SUPPORTING INFORMATION FOR: "TOWARD A NEW DEFINITION OF THE SURFACE ENERGY OF LATE TRANSITION METALS"

Alexandre Boucher,[a] Glenn Jones[b] and Alberto Roldan[a]

[a] Cardiff Catalysis Institute, School of Chemistry, Cardiff University, Main Building, Park Place, Cardiff, CF10 3AT, Wales, United Kingdom.

[b] Johnson Matthey Technology Center, Blounts Ct Rd, Sonning Common, Reading RG4 9NH, United Kingdom.

Content:

Table S1: Lorentzian parameters for surface area and surface energy of transition metals.

This table shows the parameters of the Lorentzian equation describing the surface area of an atom (Å²) and its surface energy (J/m²) as a function of its CN. Lorentzian functions have the following form:

$$f(CN) = a - \frac{b + CN^c}{d} \#(1)$$

Where in this work parameters a, b, c and d were obtained from fitting functions available in the SciPy Python package.

Area parameters					
Metal	a	b	c	d	R^2
Pd	114.7918	57.4572	0.7181	0.5759	0.9794
Ag	17.8015	4.6483	1.1138	1.5625	0.9621
Ir	9.9810	-5.1590	2.2389	380784	0.8317
Cu	675.4554	-1.0408	-0.0005	-0.0001	0.9423
Pt	5.6015	-3.8436	0.5865	0.3142	0.9528
Au	-21.0411	-72.2115	1.1591	2.1030	0.9559
Ru hcp	9.9397	-3.1276	2.5862	78.6354	0.9852
Ru fcc	7.1547	107685.4046	6.7125	4079328.7943	0.8195
W	9.1743	-514.4266	4.0125	449.9303	0.9829
Surface energy parameters					
Pd	2.5958	-1897.0355	4.4287	22118.5298	0.9771
Ag	1.9391	-5.9966	1.1345	6.0697	0.9390
Ir	33.5081	438.5018	1.9294	16.6052	0.9701
Cu	2.2952	514500807741.7106	12.3881	9899241901288.1400	0.7406
Pt	4.2498	-16.4891	2.6691	163.9623	0.9783
Au	2.3787	31.0056	2.8897	556.5603	0.9913
Ru hcp	3.9568	6723228.021	9.1560	1951497087.0471	0.9868
Ru fcc	-184.1913	-237.9911	1.0567	1.2188	0.9745
W	4.3964	-7669.2043	7.0222	490623.7437	0.9418

Table 1: Lorentzian parameters describing the surface are and surface energy of transition metal atoms forming a surface.

Table S2: Validation set for Lorentzian trends.

The table provide details on the nature of the slabs used in the validation set for the metal slabs. Predictions were obtained using the parameters given in the table S1 and the average CN on the surface of the slab, $\langle CN \rangle$:

$$\gamma_{val} = a - \frac{b + \langle CN \rangle^c}{d} \#(2)$$

Metal	Surface, dimension	Defect	DFT-γ (J/m²)	Predicted-γ (J/m²)
Ir	(100), *5x5*	1 adatom	3.545	3.430
Ir		2 adatoms	3.738	3.653
Ir		3 adatoms	3.685	3.597
Ir	(100), *5x5*	Pristine	3.218	2.863
Ir		1 vacancy	3.232	2.899
Ir	(014), *1x3*	Pristine	3.381	3.084
Ir	(611), *1x3*	Pristine	3.244	2.863
Pd	(100), *5x5*	2 vacancies	2.001	2.136
Pd		4 adatoms, square	1.947	2.192
Pd		1 adatom	2.137	2.229
Pd		2 adatoms	2.123	2.210
Pd		5 adatoms, tetrahedron	2.137	2.193
Pd	(111), *5x5*	3 vacancies, linear	1.916	1.945
Pd		2 vacancies non-adjacent	1.545	1.919
Pd		3 vacancies, triangular	1.947	1.959
Pd	(110), *3x4*	Pristine	1.881	1.950
Pd		1 vacancy	1.890	1.980
Pd		2 vacancies	1.863	1.919
Pd	(210), *3x3*	Pristine	2.020	2.090
Pd	(310), *3x3*	Pristine	2.002	2.037
Pd	(730), *1x4*	Pristine	2.018	2.067
Pd	(311), *2x4*	Pristine	1.926	1.919
Pt	(100), *5x5*	1 adatom	2.702	2782
Pt		2 adatoms	2.682	2.743
Pt		3 adatoms	2.646	2.706
Pt	(100), *5x5*	Pristine	2.405	2.202
Pt		1 vacancy	2.398	2.227
Pt	(014), *1x3*	Pristine	2.429	2.358
Pt	(611), *1x3*	Pristine	2.353	2.202
Cu	(100), *5x5*	1 adatom	2.304	2.228
Cu		2 adatoms	2.285	2.226
Cu		3 adatoms	2.263	2.224
Cu	(100), *5x5*	Pristine	1.992	2.176
Cu		1 vacancy	2.164	2.180
Cu	(014), *1x3*	Pristine	2.195	2.196
Cu	(611), *1x3*	Pristine	2.120	2.176
Ag	(100), *5x5*	1 adatom	1.283	1.184
Ag		2 adatoms	1.278	1.165
Ag		3 adatoms	1.271	1.148
Ag	(100), *5x5*	Pristine	1.130	0.934
Ag		1 vacancy	1.137	0.944
Ag	(014), *1x3*	Pristine	1.218	0.997

