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

Supplementary Information

Robustness of Surface Activity Electronic Structure-Based Descriptors of Transition Metals

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Figure S1. Exemplary *d*-PDOS representation of bulk and (0001) surface of Ti obtained by PBE and the absolute difference between them. The red area belongs to the integral of this difference.

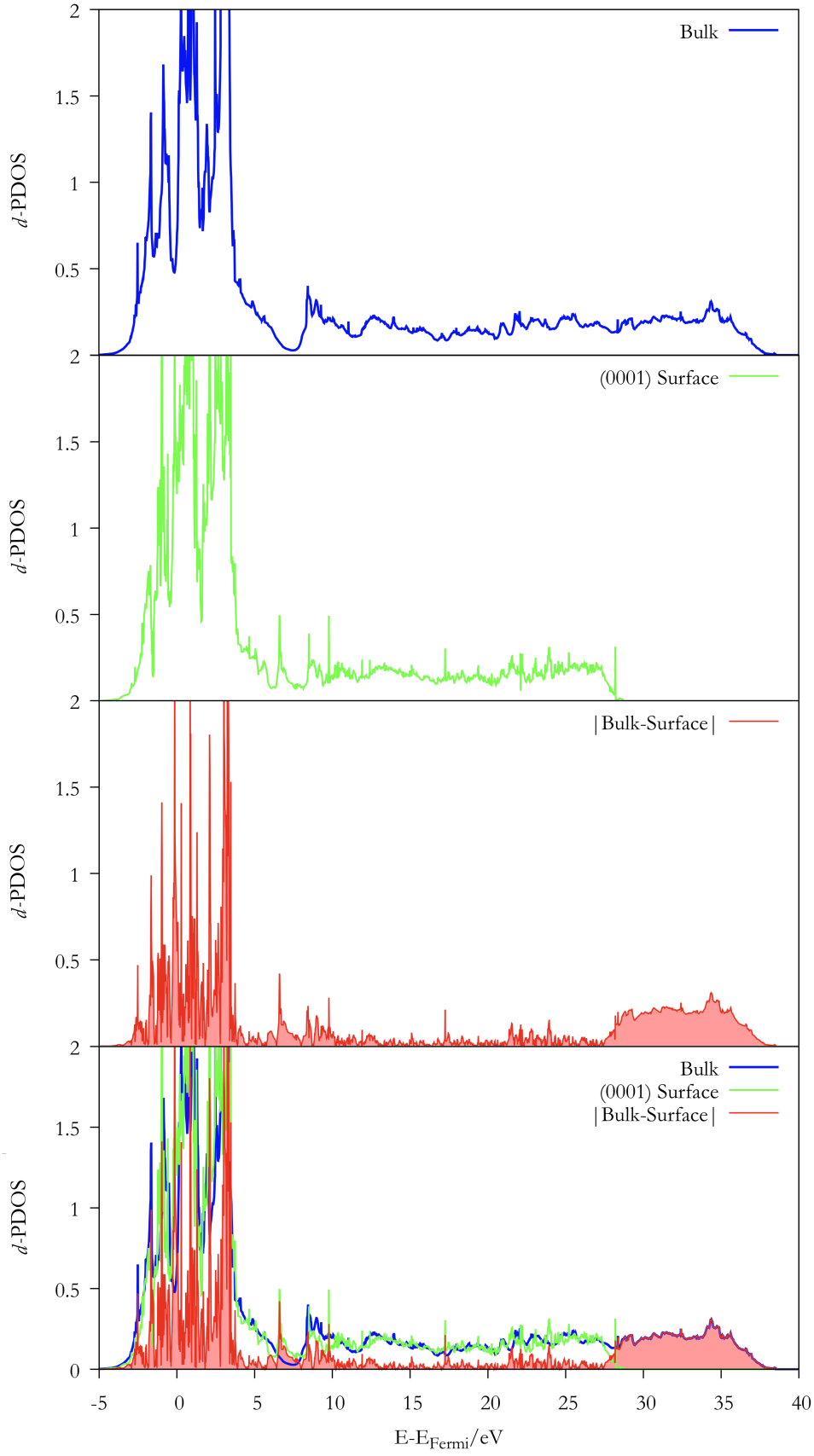

Table S1. Calculated values of ε_d (eV) for all TMs surfaces and density functionals.

