SUPPORTING INFORMATION

Computer-Aided Bimetallic Catalyst Screening for Ester Selective Hydrogenation

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1. The formation energy approach

Hence, the formation energy of species $C_xH_yO_z$ is defined as

$$E_{C_xH_yO_z} = E_{surf+C_xH_yO_z} - E_{surf} - (xE_C + yE_H + zE_O) \quad \text{(S1)}$$

where is the total energy of the surface with adsorbate, E_{surf} is the total energy of the clean surface, E_C is calculated as $E_{CH_4(g)} - 2E_{H_2(g)}$, E_H is calculated as $0.5E_{H_2(g)}$, and E_O is calculated as $E_{H_2O(g)} - E_{H_2(g)}$.

2. Scaling relations of transition states

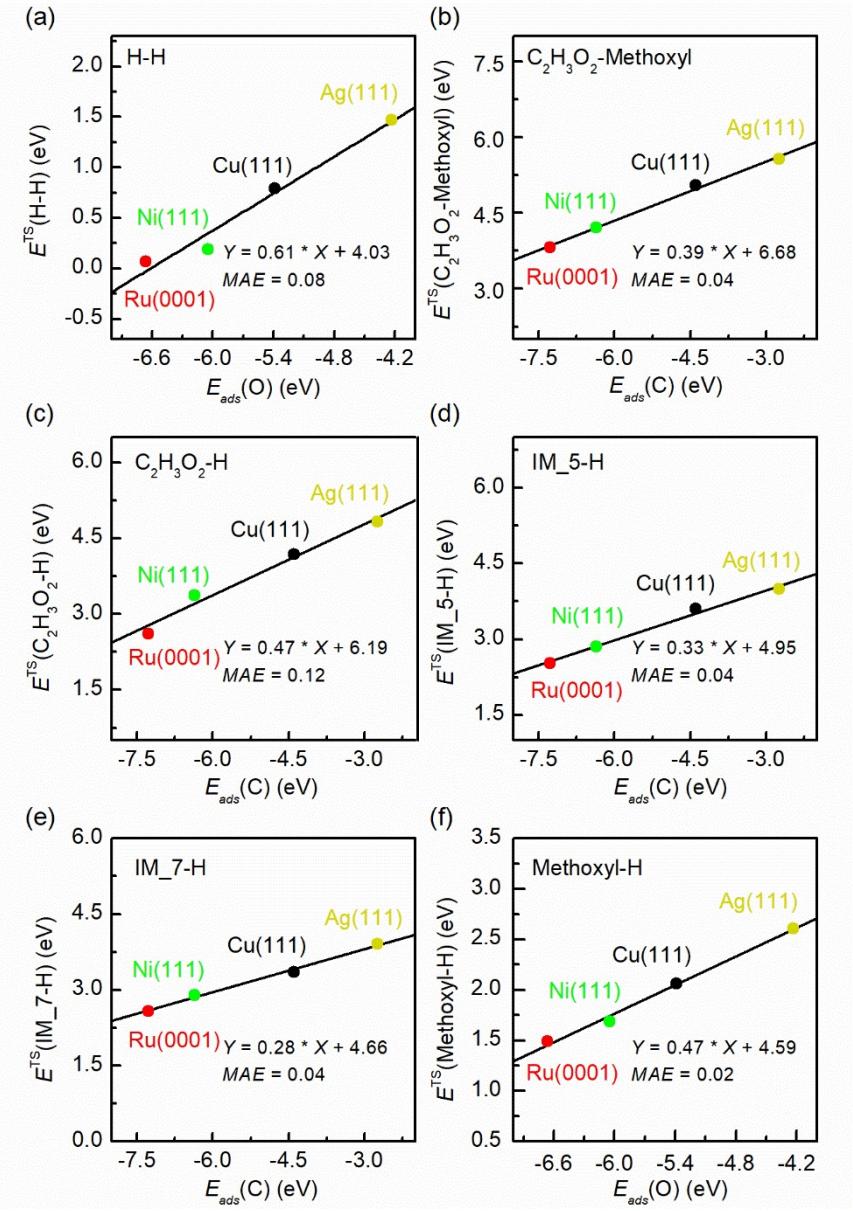

Figure S1 Calculated adsorption energies of transition states as a function of the adsorption energy of atomic carbon or oxygen.

3. Scaling relations of *bimetallic catalysts and* elemental metals

To see if the established scaling relations can be applied to the *d*-block&*d*-block (*d*&*d*), *d*-block&*s*-block (*d*&*s*) and *d*-block&*p*-block (*d*&*p*) bimetallic catalysts, the formation energies of acyl(1) over $Ag_3Zn_1(111)$, $Ag_3Sn_1(111)$, $Ag_3Mg_1(111)$, $Cu_3Ni_1(111)$ and $Cu_3Mg_1(111)$ have been calculated and plotted in in Figure S3, where the black straight lines indicate the scaling relations obtained by making linear regressions on the 4 elemental metals. From the figure, one can see that the data fit the scaling relations quite well, and the formation energies of atomic C and O are only needed to predict the catalytic performance of bimetallic catalysts.

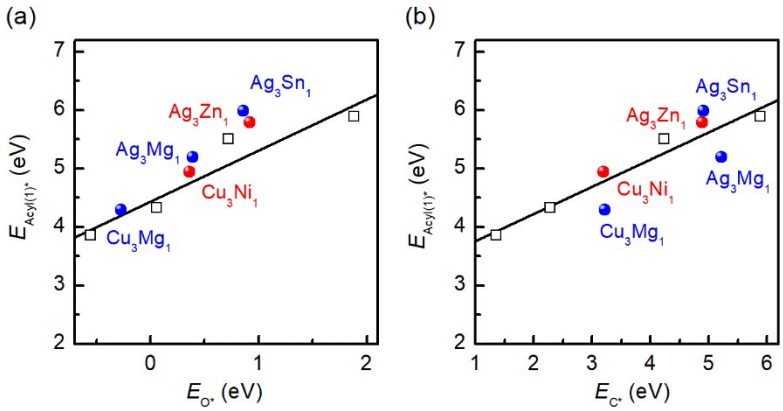

Figure S2 Calculated formation energies of acyl(1) as a function of the formation energies of (a) atomic carbon or oxygen on d&d (red spheres), d&s and d&p (blue spheres) bimetallic catalysts and elemental metals (black squares); the black straight lines indicate the scaling relations obtained by making linear regressions on the 4 elemental metals.

4，Shomate parameters of gas-phase species calculated by ASPEN PLUS V9

Table S1. Shomate parameters of gas-phase species

	DMO	MG	EG
A	71.88	-12.97	-18.03
B	165.54	467.00	368.90
C	149.63	-392.94	-286.98
D	-145.11	137.78	94.89
E	0.46	0.79	0.91
F	-28.30	-11.18	-5.63
G	518.83	242.16	190.05
H	0.00	0.00	0.00

5. The details of clustering algorithm

The bimetallic catalysts are all composed of two elements among the 39 selected elements as shown in Figure S2. The clustering algorithm used in this work is a bisecting k-means clustering algorithm, which can overcome the problem of poor clusters arising from k-means getting caught in a local minimum. Since the optimization process is a dynamic iterative process moving from the unreasonable partition to the "optimal" partition, this method is taken as a dynamic clustering method. Bisecting k-means clustering algorithm starts out with one cluster and then splits the cluster in two. After that, it chooses a cluster to split. The cluster to split is determined by minimizing the sum of squared error (SSE). This splitting based on the SSE is repeated until the user-defined number of clusters is attained. The process of clustering is as follows. First, all the data points start with one cluster. Although the number of clusters is less than k (k is the user-defined number of clusters to be divided), for every cluster, it measures total error and performs k-means clustering with k=2 on the given cluster (k-means clustering will split the cluster in two). Then, it chooses the cluster split that gives the lowest error and commits this split. Finally, the calculation stops until the number of clusters equals k.

