.1795897854391633 F F F
0.7777777777777787 0.4444444444444428 0.1795897854391633 F F F
0.1111111111111150 0.7777777777777778 0.1795897854391633 F F F
0.4444444444444454 0.7777777777777778 0.1795897854391633 F F F
0.7777777777777806 0.7777777777777778 0.1795897854391633 F F F
0.8888888752855114 0.2222222070093568 0.2667014493011255 T T T
0.2222222081480872 0.2222222101755627 0.2667014498880764 T T T
0.5555555442885847 0.2222222081859509 0.2667014457237204 T T T
0.8888888733972684 0.5555555468062763 0.2667014476092278 T T T
0.2222222072473073 0.5555555394819613 0.2667014472298071 T T T
0.5555555418348375 0.5555555431049960 0.2667014465764869 T T T
0.8888888777475312 0.8888888742505837 0.2667014475198846 T T T
0.2222222096896887 0.8888888778540504 0.2667014494021222 T T T
0.5555555404135117 0.8888888789670559 0.2667014454419004 T T T
-0.0000000093291846 -0.0000000095020838 0.3552884872196608 T T T
0.3333333300228480 -0.0000000062924080 0.3552884875617840 T T T
0.6666666560547367 -0.0000000072155248 0.3552884880341498 T T T
-0.0000000093391197 0.3333333257297619 0.3552884864600340 T T T
0.3333333309683794 0.3333333285767561 0.3552884875690537 T T T
0.6666666655466773 0.3333333236851794 0.3552884870158309 T T T
-0.0000000043142726 0.6666666610389311 0.3552884876976051 T T T
0.3333333278712379 0.6666666585164227 0.3552884856511891 T T T
0.6666666599060103 0.6666666606544034 0.3552884852609683 T T T

Ag111 (2x2x1) supercell

Ag
1.00000000000000
5.7558491988584972 0.0000000000000000 0.0000000000000000
2.8779245994292486 4.9847116265637670 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.0494467868053334
Ag
16
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0850294654130223 F F F
0.5000000000000000 0.0000000000000000 0.0850294654130223 F F F
-0.0000000000000000 0.5000000000000000 0.0850294654130223 F F F
0.4999999999999999 0.5000000000000000 0.0850294654130223 F F F
0.1666666666666643 0.1666666666666643 0.1719005801578888 F F F
0.6666666666666642 0.1666666666666643 0.1719005801578888 F F F
0.1666666666666643 0.6666666666666643 0.1719005801578888 F F F
0.6666666666666643 0.6666666666666643 0.1719005801578888 F F F
0.8333333248032478 0.3333333305712949 0.2585184823258445 T T T
0.3333333265956561 0.3333333251001243 0.2585184814609473 T T T
0.8333333250211756 0.8333333257177051 0.2585184824075382 T T T
0.3333333315144240 0.8333333204320192 0.2585184827022645 T T T
-0.0000000064174232 -0.0000000013301591 0.3457906417277204 T T T
0.4999999949600265 -0.0000000055976585 0.3457906423121225 T T T
-0.0000000057464452 0.4999999962880696 0.3457906417202528 T T T
0.4999999961758383 0.4999999945947776 0.3457906422412195 T T T

Ag111 (3x31 supercell)

Ag
1.00000000000000
8.6380164389748657 0.0000000000000000 0.0000000000000000
4.3190082194874329 7.4807416744598259 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.0529108884204703
Ag
36
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.1035008769129745 F F F
0.3333333333333357 0.0000000000000000 0.1035008769129745 F F F
0.6666666666666643 0.0000000000000000 0.1035008769129745 F F F
0.0000000000000001 0.3333333333333354 0.1035008769129745 F F F
0.3333333333333358 0.3333333333333354 0.1035008769129745 F F F
0.6666666666666644 0.3333333333333354 0.1035008769129745 F F F
0.0000000000000004 0.6666666666666634 0.1035008769129745 F F F
0.3333333333333361 0.6666666666666634 0.1035008769129745 F F F
0.6666666666666649 0.6666666666666634 0.1035008769129745 F F F
0.1111111111111143 0.1111111111111142 0.1904035509297088 F F F
0.4444444444444429 0.1111111111111142 0.1904035509297088 F F F
0.7777777777777788 0.1111111111111142 0.1904035509297088 F F F
0.1111111111111144 0.4444444444444425 0.1904035509297088 F F F
0.4444444444444430 0.4444444444444425 0.1904035509297088 F F F