ε_d	surfaces	VWN	PBE_{sol}	PBE	RPBE	TPSS
Zr	(0001)	3.52	3.23	3.00	3.01	2.73
	$(10\bar{1}0)$	3.43	3.40	3.04	2.83	2.52
	$(11\bar{2}0)$	3.19	2.93	2.41	2.55	2.19
Zn	(0001)	-7.40	-7.26	-7.21	-7.12	-7.54
	$(10\bar{1}0)$	-7.14	-7.00	-6.97	-6.92	-7.45
	$(11\bar{2}0)$	-7.34	-7.18	-7.12	-7.01	-7.47
Y	(0001)	4.83	4.26	3.80	3.42	3.17
	$(10\bar{1}0)$	4.56	3.94	3.63	3.12	3.09
	$(11\bar{2}0)$	3.82	3.34	3.08	2.76	2.65
Ti	(0001)	3.74	3.38	3.07	2.91	3.42
	$(10\bar{1}0)$	3.73	3.33	2.96	2.72	3.30
	$(11\bar{2}0)$	3.15	2.70	2.42	2.36	2.94
Tc	(0001)	-0.62	-0.52	-0.50	-0.50	-0.51
	$(10\bar{1}0)$	-0.64	-0.55	-0.68	-0.53	-0.56
	$(11\bar{2}0)$	-0.94	-0.87	-0.84	-0.86	-0.83
Sc	(0001)	5.07	4.32	3.61	3.28	3.92
	$(10\bar{1}0)$	4.33	4.08	3.71	3.15	3.72
	$(11\bar{2}0)$	3.83	3.35	3.16	2.74	2.97
Ru	(0001)	-1.53	-1.47	-1.42	-1.37	-1.45
	$(10\bar{1}0)$	-1.40	-1.38	-1.29	-1.27	-1.77
	$(11\bar{2}0)$	-1.37	-1.34	-1.27	-1.24	-1.32
Re	(0001)	1.34	1.27	1.22	1.04	1.46
	$(10\bar{1}0)$	1.22	1.09	0.99	1.11	0.64
	$(11\bar{2}0)$	1.03	0.93	0.84	0.68	1.13
Os	(0001)	-0.42	-0.42	-0.43	-0.41	-0.41
	$(10\bar{1}0)$	-0.33	-0.36	-0.35	-0.32	-0.38
	$(11\bar{2}0)$	-0.24	-0.45	-0.41	-0.35	-0.30
Hf	(0001)	3.50	3.15	2.91	2.81	3.80
	$(10\bar{1}0)$	3.34	2.98	2.71	2.56	3.50
	$(11\bar{2}0)$	2.82	2.56	2.26	2.16	3.06
Co	(0001)	-0.58	-0.58	-0.51	-0.51	-1.05
	$(10\bar{1}0)$	-0.74	-0.71	-0.60	-0.61	-1.21
	$(11\bar{2}0)$	-0.95	-0.74	-0.74	-0.74	-0.44
Cd	(0001)	-8.76	-8.71	-8.70	-8.71	-7.60
	$(10\bar{1}0)$	-8.51	-8.49	-8.63	-8.54	-7.36
	$(11\bar{2}0)$	-8.64	-8.58	-8.48	-8.48	-7.64
Rh	(001)	-1.70	-1.63	-1.52	-1.46	-1.64
	(011)	-1.73	-1.68	-1.56	-1.53	-1.90
	(111)	-1.85	-1.77	-1.64	-1.60	-1.76
Pt	(001)	-2.28	-2.19	-2.03	-1.97	-2.01
	(011)	-2.26	-2.19	-2.04	-1.97	-1.99
	(111)	-2.39	-2.31	-2.16	-2.08	-2.15
Pd	(001)	-2.00	-1.90	-1.72	-1.64	-1.70
	(011)	-1.96	-1.87	-1.72	-1.66	-1.73
	(111)	-2.10	-2.01	-1.83	-1.74	-1.90