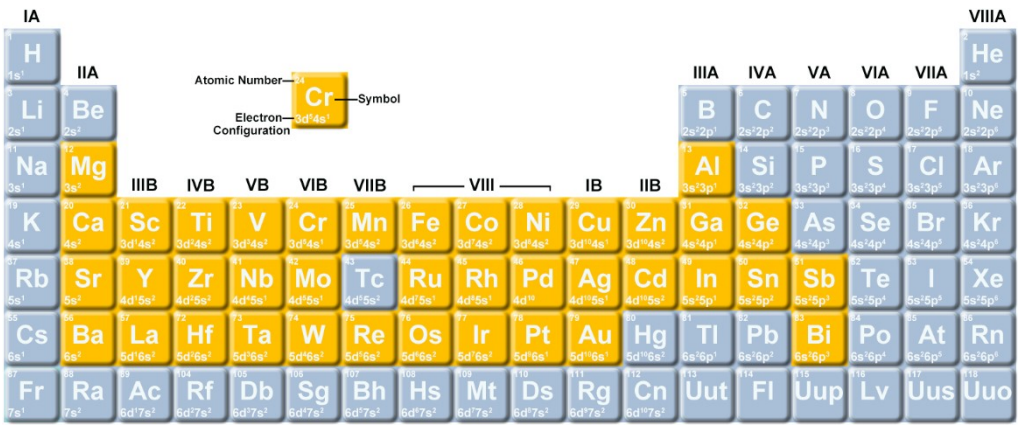

Figure S3. Constituent elements of the alloys of interest, which are colored yellow in the periodic table.

6. Summary of calculated data for screening for bimetallic catalysts

Table S2. Summary of calculated data for screening for alloy catalysts.

Alloy	C [eV]	O [eV]	cost [$ per kg]
Ag3Al1	5.84	-0.36	939.5
Ag3As1	3.71	1.00	1700
Ag3Au1	5.12	1.88	14750
Ag3Bi1	5.36	1.42	997.5
Ag3Ca1	4.91	-0.02	950
Ag3Cd1	5.55	1.37	1015
Ag3Ga1	5.80	0.51	1450
Ag3Ge1	5.69	0.56	1800
Ag3In1	5.26	1.02	3320
Ag3Mg1	5.22	0.39	909.25
Ag3P1	5.37	-0.54	975
Ag3Pd1	4.52	1.77	15482.5
Ag3Pt1	3.74	1.55	33400
Ag3Sb1	5.01	1.14	911.25
Ag3Sn1	4.91	0.86	960
Ag3Y1	4.13	-1.15	1007.5
Ag3Zn1	4.89	0.92	913.25
Al3Au1	2.13	-2.51	13968.5
Al3Ca1	1.53	-2.42	168.5
Al3Co1	3.49	-1.88	171
Al3Cr1	2.57	-1.83	198.5
Al3Cu1	2.33	-2.33	143
Al3Fe1	3.47	-1.90	136.5
Al3Ga1	2.29	-2.21	668.5
Al3Ge1	2.38	-2.32	1018.5
Al3Hf1	2.63	-2.04	418.5
Al3Ir1	3.57	-2.06	10618.5
Al3La1	1.94	-2.24	318.5
Al3Mg1	2.68	-2.37	127.75
Al3Mn1	3.20	-1.56	134.75
Al3Mo1	2.82	-1.93	228.5
Al3Nb1	2.72	-1.43	163.5
Al3Ni1	2.75	-2.12	137.75
Al3Os1	3.84	-2.11	19368.5
Al3Pd1	2.43	-2.22	14701
Al3Pt1	2.67	-2.41	32618.5
Al3Re1	2.20	-1.96	4118.5
Al3Rh1	3.42	-1.96	32618.5
Al3Ru1	3.48	-2.02	3618.5
Al3Sc1	2.98	-2.42	468.5

Al3Si1	2.42	-2.42	132
Al3Ta1	2.49	-1.55	1243.5
Al3Ti1	2.66	-1.96	283.75
Al3V1	2.53	-1.54	668.5
Al3W1	1.47	-1.78	146
Al3Y1	2.59	-1.53	226
Al3Zn1	2.54	-2.35	131.75
Al3Zr1	2.83	-1.88	511
Au3Ag1	4.44	2.10	41850
Au3Bi1	4.20	1.36	41647.5
Au3Ca1	3.77	0.72	41600
Au3Cd1	4.62	1.70	41665
Au3Cu1	4.49	1.69	41574.5
Au3Ge1	4.11	1.08	42450
Au3In1	4.47	1.44	43970
Au3Mg1	4.59	0.96	41559.25
Au3Mn1	3.99	0.84	41566.25
Au3Pb1	3.96	1.50	41556.25
Au3Pd1	4.04	2.21	56132.5
Au3Pt1	3.41	1.97	74050
Au3Sb1	4.31	1.18	41561.25
Au3Sc1	3.97	-0.79	41900
Au3Sn1	4.26	1.26	41610
Au3Sr1	2.90	-0.36	41800
Au3Ti1	2.65	-2.05	41715.25
Au3Y1	4.00	-0.41	41657.5
Au3Zn1	4.58	1.30	41563.25
Ba3Pb1	2.03	-2.91	418.75
Ba3Sn1	1.88	-2.84	472.5
Bi3Ba1	4.52	-0.02	430
Bi3Ca1	4.49	0.05	342.5
Bi3Cd1	3.38	-0.40	407.5
Bi3Ga1	4.64	0.77	842.5
Bi3In1	4.51	0.00	2712.5
Bi3La1	4.29	-0.31	492.5
Bi3Sc1	3.87	-1.40	642.5
Bi3Sr1	4.59	0.17	542.5
Bi3Tl1	4.42	0.40	412.5
Bi3Y1	4.16	-0.60	400
Ca3Al1	4.00	-3.51	189.5
Ca3Cd1	3.53	-3.83	265
Ca3Pb1	4.01	-3.82	156.25
Ca3Sn1	4.07	-3.79	210
Cd3Ag1	5.32	0.67	645
Cd3Au1	5.31	0.59	14195
Cd3Bi1	3.96	0.33	442.5

Cd3Ca1	3.88	-0.67	395
Cd3Ga1	5.22	0.17	895
Cd3Hf1	2.78	-2.40	645
Cd3Hg1	5.41	0.45	465
Cd3Mg1	5.45	-0.41	354.25
Cd3Pb1	4.22	0.26	351.25
Cd3Pd1	4.97	0.84	14927.5
Cd3Pt1	4.26	0.87	32845
Cd3Rh1	3.67	0.93	32845
Cd3Sc1	3.75	-1.70	695
Cd3Sn1	4.77	0.37	405
Cd3Ti1	2.81	-2.07	510.25
Cd3Y1	3.87	-1.50	452.5
Cd3Zn1	5.40	0.24	358.25
Cd3Zr1	2.93	-1.99	737.5
Co3Al1	1.69	-0.67	197
Co3As1	2.19	-0.41	957.5
Co3Cr1	0.89	-2.24	237.5
Co3Fe1	1.92	-0.54	175.5
Co3Ga1	1.98	-0.30	707.5
Co3Ge1	2.14	-0.25	1057.5
Co3Hf1	0.66	-1.51	457.5
Co3Ir1	1.81	-0.13	10657.5
Co3Mo1	1.47	-1.10	267.5
Co3Nb1	1.14	-1.19	202.5
Co3Ni1	2.15	-0.37	176.75
Co3P1	1.18	-1.37	232.5
Co3Pt1	2.29	-0.24	32657.5
Co3Rh1	2.02	-0.31	32657.5
Co3Sb1	2.16	-0.19	168.75
Co3Sc1	0.55	-1.58	507.5
Co3Si1	2.10	-0.36	171
Co3Ta1	1.24	-1.33	1282.5
Co3Ti1	1.04	-1.41	322.75
Co3V1	1.55	-1.23	707.5
Co3W1	1.48	-1.45	185
Co3Zr1	0.58	-1.45	550
Cr3Al1	0.91	-2.00	279.5
Cr3As1	1.44	-2.12	1040
Cr3Co1	0.58	-2.63	292.5
Cr3Cu1	0.98	-2.63	264.5
Cr3Fe1	-0.60	-3.26	258
Cr3Ga1	1.39	-2.02	790
Cr3Ge1	1.83	-1.98	1140
Cr3Ir1	0.83	-2.27	10740
Cr3Mn1	-1.39	-4.17	256.25