Ag	(611), *1x3*	Pristine	1.180	0.934
Au	(100), *5x5*	1 adatom	1.513	1.592
Au		2 adatoms	1.502	1.172
Au		3 adatoms	1.491	1.553
Au	(100), *5x5*	Pristine	1.343	1.295
Au		1 vacancy	1.350	1.308
Au	(014), *1x3*	Pristine	1.400	1.375
Au	(611), *1x3*	Pristine	1.363	1.295
Ru, fcc	(111), *5x5*	2 vacancies	2.912	2.746
Ru, fcc		3 vacancies	2.896	2.817
Ru, fcc	(100), *5x5*	1 adatom	3.674	3.690
Ru, fcc		2 adatoms	3.612	3.618
Ru, fcc		3 adatoms	3.561	3.376
Ru, fcc	(611), *1x3*	Pristine	3.104	2.711
Ru, hcp	(010), *3x4*	Pristine	3.685	3.802
Ru, hcp		1 vacancy	3.472	3.787
Ru, hcp	(011), *4x3*	1 vacancy	3.528	3.724
Ru, hcp		2 vacancies	3.430	3.707
Ru, hcp	(012), *4x2*	Pristine	3.432	3.715
Ru, hcp	(023), *4x1*	Pristine	3.538	3.727
W	(013), *4x1*	Pristine	4.449	4.247
W	(121), *4x2*	Pristine	3.934	3.818
W	(210), *2x4*	Pristine	4.407	4.152
W	(110), *3x4*	1 adatom	4.185	3.760
W		2 adatoms	4.237	3.760
W		3 adatoms	4.188	3.870
W	(111), *3x4*	Pristine	4.185	3.818
W		1 vacancy	3.911	3.703

Table 2: Slabs used to validate the Lorentzian trends predicting surface energy of a metal atom on a slab.

Table S3: Surface energy of low-index fcc-surfaces computed from DFT + tilling scheme, predicted and from literature.

The table S3 compares the surface energies of low-index surfaces of fcc-metals ((111), (001) and (110) surfaces) predicted by 1) the Lorentzian trends, 2) the DFT + tilling scheme developed in this work, and 3) the surface energy taken from literature (Vitos *et al.*, ref. 26 on the main article).

	γ-prediction (J/m²)	**γ-DFT (J/m²)**	**γ-literature (J/m²)**
Ir(111)	2.863	3.280	2.971
Ir(100)	3.818	3.712	3.722
Ir(110)	2.863	3.218	3.606
Pd(111)	1.919	2.003	1.920
Pd(100)	2.229	2.130	2.326
Pd(110)	1.919	1.863	2.225
Pt(111)	2.202	2.402	2.229
Pt(100)	2.782	2.723	2.734

Pt(110)	2.202	2.405	2.819
Cu(111)	2.176	2.210	1.952
Cu(100)	2.228	2.292	2.166
Cu(110)	2.176	2.192	2.237
Ag(111)	0.934	1.218	1.172
Ag(100)	1.184	1.210	1.200
Ag(110)	0.934	1.130	1.238
Au(111)	1.295	1.367	1.283
Au(100)	1.592	1.510	1.627
Au(110)	1.295	1.343	1.321

Table 3: Comparison of the fcc low-index surface energy predicted by the Lorentzian trends, DFT + tiling scheme vs. the literature data taken from Vitos et al.