Ni	(001)	-1.54	-1.49	-1.39	-1.34	-1.72
	(011)	-1.36	-1.33	-1.26	-1.21	-1.47
	(111)	-1.82	-1.77	-1.65	-1.59	-2.03
Ir	(001)	-0.78	-0.73	-0.63	-0.60	-0.47
	(011)	-0.77	-0.75	-0.69	-0.61	-0.45
	(111)	-0.94	-1.08	-0.99	-0.80	-0.75
Cu	(001)	-2.54	-2.41	-2.29	-2.25	-2.83
	(011)	-2.51	-2.35	-2.29	-2.20	-2.76
	(111)	-2.81	-2.69	-2.56	-2.48	-3.13
Au	(001)	-3.43	-3.36	-3.21	-3.14	-3.28
	(011)	-3.39	-3.34	-3.21	-3.15	-3.34
	(111)	-3.63	-3.55	-3.39	-3.32	-3.57
Ag	(001)	-4.03	-3.96	-3.87	-3.83	-3.51
	(011)	-4.04	-3.96	-3.91	-3.89	-3.32
	(111)	-4.21	-4.13	-4.05	-4.01	-3.73
W	(001)	1.88	2.74	2.54	2.40	2.61
	(011)	1.25	2.07	1.93	1.84	1.93
	(111)	1.88	2.95	2.63	2.44	2.92
V	(001)	2.83	3.32	3.26	3.05	3.08
	(011)	3.45	4.00	3.73	3.63	4.04
	(111)	3.51	4.05	3.97	3.97	2.81
Ta	(001)	2.20	2.12	1.99	1.78	2.41
	(011)	3.03	2.10	2.95	2.53	2.24
	(111)	3.08	2.97	2.77	2.64	3.44
Nb	(001)	0.56	0.54	0.50	0.51	0.49
	(011)	1.00	0.97	0.92	0.90	0.92
	(111)	1.05	1.01	0.98	0.96	0.90
Mo	(001)	0.16	0.21	0.14	0.12	0.13
	(011)	-0.27	-0.27	-0.27	-0.27	-0.26
	(111)	-0.09	-0.10	-0.12	-0.12	-0.14
Fe	(001)	-0.24	0.38	0.47	0.49	-0.84
	(011)	0.47	0.79	0.67	1.12	-0.25
	(111)	0.23	0.46	0.19	0.44	-1.11
Cr	(001)	-0.03	-0.01	0.01	0.01	-0.17
	(011)	-0.29	-0.26	-0.28	-0.28	-0.26
	(111)	-0.20	-0.12	-0.16	-0.16	-0.14

Table S2. Calculated values of ε_d^W (eV) for all TMs surfaces and density functionals