Cr3Mo1	-3.41	-5.06	350
Cr3Ni1	0.80	-2.24	259.25
Cr3Os1	0.24	-2.49	19490
Cr3P1	1.60	-2.06	315
Cr3Pd1	0.61	-2.86	14822.5
Cr3Pt1	0.97	-2.32	32740
Cr3Re1	-0.95	-3.32	4240
Cr3Rh1	0.56	-2.60	32740
Cr3Ru1	0.16	-2.71	3740
Cr3Si1	1.80	-1.94	253.5
Cr3V1	0.89	-2.49	790
Cr3W1	-0.88	-2.25	267.5
Cr3Zn1	1.03	-2.46	253.25
Cu3Al1	3.80	-0.49	113
Cu3As1	3.31	0.69	873.5
Cu3Au1	4.08	0.60	13923.5
Cu3Ga1	4.06	0.24	623.5
Cu3Ge1	3.95	0.40	973.5
Cu3In1	3.74	0.44	2493.5
Cu3Mg1	3.22	-0.27	82.75
Cu3Ni1	3.20	0.36	92.75
Cu3P1	2.53	0.15	148.5
Cu3Pd1	3.66	0.61	14656
Cu3Pt1	3.31	0.78	32573.5
Cu3Rh1	2.58	0.55	32573.5
Cu3Sc1	3.09	-1.47	423.5
Cu3Si1	3.15	-0.42	87
Cu3Sn1	4.39	0.51	133.5
Cu3Zn1	4.06	0.46	86.75
Fe3Al1	1.64	-1.27	93.5
Fe3As1	2.45	-0.73	854
Fe3Co1	1.07	-1.19	106.5
Fe3Cr1	1.60	-1.46	134
Fe3Cu1	1.78	-1.07	78.5
Fe3Ga1	1.87	-0.66	604
Fe3Ge1	2.41	-0.52	954
Fe3Hf1	-0.03	-2.54	354
Fe3In1	1.80	-0.74	2474
Fe3Ir1	1.67	-0.86	10554
Fe3Mo1	1.43	-1.36	164
Fe3Nb1	0.55	-1.87	99
Fe3Ni1	1.91	-0.81	73.25
Fe3P1	2.40	-0.71	129
Fe3Pd1	1.70	-1.07	14636.5
Fe3Pt1	2.06	-0.96	32554
Fe3Re1	1.68	-0.77	4054

Fe3Rh1	1.47	-1.01	32554
Fe3Sb1	2.53	-0.51	65.25
Fe3Sc1	0.26	-2.38	404
Fe3Si1	2.33	-0.62	67.5
Fe3Sn1	2.31	-0.44	114
Fe3Ta1	0.52	-1.98	1179
Fe3Ti1	0.11	-2.48	219.25
Fe3V1	1.13	-1.71	604
Fe3W1	1.46	-1.45	81.5
Fe3Zn1	1.61	-0.98	67.25
Fe3Zr1	0.16	-2.07	446.5
Ga3Ag1	3.41	-0.01	1950
Ga3Al1	3.34	-0.94	1689.5
Ga3Ca1	2.92	-0.29	1700
Ga3Cd1	3.40	-0.13	1765
Ga3Ge1	3.64	-0.52	2550
Ga3Hf1	3.09	-0.78	1950
Ga3La1	3.17	-1.20	1850
Ga3Mg1	4.02	-0.92	1659.25
Ga3Mn1	3.46	-0.30	1666.25
Ga3Nb1	3.21	-0.09	1695
Ga3Sb1	3.88	-0.25	1661.25
Ga3Sc1	3.53	-1.09	2000
Ga3Ta1	2.94	-0.27	2775
Ga3Ti1	3.19	-0.49	1815.25
Ga3V1	3.05	-0.15	2200
Ga3Y1	3.63	-1.09	1757.5
Ga3Zn1	3.81	-0.23	1663.25
Ga3Zr1	3.33	-0.46	2042.5
Ge3Ag1	3.96	0.10	3000
Ge3Ca1	3.60	-0.47	2750
Ge3Cd1	3.34	-0.38	2815
Ge3Ga1	3.87	0.15	3250
Ge3Hf1	2.66	-1.56	3000
Ge3In1	3.82	-0.17	5120
Ge3La1	3.77	-0.33	2900
Ge3Mg1	3.32	-0.70	2709.25
Ge3Sc1	3.52	-0.40	3050
Ge3Sn1	3.65	-0.02	2760
Ge3Sr1	3.50	-0.50	2950
Ge3Ti1	2.84	-1.51	2865.25
Ge3Y1	3.56	-0.45	2807.5
Ge3Zr1	3.03	-0.65	3092.5
Hf3Al1	1.00	-3.91	939.5
Hf3As1	0.94	-3.79	1700
Hf3Au1	0.81	-4.12	14750

Hf3Bi1	0.98	-3.77	997.5
Hf3Cd1	0.86	-4.09	1015
Hf3Cu1	0.86	-3.92	924.5
Hf3Ga1	0.98	-3.91	1450
Hf3Ge1	1.07	-3.79	1800
Hf3Hg1	0.82	-4.12	1020
Hf3In1	0.70	-4.03	3320
Hf3Ir1	-1.10	-6.34	11400
Hf3Mo1	-0.86	-5.06	1010
Hf3Nb1	0.52	-4.14	945
Hf3Os1	-0.08	-4.97	20150
Hf3Pb1	0.82	-3.85	906.25
Hf3Pd1	-0.23	-5.14	15482.5
Hf3Pt1	-0.33	-5.33	33400
Hf3Re1	1.00	-3.93	4900
Hf3Rh1	-1.48	-6.55	33400
Hf3Ru1	-2.23	-7.03	4400
Hf3Sb1	1.04	-3.75	911.25
Hf3Sc1	0.43	-3.95	1250
Hf3Si1	1.19	-3.76	913.5
Hf3Sn1	0.93	-3.81	960
Hf3Ta1	0.45	-4.07	2025
Hf3Ti1	0.89	-3.96	1065.25
Hf3Tl1	0.60	-4.08	1020
Hf3Zn1	1.06	-3.98	913.25
Hf3Zr1	0.59	-3.98	1292.5
Hg3In1	6.03	2.31	2780
Hg3La1	3.94	-1.45	560
Hg3Sc1	5.64	-1.46	710
Hg3Y1	4.16	-1.10	467.5
In3Ag1	4.73	0.35	7560
In3Bi1	4.62	0.26	7357.5
In3Ca1	4.54	-0.77	7310
In3Cd1	4.64	0.20	7375
In3Ga1	4.69	0.03	7810
In3Ge1	4.02	-0.07	8160
In3Hf1	3.11	-1.13	7560
In3La1	3.98	-1.12	7460
In3Mg1	4.79	-0.69	7269.25
In3Sb1	4.32	0.25	7271.25
In3Sc1	3.76	-1.05	7610
In3Sn1	4.37	0.09	7320
In3Sr1	4.27	-0.73	7510
In3Ti1	3.08	-1.16	7425.25
In3Y1	3.98	-0.95	7367.5
In3Zr1	3.42	-0.61	7652.5

Ir3Al1	1.10	-0.28	31539.5
Ir3As1	-0.70	-1.73	32300
Ir3Cr1	1.68	-0.33	31580
Ir3Fe1	0.81	-0.35	31518
Ir3Ga1	1.09	0.17	32050
Ir3Ge1	0.26	-0.80	32400
Ir3Hf1	0.57	-0.80	31800
Ir3Mg1	0.74	-0.24	31509.25
Ir3Mn1	1.22	-0.02	31516.25
Ir3Mo1	1.81	-0.31	31610
Ir3Nb1	1.08	-0.66	31545
Ir3Os1	1.46	0.21	50750
Ir3Re1	1.58	-0.12	35500
Ir3Rh1	1.35	0.33	64000
Ir3Ru1	1.54	0.20	35000
Ir3Sb1	1.18	0.46	31511.25
Ir3Sc1	0.59	-0.75	31850
Ir3Si1	-1.11	-2.48	31513.5
Ir3Sn1	1.13	0.32	31560
Ir3Ta1	1.14	-0.81	32625
Ir3Ti1	0.81	-0.71	31665.25
Ir3V1	1.35	-0.62	32050
Ir3W1	1.81	-1.23	31527.5
Ir3Y1	0.15	-0.88	31607.5
Ir3Zn1	1.05	0.09	31513.25
Ir3Zr1	0.44	-0.78	31892.5
La3Al1	2.10	-3.30	639.5
La3Bi1	1.58	-3.56	697.5
La3Cd1	1.59	-3.54	715
La3Ga1	2.04	-3.32	1150
La3Ge1	1.94	-3.35	1500
La3Hg1	1.44	-3.74	720
La3In1	1.82	-3.46	3020
La3Mg1	1.68	-3.44	609.25
La3Pb1	1.67	-3.52	606.25
La3Sb1	1.72	-3.49	611.25
La3Si1	2.05	-3.30	613.5
La3Sn1	1.81	-3.45	660
La3Tl1	1.70	-3.52	720
Mg3Ag1	4.52	-2.36	327.75
Mg3Au1	4.62	-2.37	13877.75
Mg3Bi1	4.44	-2.78	125.25
Mg3Cu1	4.65	-2.31	52.25
Mg3Ge1	4.49	-2.63	927.75
Mg3Ir1	5.18	-1.86	10527.75
Mg3Ni1	4.67	-2.17	47