0.7777777777777788 0.4444444444444425 0.1904035509297088 F F F
0.1111111111111145 0.7777777777777780 0.1904035509297088 F F F
0.4444444444444431 0.7777777777777780 0.1904035509297088 F F F
0.7777777777777788 0.7777777777777780 0.1904035509297088 F F F
0.8888888530280930 0.2222221839578483 0.2770536779505749 T T T
0.2222221849477797 0.2222221813079360 0.2770536799860496 T T T
0.5555555166441265 0.2222221862142236 0.2770536775651041 T T T
0.8888888502984020 0.5555555196496842 0.2770536786266509 T T T
0.2222221893038395 0.5555555135006405 0.2770536802479278 T T T
0.5555555188216410 0.5555555177887050 0.2770536775595658 T T T
0.8888888521774285 0.8888888518197774 0.2770536790370572 T T T
0.2222221883633901 0.8888888521233121 0.2770536791859164 T T T
0.5555555160510776 0.8888888488956932 0.2770536784538555 T T T
-0.0000000005655671 0.0000000007793520 0.3643422874196506 T T T
0.3333333333142646 0.0000000013986913 0.3643422876774339 T T T
0.6666666638086874 0.0000000012292252 0.3643422876968596 T T T
-0.0000000021204447 0.3333333339554644 0.3643422877071616 T T T
0.3333333314303652 0.3333333322684880 0.3643422888216912 T T T
0.6666666682253886 0.3333333324757837 0.3643422888837408 T T T
-0.0000000014389592 0.6666666651267951 0.3643422876857258 T T T
0.3333333319057362 0.6666666682223712 0.3643422873277074 T T T
0.6666666684548713 0.6666666659496925 0.3643422880023126 T T T

Ru1000 (2x2x1 supercell)

Ru
1.00000000000000
5.3959999999999999 0.0000000000000000 0.0000000000000000
0.0000000000000000 4.6730730788208303 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.3585000000000136
Ru
16
Selective dynamics
Direct
0.9478945918263788 0.2384671836355981 0.6996168202162413 T T T
0.4478955888836150 0.2384674258392305 0.6996167900012332 T T T
0.1980899520454035 0.7391382077831928 0.6996191603685507 T T T
0.6980893336621211 0.7391474457383422 0.6996180451927324 T T T
0.9479820951850599 0.9059572449406431 0.7675916021309903 T T T
0.4479803891105922 0.9059587366841269 0.7675919589135329 T T T
0.1981582030988638 0.4059005209307382 0.7676138995501760 T T T
0.6981566659774300 0.4058988712967258 0.7676129986656403 T T T
0.9480954665243431 0.2401140593212859 0.8377277124406068 F F F
0.4480954665243360 0.2401140593212859 0.8377277124406068 F F F
0.1980954665243431 0.7401140593212933 0.8377277124406068 F F F
0.6980954665243431 0.7401140593212933 0.8377277124406068 F F F
0.9480954665243431 0.9067807259879503 0.9075434147974484 F F F
0.4480954665243360 0.9067807259879503 0.9075434147974484 F F F
0.1980954665243431 0.4067807259879587 0.9075434147974484 F F F
0.6980954665243431 0.4067807259879587 0.9075434147974484 F F F

Co111 (2x2x1 supercell)

```
Co
  1.00000000000000
    4.9260000000000002    0.0000000000000000    0.0000000000000000
    0.0000000000000000    4.2660411390421444    0.0000000000000000
    0.0000000000000000    0.0000000000000000   35.9774999999999991
  Co
   16
Selective dynamics
Direct
  0.0010733722163123  0.3332007300715120  0.7537321292013630   T   T   T
  0.4989456208251118  0.3332204003127698  0.7537260037213500   T   T   T
  0.2499761977839875  0.8325601408864957  0.7534600658769329   T   T   T
  0.7500002873918765  0.8327607294588447  0.7524406731994943   T   T   T
 -0.0014321643310377 -0.0012174855253035  0.8088622033764065   T   T   T
  0.5014299176286391 -0.0012430472200869  0.8088647714936072   T   T   T
  0.2500112171702867  0.5016652061069025  0.8083212225618738   T   T   T
  0.7499891770443194  0.5015136210752131  0.8088718146963036   T   T   T
  0.0000000000000000  0.3333333333333354  0.8640122298658923   F   F   F
  0.5000000000000000  0.3333333333333354  0.8640122298658923   F   F   F
  0.2500000000000000  0.8333333333333350  0.8640122298658923   F   F   F
  0.7500000000000000  0.8333333333333350  0.8640122298658923   F   F   F
  0.0000000000000000  0.0000000000000000  0.9193940657355314   F   F   F
  0.5000000000000000  0.0000000000000000  0.9193940657355314   F   F   F
  0.2500000000000000  0.4999999999999996  0.9193940657355314   F   F   F
  0.7500000000000000  0.4999999999999996  0.9193940657355314   F   F   F
```

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