ε_d^W	surfaces	VWN	PBE_{sol}	PBE	RPBE	TPSS
Zr	(0001)	13.89	12.87	12.26	12.26	11.16
	$(10\bar{1}0)$	13.83	13.73	12.58	11.84	10.61
	$(11\bar{2}0)$	13.35	12.42	10.86	11.26	9.82
Zn	(0001)	-1.76	-1.79	-2.04	-2.21	-2.07
	$(10\bar{1}0)$	-2.20	-2.21	-2.43	-2.56	-1.79
	$(11\bar{2}0)$	-2.15	-2.16	-2.35	-2.44	-2.41
Y	(0001)	15.92	13.87	12.27	11.09	10.04
	$(10\bar{1}0)$	17.07	12.79	11.93	10.33	9.89
	$(11\bar{2}0)$	12.78	11.25	10.47	9.41	8.60
Ti	(0001)	16.77	15.71	14.71	14.16	16.02
	$(10\bar{1}0)$	16.90	15.71	14.51	13.68	15.83
	$(11\bar{2}0)$	15.22	13.88	12.99	12.83	14.93
Tc	(0001)	5.19	6.41	6.15	5.98	5.99
	$(10\bar{1}0)$	4.69	5.92	5.35	5.60	5.32
	$(11\bar{2}0)$	4.78	5.85	5.73	5.37	5.28
Sc	(0001)	18.08	16.30	14.22	13.01	15.11
	$(10\bar{1}0)$	18.27	15.77	14.67	12.77	15.35
	$(11\bar{2}0)$	15.20	13.73	13.07	11.61	12.36
Ru	(0001)	4.73	5.00	4.48	4.79	4.48
	$(10\bar{1}0)$	5.09	4.99	4.83	4.88	35.86
	$(11\bar{2}0)$	5.33	5.26	5.07	5.15	5.04
Re	(0001)	14.94	14.73	14.31	13.60	14.78
	$(10\bar{1}0)$	14.60	14.04	13.50	13.95	11.77
	$(11\bar{2}0)$	14.97	14.52	14.01	13.54	14.31
Os	(0001)	12.46	12.19	12.06	11.95	12.06
	$(10\bar{1}0)$	12.42	12.75	11.95	11.99	11.84
	$(11\bar{2}0)$	12.99	12.14	11.94	12.07	12.35
Hf	(0001)	14.11	12.53	11.88	11.49	15.57
	$(10\bar{1}0)$	13.74	12.27	11.33	10.69	14.81
	$(11\bar{2}0)$	12.28	11.15	10.00	9.60	13.74
Co	(0001)	8.03	7.99	7.97	7.81	7.98
	$(10\bar{1}0)$	7.35	7.94	7.34	7.22	7.66
	$(11\bar{2}0)$	6.31	7.05	6.87	6.84	7.34
Cd	(0001)	-3.64	-3.72	-3.82	-3.90	-2.76
	$(10\bar{1}0)$	-3.67	-3.74	-3.87	-3.91	-2.83
	$(11\bar{2}0)$	-3.72	-3.75	-3.81	-3.88	-3.06
Rh	(001)	4.57	4.87	4.80	4.87	4.39
	(011)	4.63	4.57	4.57	4.36	4.54
	(111)	3.81	3.87	3.84	3.68	3.86
Pt	(001)	3.87	4.11	4.08	4.05	4.04
	(011)	3.84	3.85	3.74	3.77	3.77
	(111)	3.58	3.69	3.80	3.79	3.56

Pd	(001)	1.60	1.60	1.53	1.49	1.61
	(011)	1.50	1.50	1.42	1.94	1.44
	(111)	1.54	1.53	1.47	1.43	2.01
Ni	(001)	5.09	5.87	4.97	5.77	5.00
	(011)	5.06	5.84	4.88	5.71	4.94
	(111)	4.65	4.60	4.51	4.50	5.29
Ir	(001)	12.18	12.16	12.04	11.98	11.92
	(011)	12.19	12.08	11.84	11.96	12.10
	(111)	12.50	11.30	11.22	12.11	11.34
Cu	(001)	2.24	3.11	2.14	2.92	2.26
	(011)	2.17	3.05	2.06	2.87	1.96
	(111)	2.10	2.09	2.00	1.94	2.92
Au	(001)	1.42	1.34	1.20	1.11	1.22
	(011)	1.32	1.24	1.09	0.99	1.10
	(111)	1.34	1.25	1.12	1.03	1.10
Ag	(001)	-0.08	-0.18	-0.34	-0.48	0.71
	(011)	-0.16	-0.24	-0.44	-0.57	0.45
	(111)	-0.14	-0.24	-0.41	-0.54	0.62
W	(001)	14.16	17.57	16.84	16.21	16.48
	(011)	12.65	15.93	15.27	14.92	15.27
	(111)	8.44	11.92	10.77	10.52	11.79
V	(001)	15.79	16.67	15.83	15.95	15.29
	(011)	16.99	17.89	16.66	16.98	17.80
	(111)	12.21	12.40	12.29	12.77	10.05
Ta	(001)	12.38	11.98	11.39	10.13	13.55
	(011)	14.33	11.86	13.88	12.30	14.02
	(111)	10.22	9.80	9.10	9.59	12.22
Nb	(001)	5.90	5.78	5.50	5.41	5.42
	(011)	6.81	6.62	6.32	6.18	6.24
	(111)	3.75	6.85	3.23	3.16	2.92
Mo	(001)	6.22	6.61	5.89	5.72	5.78
	(011)	5.45	5.38	5.12	4.96	5.00
	(111)	2.24	2.15	1.96	1.97	0.16
Fe	(001)	7.63	9.46	10.01	9.46	7.32
	(011)	9.94	10.79	10.22	10.63	7.22
	(111)	7.34	6.04	8.58	8.99	4.40
Cr	(001)	5.33	5.41	5.55	5.38	4.86
	(011)	5.64	5.46	5.33	4.97	6.31
	(111)	0.98	0.55	-0.09	-0.16	0.55