Mg3Pb1	4.64	-2.59	34
Mg3Pd1	4.61	-2.23	14610.25
Mg3Pt1	4.79	-2.18	32527.75
Mg3Rh1	4.85	-2.03	32527.75
Mg3Ru1	2.24	-1.77	3527.75
Mg3Sb1	4.26	-2.94	39
Mg3Sc1	2.83	-3.29	377.75
Mg3Si1	4.60	-2.62	41.25
Mg3Zn1	4.45	-2.38	41
Mg3Zr1	1.82	-3.39	420.25
Mn3Co1	0.31	-2.45	101.25
Mn3Cr1	0.77	-2.54	128.75
Mn3Fe1	0.50	-2.48	66.75
Mn3Ga1	1.33	-2.05	598.75
Mn3Ge1	1.62	-1.91	948.75
Mn3Hf1	1.06	-2.24	348.75
Mn3Ir1	0.55	-2.17	10548.75
Mn3Mo1	0.71	-2.17	158.75
Mn3Nb1	1.19	-1.76	93.75
Mn3Ni1	1.38	-2.36	68
Mn3Os1	0.71	-2.02	19298.75
Mn3P1	1.64	-1.91	123.75
Mn3Pt1	1.91	-1.35	32548.75
Mn3Re1	-0.79	-3.29	4048.75
Mn3Rh1	-0.56	-3.64	32548.75
Mn3Ru1	0.20	-2.27	3548.75
Mn3Sb1	1.87	-1.20	60
Mn3Sc1	0.78	-2.21	398.75
Mn3Si1	1.24	-1.88	62.25
Mn3Sn1	1.80	-1.17	108.75
Mn3Ta1	1.07	-1.93	1173.75
Mn3Ti1	0.45	-2.17	214
Mn3V1	-0.36	-2.89	598.75
Mn3W1	0.78	-1.98	76.25
Mn3Zr1	1.08	-2.07	441.25
Mo3Al1	1.34	-1.85	369.5
Mo3As1	-1.64	-4.63	1130
Mo3Au1	0.79	-2.32	14180
Mo3Co1	1.22	-2.00	382.5
Mo3Cr1	-2.88	-5.85	410
Mo3Cu1	0.82	-2.30	354.5
Mo3Fe1	-0.07	-2.30	348
Mo3Ga1	1.36	-1.84	880
Mo3Ge1	1.60	-1.88	1230
Mo3In1	1.35	-1.82	2750
Mo3Ir1	1.38	-1.94	10830

Mo3Mn1	-0.60	-3.01	346.25
Mo3Nb1	0.16	-2.23	375
Mo3Ni1	1.13	-2.17	349.25
Mo3Os1	1.02	-2.01	19580
Mo3Pd1	0.91	-2.27	14912.5
Mo3Pt1	1.14	-2.09	32830
Mo3Re1	-0.25	-2.56	4330
Mo3Rh1	1.24	-2.07	32830
Mo3Ru1	1.16	-2.09	3830
Mo3Sb1	0.87	-1.84	341.25
Mo3Si1	1.56	-1.85	343.5
Mo3Sn1	1.64	-1.81	390
Mo3Ta1	0.62	-2.35	1455
Mo3Ti1	0.66	-2.82	495.25
Mo3V1	0.03	-2.71	880
Mo3W1	-2.92	-6.16	357.5
Mo3Zn1	0.91	-2.12	343.25
Nb3Al1	1.18	-2.84	174.5
Nb3As1	0.78	-2.91	935
Nb3Au1	0.42	-3.34	13985
Nb3Bi1	0.87	-2.77	232.5
Nb3Cd1	0.50	-3.07	250
Nb3Cu1	0.76	-3.19	159.5
Nb3Fe1	-0.84	-4.17	153
Nb3Ga1	1.18	-3.00	685
Nb3Ge1	1.03	-3.10	1035
Nb3Hf1	-2.02	-6.19	435
Nb3Hg1	0.49	-3.19	255
Nb3In1	0.90	-2.75	2555
Nb3Ir1	-0.17	-3.98	10635
Nb3Mg1	0.50	-3.11	144.25
Nb3Mo1	1.24	-2.67	245
Nb3Ni1	0.00	-3.33	154.25
Nb3Os1	0.31	-3.83	19385
Nb3P1	0.79	-2.92	210
Nb3Pb1	1.03	-2.87	141.25
Nb3Pd1	0.86	-2.97	14717.5
Nb3Pt1	0.54	-3.15	32635
Nb3Rh1	-0.07	-3.87	32635
Nb3Ru1	1.33	-2.57	3635
Nb3Sb1	1.04	-2.74	146.25
Nb3Sc1	0.55	-3.85	485
Nb3Si1	1.44	-2.58	148.5
Nb3Sn1	1.12	-2.82	195
Nb3Ta1	0.98	-2.83	1260
Nb3Ti1	1.01	-2.96	300.25

Nb3Tl1	0.84	-2.87	255
Nb3V1	1.02	-2.81	685
Nb3W1	0.90	-2.67	162.5
Nb3Zn1	0.90	-3.07	148.25
Ni3Al1	2.05	-0.42	97.25
Ni3As1	2.85	0.25	857.75
Ni3Co1	2.30	-0.12	110.25
Ni3Cr1	2.09	-0.95	137.75
Ni3Cu1	1.96	-0.16	82.25
Ni3Fe1	2.34	-0.28	75.75
Ni3Ga1	2.15	0.07	607.75
Ni3Ge1	2.53	0.23	957.75
Ni3Hf1	2.56	-1.21	357.75
Ni3In1	1.88	-0.03	2477.75
Ni3Ir1	1.78	0.10	10557.75
Ni3La1	1.57	-0.29	257.75
Ni3Mg1	1.70	-0.61	67
Ni3Mn1	1.92	-0.41	74
Ni3Mo1	2.04	-1.00	167.75
Ni3Nb1	2.29	-1.18	102.75
Ni3Pd1	2.14	-0.09	14640.25
Ni3Pt1	2.24	0.10	32557.75
Ni3Rh1	2.03	0.16	32557.75
Ni3Sb1	2.94	0.53	69
Ni3Sc1	0.97	-1.11	407.75
Ni3Si1	2.61	-0.26	71.25
Ni3Sn1	2.41	0.23	117.75
Ni3Ta1	2.39	-1.52	1182.75
Ni3Ti1	2.27	-1.20	223
Ni3V1	2.43	-1.16	607.75
Ni3W1	1.89	-1.39	85.25
Ni3Y1	1.43	-1.37	165.25
Ni3Zn1	1.89	-0.11	71
Ni3Zr1	2.58	-1.08	450.25
Os3Cr1	1.20	-1.03	57830
Os3Fe1	1.36	-0.59	57768
Os3Hf1	0.55	-1.39	58050
Os3Ir1	1.19	-0.71	68250
Os3Mn1	1.23	-0.74	57766.25
Os3Mo1	0.89	-0.94	57860
Os3Nb1	0.66	-1.12	57795
Os3Re1	1.25	-0.87	61750
Os3Rh1	1.07	-0.83	90250
Os3Ru1	1.02	-0.87	61250
Os3Sc1	0.70	-1.57	58100
Os3Ta1	0.73	-1.23	58875