Table S3. Calculated values of ε_u (eV) for all TMs surfaces and density functionals.

ε_u	surfaces	VWN	PBE_{sol}	PBE	RPBE	TPSS
Zr	(0001)	4.97	12.23	4.60	4.72	5.21
	$(10\bar{1}0)$	3.15	-0.91	-0.38	5.57	1.23
	$(11\bar{2}0)$	3.29	2.91	0.08	2.69	2.93
Zn	(0001)	-7.04	-6.92	-6.92	-6.84	-7.24
	$(10\bar{1}0)$	-6.72	-6.61	-6.80	-6.83	-6.94
	$(11\bar{2}0)$	-6.89	-6.77	-6.76	-6.68	-7.12
Y	(0001)	2.29	2.44	5.51	5.16	0.42
	$(10\bar{1}0)$	3.94	2.40	4.38	3.33	5.68
	$(11\bar{2}0)$	3.36	3.14	2.98	2.89	3.19
Ti	(0001)	3.77	3.66	2.95	1.51	3.34
	$(10\bar{1}0)$	0.66	3.45	3.20	3.16	3.32
	$(11\bar{2}0)$	3.71	3.55	3.36	3.24	2.31
Tc	(0001)	3.25	-0.59	-0.59	-0.56	-0.57
	$(10\bar{1}0)$	2.13	2.12	2.13	2.57	1.94
	$(11\bar{2}0)$	3.27	-1.39	1.21	1.18	2.93
Sc	(0001)	3.59	4.07	3.27	3.19	3.36
	$(10\bar{1}0)$	3.18	2.12	2.77	2.78	3.83
	$(11\bar{2}0)$	2.63	2.48	2.36	2.32	2.50
Ru	(0001)	0.92	1.75	0.84	-1.47	0.88
	$(10\bar{1}0)$	-1.62	-1.59	0.88	0.86	-1.46
	$(11\bar{2}0)$	-0.37	1.26	1.58	-2.68	1.50
Re	(0001)	4.44	3.77	16.41	0.58	4.75
	$(10\bar{1}0)$	-2.10	2.69	3.37	-3.54	4.06
	$(11\bar{2}0)$	-4.32	-1.58	2.28	2.01	0.23
Os	(0001)	2.30	-1.68	2.18	2.15	-1.71
	$(10\bar{1}0)$	1.43	-3.01	1.34	2.66	-2.26
	$(11\bar{2}0)$	0.66	1.57	-0.10	0.60	-0.10
Hf	(0001)	11.87	11.38	5.70	-1.22	7.37
	$(10\bar{1}0)$	3.71	6.66	2.61	2.56	7.65
	$(11\bar{2}0)$	3.55	3.25	3.30	3.22	3.28
Co	(0001)	-1.10	-2.35	-3.81	-2.38	-1.75
	$(10\bar{1}0)$	-1.50	-0.41	-1.66	-1.72	-1.54
	$(11\bar{2}0)$	-2.93	-3.61	-0.73	-1.54	-0.38
Cd	(0001)	-8.32	-8.29	-8.38	-8.40	-6.99
	$(10\bar{1}0)$	-8.25	-8.35	-8.30	-8.40	-6.96
	$(11\bar{2}0)$	-8.76	-8.11	-8.09	-8.13	-7.28
Rh	(001)	0.49	0.47	0.79	0.76	0.89
	(011)	0.47	0.64	0.25	0.23	0.71
	(111)	-4.44	0.37	-3.64	0.34	-0.37
Pt	(001)	-3.31	-3.23	-0.85	0.19	0.14
	(011)	-0.26	0.09	0.09	-0.27	0.10
	(111)	0.31	0.30	-0.19	-0.19	0.30