Os3Ti1	0.89	-1.30	57915.25
Os3V1	1.05	-1.17	58300
Os3W1	0.98	-1.03	57777.5
Os3Zr1	0.81	-1.29	58142.5
Pb3Ba1	4.82	-0.03	156.25
Pb3Bi1	4.88	0.32	116.25
Pb3Ca1	4.65	-0.29	68.75
Pb3Cd1	5.02	0.53	133.75
Pb3Ga1	4.20	0.19	568.75
Pb3Hg1	5.01	0.44	138.75
Pb3In1	5.01	0.45	2438.75
Pb3La1	4.13	-0.67	218.75
Pb3Mg1	5.18	-0.54	28
Pb3Sb1	4.76	0.23	30
Pb3Sc1	3.92	-1.17	368.75
Pb3Sn1	4.58	0.25	78.75
Pb3Sr1	4.74	-0.17	268.75
Pb3Tl1	4.97	0.50	138.75
Pb3Y1	4.13	-0.73	126.25
Pd3Ag1	2.11	1.21	44047.5
Pd3Al1	2.67	0.31	43787
Pd3Au1	2.15	1.23	57597.5
Pd3Bi1	3.70	1.31	43845
Pd3Ca1	2.62	0.31	43797.5
Pd3Cd1	2.29	1.31	43862.5
Pd3Co1	2.48	0.61	43800
Pd3Cu1	2.37	1.14	43772
Pd3Fe1	2.78	0.47	43765.5
Pd3Ga1	2.74	0.90	44297.5
Pd3Ge1	2.38	0.20	44647.5
Pd3Hf1	3.70	-0.84	44047.5
Pd3Hg1	2.36	1.38	43867.5
Pd3In1	2.72	1.37	46167.5
Pd3La1	3.12	-0.17	43947.5
Pd3Mg1	2.31	0.58	43756.75
Pd3Mn1	2.45	0.54	43763.75
Pd3Mo1	1.99	-1.53	43857.5
Pd3Nb1	2.58	-1.83	43792.5
Pd3Ni1	2.33	0.74	43766.75
Pd3Pb1	3.25	1.42	43753.75
Pd3Pt1	2.00	1.04	76247.5
Pd3Sb1	3.78	1.12	43758.75
Pd3Sc1	2.52	-0.25	44097.5
Pd3Sn1	3.39	1.20	43807.5
Pd3Ta1	2.52	-2.31	44872.5
Pd3Ti1	3.27	-0.89	43912.75

Pd3Tl1	2.72	1.61	43867.5
Pd3V1	2.55	-1.46	44297.5
Pd3Y1	2.82	-0.01	43855
Pd3Zn1	2.43	1.13	43760.75
Pd3Zr1	3.66	-0.68	44140
Pt3Ag1	1.60	1.23	97800
Pt3Al1	2.14	0.42	97539.5
Pt3Cd1	1.68	1.10	97615
Pt3Co1	2.25	0.81	97552.5
Pt3Cr1	2.10	-0.73	97580
Pt3Cu1	1.95	1.15	97524.5
Pt3Fe1	2.33	0.69	97518
Pt3Ga1	1.85	0.95	98050
Pt3Ge1	1.24	0.02	98400
Pt3Hf1	2.95	-0.18	97800
Pt3In1	2.05	1.13	99920
Pt3Mg1	1.72	0.41	97509.25
Pt3Mn1	1.93	0.65	97516.25
Pt3Mo1	2.09	-1.28	97610
Pt3Nb1	2.66	-1.50	97545
Pt3Ni1	2.03	0.86	97519.25
Pt3Pb1	2.53	1.14	97506.25
Pt3Pd1	1.74	1.08	112082.5
Pt3Ru1	1.73	0.57	101000
Pt3Sc1	1.67	-0.03	97850
Pt3Sn1	2.56	1.08	97560
Pt3Ta1	2.64	-1.98	98625
Pt3Ti1	2.92	-0.35	97665.25
Pt3Tl1	1.91	1.12	97620
Pt3V1	2.47	-1.17	98050
Pt3W1	1.99	-1.95	97527.5
Pt3Y1	1.95	0.07	97607.5
Pt3Zn1	1.92	0.97	97513.25
Pt3Zr1	2.81	-0.08	97892.5
Re3Co1	1.15	-1.37	12052.5
Re3Cr1	1.13	-1.70	12080
Re3Fe1	1.17	-1.36	12018
Re3Ir1	1.19	-1.47	22500
Re3Mn1	1.02	-1.40	12016.25
Re3Mo1	0.94	-1.61	12110
Re3Nb1	0.63	-1.82	12045
Re3Ni1	1.20	-1.61	12019.25
Re3Os1	1.27	-1.28	31250
Re3Pt1	1.17	-1.74	44500
Re3Rh1	1.04	-1.63	44500
Re3Ru1	1.22	-1.38	15500

Re3Ta1	0.64	-1.95	13125
Re3Ti1	0.32	-2.21	12165.25
Re3V1	0.85	-1.89	12550
Re3W1	0.93	-1.69	12027.5
Rh3Al1	1.45	-0.27	97539.5
Rh3As1	0.96	-0.25	98300
Rh3Bi1	1.43	0.56	97597.5
Rh3Cd1	1.10	0.05	97615
Rh3Cr1	1.73	-0.80	97580
Rh3Ga1	1.52	0.31	98050
Rh3Ge1	1.36	0.11	98400
Rh3Hf1	0.94	-0.89	97800
Rh3In1	1.27	0.33	99920
Rh3Ir1	1.54	0.25	108000
Rh3La1	1.42	-0.64	97700
Rh3Mg1	1.03	-0.11	97509.25
Rh3Mn1	1.46	-0.14	97516.25
Rh3Mo1	1.85	-0.77	97610
Rh3Nb1	1.31	-0.93	97545
Rh3Ni1	1.83	0.22	97519.25
Rh3Pb1	1.37	0.49	97506.25
Rh3Pt1	1.65	0.18	130000
Rh3Re1	1.56	-0.96	101500
Rh3Ru1	1.59	-0.02	101000
Rh3Sb1	1.57	0.65	97511.25
Rh3Sc1	1.06	-0.72	97850
Rh3Si1	0.49	-1.45	97513.5
Rh3Sn1	1.49	0.55	97560
Rh3Ta1	1.36	-1.10	98625
Rh3Ti1	1.19	-0.91	97665.25
Rh3V1	1.54	-1.00	98050
Rh3Zn1	1.41	0.19	97513.25
Rh3Zr1	0.89	-0.85	97892.5
Ru3Al1	1.21	-0.66	10539.5
Ru3Cr1	1.41	-1.24	10580
Ru3Ga1	1.37	-0.47	11050
Ru3Ge1	-0.19	-2.14	11400
Ru3Hf1	0.67	-1.39	10800
Ru3Ir1	1.40	-0.58	21000
Ru3Mn1	1.34	-0.75	10516.25
Ru3Mo1	1.11	-1.14	10610
Ru3Nb1	0.87	-1.29	10545
Ru3Os1	1.21	-0.75	29750
Ru3Pt1	1.30	-0.64	43000
Ru3Re1	1.34	-1.10	14500
Ru3Rh1	1.25	-0.80	43000

Ru3Sc1	0.36	-1.75	10850
Ru3Ta1	0.88	-1.44	11625
Ru3Ti1	1.00	-1.37	10665.25
Ru3V1	1.21	-1.39	11050
Ru3W1	1.15	-1.24	10527.5
Ru3Zr1	0.63	-1.27	10892.5
Sb3Ca1	4.10	0.76	83.75
Sb3Sr1	4.23	-0.07	283.75
Sc3Ag1	1.08	-5.70	1350
Sc3Al1	1.62	-4.05	1089.5
Sc3As1	1.36	-4.14	1850
Sc3Au1	-0.14	-5.85	14900
Sc3Bi1	0.92	-4.22	1147.5
Sc3Cd1	1.22	-4.29	1165
Sc3Ga1	1.58	-4.11	1600
Sc3Ge1	1.51	-4.08	1950
Sc3Hf1	1.21	-4.09	1350
Sc3Hg1	1.09	-4.51	1170
Sc3In1	1.27	-4.21	3470
Sc3Mg1	1.16	-4.27	1059.25
Sc3Mn1	1.37	-4.14	1066.25
Sc3Mo1	2.25	-3.83	1160
Sc3Nb1	1.08	-3.73	1095
Sc3P1	1.55	-4.09	1125
Sc3Pb1	1.03	-4.23	1056.25
Sc3Sb1	1.14	-4.16	1061.25
Sc3Si1	1.69	-4.01	1063.5
Sc3Sn1	1.23	-4.14	1110
Sc3Tl1	1.15	-4.29	1170
Sc3Y1	1.50	-4.03	1157.5
Sc3Zr1	1.36	-3.93	1442.5
Si3Ca1	2.72	-1.12	90.5
Si3Hf1	2.02	-1.69	340.5
Si3La1	3.10	-0.87	240.5
Si3Nb1	0.76	-2.59	85.5
Si3Sc1	2.67	-1.59	390.5
Si3Ta1	2.06	-2.91	1165.5
Si3V1	2.71	-2.10	590.5
Si3Y1	2.63	-1.16	148
Si3Zr1	1.53	-1.97	433
Sn3Ag1	4.42	0.26	480
Sn3Ba1	4.17	-0.38	317.5
Sn3Bi1	3.73	-0.36	277.5
Sn3Ca1	4.13	-0.50	230
Sn3Cd1	4.34	0.13	295
Sn3Ga1	4.17	0.01	730

Sn3Ge1	3.78	-0.02	1080
Sn3Hf1	2.41	-0.40	480
Sn3In1	4.32	0.07	2600
Sn3La1	3.79	-0.56	380
Sn3Mg1	3.91	-0.74	189.25
Sn3Pb1	4.16	0.07	186.25
Sn3Sc1	3.66	-0.82	530
Sn3Sr1	4.31	-0.40	430
Sn3Tl1	4.31	0.07	300
Sn3Y1	3.83	-0.56	287.5
Sn3Zr1	2.54	-1.34	572.5
Ta3Al1	0.92	-2.87	3414.5
Ta3As1	-0.92	-3.83	4175
Ta3Au1	0.22	-3.47	17225
Ta3Co1	-1.22	-5.17	3427.5
Ta3Cu1	0.51	-3.53	3399.5
Ta3Fe1	-1.32	-4.70	3393
Ta3Ga1	0.89	-3.14	3925
Ta3Ge1	0.96	-3.30	4275
Ta3Hf1	-1.26	-4.59	3675
Ta3In1	0.75	-2.90	5795
Ta3Ir1	-0.45	-4.30	13875
Ta3Mn1	0.41	-4.04	3391.25
Ta3Mo1	0.91	-2.96	3485
Ta3Nb1	0.77	-2.92	3420
Ta3Ni1	0.27	-3.67	3394.25
Ta3Os1	0.58	-3.02	22625
Ta3Pd1	0.38	-3.32	17957.5
Ta3Pt1	0.54	-3.37	35875
Ta3Re1	0.68	-2.97	7375
Ta3Rh1	-0.31	-4.07	35875
Ta3Ru1	0.86	-3.86	6875
Ta3Sb1	0.62	-3.11	3386.25
Ta3Si1	1.09	-3.17	3388.5
Ta3Sn1	0.87	-2.88	3435
Ta3Ti1	0.59	-3.17	3540.25
Ta3V1	0.90	-2.93	3925
Ta3W1	0.97	-2.91	3402.5
Ta3Zn1	0.54	-3.25	3388.25
Ti3Al1	1.11	-3.75	535.25
Ti3As1	1.41	-3.52	1295.75
Ti3Au1	1.04	-3.91	14345.75
Ti3Bi1	1.24	-3.60	593.25
Ti3Cd1	0.94	-3.92	610.75
Ti3Co1	1.23	-3.54	548.25
Ti3Cu1	1.30	-3.78	520.25

Ti3Fe1	-0.81	-6.27	513.75
Ti3Ga1	1.12	-3.78	1045.75
Ti3Ge1	1.43	-3.52	1395.75
Ti3Hf1	0.86	-3.71	795.75
Ti3Hg1	0.94	-3.94	615.75
Ti3In1	0.85	-3.86	2915.75
Ti3Ir1	0.61	-4.30	10995.75
Ti3Mn1	0.39	-4.73	512
Ti3Mo1	1.14	-3.90	605.75
Ti3Nb1	0.85	-3.83	540.75
Ti3Ni1	0.21	-4.85	515
Ti3Os1	0.89	-4.06	19745.75
Ti3P1	1.47	-3.51	570.75
Ti3Pb1	1.08	-3.63	502
Ti3Pd1	0.70	-4.16	15078.25
Ti3Pt1	0.75	-4.20	32995.75
Ti3Re1	-0.66	-3.96	4495.75
Ti3Rh1	0.93	-3.96	32995.75
Ti3Ru1	1.23	-3.52	3995.75
Ti3Sb1	1.36	-3.52	507
Ti3Si1	1.55	-3.45	509.25
Ti3Sn1	1.18	-3.57	555.75
Ti3Ta1	0.74	-3.78	1620.75
Ti3Tl1	0.77	-3.91	615.75
Ti3V1	0.73	-3.85	1045.75
Ti3W1	0.75	-4.26	523.25
Ti3Zn1	1.22	-3.82	509
Ti3Zr1	0.75	-3.64	888.25
Tl3As1	3.68	0.30	1160
Tl3Ba1	4.78	-0.33	497.5
Tl3Bi1	5.13	0.86	457.5
Tl3Ca1	5.52	-0.45	410
Tl3Cd1	5.52	0.64	475
Tl3Hg1	5.37	0.59	480
Tl3La1	4.30	-1.07	560
Tl3Pb1	5.30	0.81	366.25
Tl3Sb1	4.67	0.56	371.25
Tl3Sc1	5.91	-1.11	710
Tl3Sn1	6.05	0.43	420
Tl3Y1	5.74	-0.85	467.5
V3Al1	1.14	-2.73	1689.5
V3As1	1.28	-2.91	2450
V3Co1	0.10	-4.26	1702.5
V3Cu1	1.12	-3.40	1674.5
V3Ge1	1.46	-2.71	2550
V3In1	1.00	-2.80	4070

V3Mn1	-2.01	-6.34	1666.25
V3Nb1	-2.45	-7.74	1695
V3Ni1	0.57	-3.39	1669.25
V3Os1	-1.08	-5.60	20900
V3P1	1.43	-2.92	1725
V3Pd1	0.20	-3.84	16232.5
V3Pt1	0.39	-3.74	34150
V3Sb1	1.27	-2.70	1661.25
V3Si1	1.59	-2.69	1663.5
V3Sn1	1.23	-2.64	1710
V3Zn1	0.76	-3.22	1663.25
W3Al1	1.23	-1.96	122
W3Au1	0.62	-2.48	13932.5
W3Co1	0.92	-2.23	135
W3Cr1	-3.85	-5.15	162.5
W3Cu1	0.63	-2.37	107
W3Fe1	-0.07	-2.65	100.5
W3Ga1	1.21	-1.99	632.5
W3Ge1	1.30	-2.07	982.5
W3Ir1	1.03	-2.19	10582.5
W3Mn1	0.22	-3.01	98.75
W3Ni1	0.78	-2.36	101.75
W3Os1	0.95	-2.20	19332.5
W3Pd1	0.64	-2.41	14665
W3Pt1	0.84	-2.29	32582.5
W3Re1	-0.02	-2.54	4082.5
W3Rh1	0.89	-2.28	32582.5
W3Ru1	0.82	-2.40	3582.5
W3Si1	1.26	-2.05	96
W3Ta1	-2.52	-2.35	1207.5
W3Ti1	-4.26	-6.23	247.75
W3V1	-1.96	-4.27	632.5
W3Zn1	0.77	-2.15	95.75
Y3Al1	2.04	-3.86	362
Y3Bi1	1.43	-3.99	420
Y3Ga1	1.98	-3.90	872.5
Y3Ge1	1.92	-3.87	1222.5
Y3Hg1	0.77	-4.92	442.5
Y3In1	1.76	-3.98	2742.5
Y3Mg1	1.65	-3.99	331.75
Y3Pb1	1.53	-4.01	328.75
Y3Sb1	1.63	-3.94	333.75
Y3Sc1	1.73	-3.94	672.5
Y3Sn1	1.72	-3.93	382.5
Y3Tl1	1.63	-4.04	442.5
Zn3Al1	3.85	-1.15	79.25

Zn3Au1	4.61	-0.30	13889.75
Zn3Co1	4.99	0.20	92.25
Zn3Cr1	2.00	-1.45	119.75
Zn3Cu1	4.53	0.02	64.25
Zn3Fe1	2.71	-0.45	57.75
Zn3Ga1	4.11	-0.46	589.75
Zn3Ge1	3.98	-0.54	939.75
Zn3Hf1	2.70	-2.26	339.75
Zn3Ir1	5.09	0.28	10539.75
Zn3Mn1	3.08	-0.38	56
Zn3Mo1	1.95	-1.43	149.75
Zn3Nb1	2.23	-1.91	84.75
Zn3Ni1	4.81	0.21	59
Zn3Pd1	4.61	-0.08	14622.25
Zn3Pt1	4.18	0.04	32539.75
Zn3Rh1	3.69	0.23	32539.75
Zn3Ru1	3.03	0.23	3539.75
Zn3Sc1	3.17	-1.70	389.75
Zn3Si1	3.29	-0.75	53.25
Zn3Ta1	1.92	-2.40	1164.75
Zn3Ti1	2.80	-1.95	205
Zn3V1	2.17	-1.98	589.75
Zn3W1	1.70	-1.97	67.25
Zn3Zr1	2.79	-1.81	432.25
Zr3Ag1	1.15	-3.66	1477.5
Zr3Al1	1.25	-3.58	1217
Zr3As1	1.27	-3.58	1977.5
Zr3Au1	1.13	-3.71	15027.5
Zr3Bi1	1.27	-3.45	1275
Zr3Cd1	1.10	-3.72	1292.5
Zr3Cu1	1.30	-3.68	1202
Zr3Ga1	1.20	-3.59	1727.5
Zr3Ge1	1.39	-3.41	2077.5
Zr3Hf1	1.02	-3.74	1477.5
Zr3Hg1	1.07	-3.76	1297.5
Zr3In1	0.96	-3.70	3597.5
Zr3Mg1	1.18	-3.60	1186.75
Zr3Nb1	1.31	-3.59	1222.5
Zr3Pb1	1.21	-3.47	1183.75
Zr3Pd1	0.37	-4.41	15760
Zr3Pt1	0.17	-4.75	33677.5
Zr3Sb1	1.35	-3.40	1188.75
Zr3Sc1	1.19	-3.56	1527.5
Zr3Si1	1.49	-1.73	1191
Zr3Sn1	1.32	-3.43	1237.5
Zr3Ti1	1.03	-3.59	1342.75

Zr3Tl1	0.85	-3.76	1297.5
Zr3Zn1	1.33	-3.60	1190.75
Ag1Au1	4.42	1.78	28300
Ag1Hf1	1.15	-3.51	1200
Ag1Pd1	3.00	1.45	29765
Ag1Sb1	2.53	-0.69	622.5
Al1Co1	2.00	-0.95	184
Al1Nb1	-1.07	-3.98	169
Al1Rh1	3.05	-0.86	65079
As1Cr1	2.54	-0.28	1760
As1Hf1	2.23	-2.53	2200
As1Mn1	2.13	-0.33	1632.5
As1Mo1	2.3	-0.57	1820
As1Nb1	2.43	-0.55	1690
As1Ni1	2.64	-0.23	1638.5
As1Rh1	3.24	0.73	66600
As1Ta1	2.05	-1.34	3850
As1V1	2.62	-0.62	2700
As1W1	2.02	-0.92	1655
As1Zr1	2.58	-1.98	2385
Au1Ca1	4.2	-1.46	27800
Au1Cd1	5.08	1.21	27930
Au1Cu1	3.98	1.3	27749
Au1Hf1	1.46	-3.48	28300
Au1La1	2.82	-2.98	28100
Au1Mg1	4.83	-0.43	27718.5
Au1Mn1	2.91	-0.38	27732.5
Au1Ni1	2.29	0.56	27738.5
Au1Pd1	2.89	1.79	56865
Au1Pt1	1.86	1.05	92700
Au1Sc1	2.73	-2.93	28400
Au1Sn1	3.6	0.23	27820
Au1Ti1	1.51	-2.86	28030.5
Au1Tl1	4.82	1.29	27940
Au1Y1	3.07	-2.78	27915
Au1Zr1	1.62	-3.09	28485
Bi1Ti1	2.34	-2.87	525.5
Bi1Zn1	3.01	-0.66	221.5
Cd1Hf1	1.16	-3.58	830
Cd1Pd1	4.03	1.21	29395
Cd1Ti1	1.14	-3.28	560.5
Co1Fe1	1.66	-0.8	141
Co1Ga1	2.57	0.05	1205
Co1Ge1	3.28	0.44	1905
Co1Hf1	2.04	-2.92	705
Co1In1	3.55	-0.12	4945

Co1Ir1	-0.28	-1.17	21105
Co1Mn1	1.17	-1.25	137.5
Co1Nb1	1.19	-2.42	195
Co1Ni1	1.42	-1.41	143.5
Co1Os1	0.27	-1.82	38605
Co1Pt1	0.89	-0.41	65105
Co1Ru1	-0.71	-2.22	7105
Co1Sc1	2.29	-2.42	805
Co1Si1	3.24	-0.15	132
Co1Sn1	4.09	0.41	225
Co1Ta1	0.89	-2.73	2355
Co1Ti1	1.93	-2.74	435.5
Co1V1	1.31	-2.46	1205
Co1Y1	2.09	-2.37	320
Co1Zn1	1.9	-0.27	131.5
Co1Zr1	2.04	-2.61	890
Cr1Ir1	-1.87	-3.93	21160
Cr1Mo1	0.9	-2.12	380
Cr1Nb1	1.65	-2.43	250
Cr1Os1	-1.18	-2.91	38660
Cr1P1	2.26	-0.76	310
Cr1Re1	0.5	-1.63	8160
Cr1Ru1	-0.76	-3.39	7160
Cr1Ta1	1.47	-2.55	2410
Cr1Ti1	1.57	-2.89	490.5
Cr1W1	0.7	-2.27	215
Cu1Hf1	1.63	-3.44	649
Cu1Ir1	0.11	-0.88	21049
Cu1Mn1	2.22	-0.87	81.5
Cu1Ni1	1.68	-0.1	87.5
Cu1Pd1	2.69	1.01	29214
Cu1Pt1	1.72	0.92	65049
Cu1Rh1	1.09	0.21	65049
Cu1Sc1	2.54	-2.91	749
Cu1Y1	2.73	-2.69	264
Cu1Zr1	1.89	-2.95	834
Fe1Ga1	2.4	-0.22	1136
Fe1Ge1	2.94	0.14	1836
Fe1Hf1	0.7	-2.76	636
Fe1Ir1	1.16	-0.45	21036
Fe1Mn1	1.11	-1.76	68.5
Fe1Nb1	1.49	-2.55	126
Fe1Ni1	1.49	-1.37	74.5
Fe1Os1	0.73	-1.64	38536
Fe1Pt1	1.6	-1.24	65036
Fe1Re1	-0.4	-2.15	8036

Fe1Rh1	1.7	-0.5	65036
Fe1Ru1	0.97	-0.86	7036
Fe1Sc1	1.72	-3.23	736
Fe1Si1	2.62	-0.5	63
Fe1Ta1	1.44	-2.77	2286
Fe1Ti1	0.82	-2.59	366.5
Fe1Zn1	2.04	-1.15	62.5
Fe1Zr1	2.02	-2.45	821
Ga1Hf1	1.19	-3.54	1700
Ga1Mn1	2.29	-0.81	1132.5
Ga1Nb1	0.21	-3.19	1190
Ga1Ni1	3.17	0.44	1138.5
Ga1Os1	1.47	-0.26	39600
Ga1Pt1	3.57	0.46	66100
Ga1Ru1	2.62	-0.02	8100
Ga1Sc1	2.67	-2.77	1800
Ga1Ti1	1.02	-3.1	1430.5
Ga1V1	-0.05	-3.36	2200
Ga1Zr1	1.4	-3	1885
Ge1Ir1	2.74	0.43	22800
Ge1Mn1	3.14	0.18	1832.5
Ge1Mo1	2.17	-0.72	2020
Ge1Nb1	2.13	-1.28	1890
Ge1Pd1	4.12	0.4	30965
Ge1Pt1	1.73	-1.87	66800
Ge1Re1	1.65	-0.46	9800
Ge1Rh1	3.54	0.61	66800
Ge1Ru1	2.58	0.28	8800
Ge1Ta1	1.88	-1.84	4050
Ge1Ti1	1.12	-3.77	2130.5
Ge1V1	1.58	-2.31	2900
Ge1Zn1	1.2	-1.49	1826.5
Hf1Hg1	1.43	-3.5	840
Hf1In1	0.38	-4	5440
Hf1Ir1	1.98	-2.64	21600
Hf1Mn1	1.73	-2.95	632.5
Hf1Ni1	1.79	-3.09	638.5
Hf1Os1	0.85	-2.51	39100
Hf1Pd1	1.51	-3.52	29765
Hf1Pt1	1.44	-3.43	65600
Hf1Re1	1.52	-2.37	8600
Hf1Rh1	1.94	-2.95	65600
Hf1Ru1	1.43	-2.71	7600
Hf1Sb1	2.19	-2.23	622.5
Hf1Sn1	0.86	-3.99	720
Hf1Zn1	1.57	-3.34	626.5

Hg1Pd1	4.36	1.91	29405
Hg1Pt1	2.58	1.43	65240
Hg1Rh1	1.69	0.76	65240
Hg1Zr1	1.75	-3	1025
In1Ir1	3.33	0.8	25840
In1Pd1	4.87	1	34005
In1Pt1	3.57	0.9	69840
In1Rh1	3.18	0.82	69840
In1Ru1	1.23	-0.12	11840
In1Ti1	0.78	-3.35	5170.5
Ir1Mg1	0.63	-0.96	21018.5
Ir1Mn1	1.34	-0.82	21032.5
Ir1Ni1	0.4	-0.38	21038.5
Ir1Ru1	-3.24	-4.63	28000
Ir1Ti1	1.76	-2.35	21330.5
Ir1Y1	2.67	-1.73	21215
Ir1Zn1	1.18	0.25	21026.5
Ir1Zr1	1.96	-2.37	21785
Mg1Pd1	3.5	-0.6	29183.5
Mg1Pt1	2.85	-0.31	65018.5
Mg1Rh1	1.36	-0.48	65018.5
Mg1Sb1	1.47	-2.18	41
Mn1Os1	1.01	-1.3	38532.5
Mn1P1	2.83	-0.28	182.5
Mn1Ru1	1.44	-1.14	7032.5
Mn1Si1	2.49	-0.93	59.5
Mn1Ta1	0.72	-2.6	2282.5
Mn1Ti1	0.73	-2.73	363
Mn1V1	1.53	-2.43	1132.5
Mn1W1	0.7	-2.43	87.5
Mn1Zn1	2.03	-1.01	59
Mn1Zr1	1.97	-2.68	817.5
Mo1Si1	1.31	-1.6	247
Mo1Ta1	1.51	-2.41	2470
Mo1V1	1.37	-2.38	1320
Mo1W1	0.87	-2.03	275
Mo1Zr1	1.71	-2.47	1005
Nb1Os1	1.17	-2.27	38590
Nb1P1	2.05	-1.04	240
Nb1Re1	0.63	-2.18	8090
Nb1Rh1	0.99	-4.17	65090
Nb1Si1	-1.3	-3.95	117
Nb1Sn1	1.88	-1.56	210
Ni1Os1	-0.65	-1.82	38538.5
Ni1P1	-0.34	-1.74	188.5
Ni1Pt1	1.35	0.18	65038.5

Ni1Rh1	1.2	-0.06	65038.5
Ni1Sc1	2.56	-2.56	738.5
Ni1Si1	3.15	-0.37	65.5
Ni1Sn1	2.86	0.62	158.5
Ni1Y1	2.6	-2.38	253.5
Ni1Zn1	2.72	0.21	65
Ni1Zr1	1.87	-2.66	823.5
Os1P1	1.29	-0.76	38650
Os1Rh1	-2.29	-3.65	103500
Os1Ru1	-3.39	-4.79	45500
Os1Sb1	3.67	0.72	38522.5
Os1Sc1	1.81	-1.7	39200
Os1Si1	2.25	-0.16	38527
Os1Sn1	3.04	0.6	38620
Os1Ta1	1.07	-2.47	40750
Os1Ti1	0.92	-2.34	38830.5
Os1V1	1	-2.19	39600
Os1Y1	0.61	-2.78	38715
Os1Zr1	0.77	-2.33	39285
P1Re1	1.09	0.31	8150
P1Ru1	2.1	-0.38	7150
P1Sc1	-2.79	-5.32	850
P1Ta1	1.68	-1.19	2400
P1Ti1	0.12	-2.37	480.5
P1V1	2.26	-1.12	1250
P1W1	1.67	-0.66	205
P1Y1	-2.4	-5.12	365
P1Zr1	2.25	-2.08	935
Pb1Pd1	4.13	1.25	29177.5
Pb1Pt1	2.81	0.49	65012.5
Pb1Rh1	2.27	0.91	65012.5
Pb1Ru1	2.26	0.38	7012.5
Pd1Rh1	1.04	-0.62	94165
Pd1Sc1	2.72	-2.69	29865
Pd1Ti1	0.7	-3.13	29495.5
Pd1Y1	2.97	-2.51	29380
Pd1Zn1	3.88	0.62	29191.5
Pd1Zr1	1.65	-3.08	29950
Pt1Rh1	0.51	-0.57	130000
Pt1Ru1	0.97	-2.35	72000
Pt1Sc1	2.79	-2.21	65700
Pt1Sn1	2.44	-0.68	65120
Pt1Sr1	2.73	-0.55	65500
Pt1Ta1	-0.54	-4.19	67250
Pt1Ti1	0.97	-3.08	65330.5
Pt1Tl1	1.1	-0.67	65240

Pt1Zn1	3.55	0.82	65026.5
Pt1Zr1	1.62	-2.91	65785
Re1Si1	1.51	-0.42	8027
Re1Ta1	0.58	-1.55	10250
Rh1Ru1	-1.48	-2.75	72000
Rh1Sb1	3.5	0.7	65022.5
Rh1Sc1	2.14	-2.3	65700
Rh1Si1	3.55	-0.83	65027
Rh1Sn1	3.63	0.76	65120
Rh1Ti1	1.73	-2.65	65330.5
Rh1Tl1	2.7	0.96	65240
Rh1Y1	3.04	-2.1	65215
Rh1Zn1	1.77	0.45	65026.5
Ru1Si1	2.84	-0.26	7027
Ru1Sn1	2.76	0.7	7120
Ru1Ta1	0.97	-2.72	9250
Ru1Zr1	2.29	-2.5	7785
Sb1Ta1	2.09	-1.33	2272.5
Sb1V1	2.49	-1.04	1122.5
Sb1Zn1	0.98	-2.15	49
Sb1Zr1	2.51	-1.7	807.5
Si1W1	1.35	-1.58	82
Sn1Ti1	0.95	-3.08	450.5
Sn1Zr1	0.82	-3.42	905
Ti1Zn1	1.36	-3.07	357
V1W1	0.9	-2.34	1155
Zn1Zr1	1.77	-2.88	811.5

7. Scaling relationships on interface

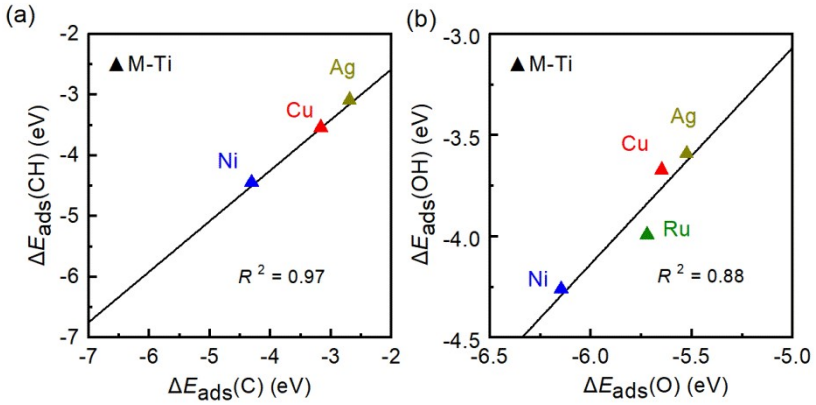

Figure S4 Scaling relationships between adsorption energies of (a) C and CH, (b) O and OH on interface (M-Ti).