Pd	(001)	-1.50	-0.21	-1.39	-0.08	-10.38
	(011)	0.00	0.00	0.00	0.00	0.00
	(111)	-0.22	-0.21	0.00	0.00	0.00
Ni	(001)	-2.13	-0.17	-2.03	-0.27	-4.35
	(011)	-2.56	-0.30	-0.45	-0.39	-0.49
	(111)	-1.78	-2.00	-2.27	-1.51	-12.91
Ir	(001)	-0.39	-0.37	-0.35	-0.35	0.80
	(011)	1.01	-0.10	1.69	1.66	0.86
	(111)	1.67	-2.65	-2.86	1.52	1.21
Cu	(001)	-2.52	-1.34	-1.46	-1.31	-1.69
	(011)	-1.51	-1.30	-1.44	-1.27	-1.68
	(111)	-1.85	-1.70	-1.72	-1.69	-1.85
Au	(001)	-1.43	-4.15	-3.09	-1.90	-3.13
	(011)	-1.68	-1.70	-1.75	-1.81	-1.88
	(111)	-2.10	-2.03	-2.08	-2.91	-4.09
Ag	(001)	-2.86	-2.86	-3.19	-2.93	-2.03
	(011)	-2.83	-3.49	-2.92	-2.96	-2.19
	(111)	-3.02	-3.02	-5.13	-4.98	-2.41
W	(001)	0.04	0.05	0.07	2.77	4.25
	(011)	3.99	4.03	3.89	2.79	3.89
	(111)	-3.13	-5.39	-1.34	2.54	-2.30
V	(001)	0.54	3.41	0.46	3.14	0.93
	(011)	2.66	3.62	3.01	3.35	2.87
	(111)	1.98	1.53	1.85	0.00	0.00
Ta	(001)	4.70	4.78	4.61	4.36	2.37
	(011)	13.16	0.54	5.04	4.86	5.08
	(111)	5.99	0.47	2.53	1.54	2.77
Nb	(001)	0.59	0.59	0.58	4.04	0.57
	(011)	4.44	4.71	4.29	4.42	4.56
	(111)	5.03	4.94	3.17	0.71	2.33
Mo	(001)	-0.24	-2.91	-0.21	-0.21	2.61
	(011)	2.31	-1.53	2.74	2.70	3.48
	(111)	3.66	3.59	2.49	-1.39	1.35
Fe	(001)	-1.34	-2.29	-2.15	-1.32	-13.58
	(011)	2.11	-4.16	0.07	-0.01	-12.08
	(111)	-0.93	-0.94	-2.77	-3.05	1.80
Cr	(001)	1.54	1.43	1.44	1.43	2.07
	(011)	2.88	-0.61	2.24	1.41	1.76
	(111)	1.51	-2.88	-0.84	-1.58	-0.40

Table S4. Calculated values of ε_d (eV) for all TMs surfaces by a set of density functionals optimized using PBE structure.

ε_d	surfaces	VWN	PBE_{sol}	RPBE	TPSS
Zr	(0001)	3.19	2.99	3.02	2.65
	$(10\bar{1}0)$	2.95	2.93	2.91	2.55
	$(11\bar{2}0)$	2.60	2.40	2.58	2.19
Zn	(0001)	-7.26	-7.17	-7.21	-7.40
	$(10\bar{1}0)$	-7.02	-6.93	-6.97	-7.24
	$(11\bar{2}0)$	-7.15	-7.08	-7.12	-7.36
Y	(0001)	3.93	3.81	3.76	3.20
	$(10\bar{1}0)$	3.65	3.67	3.42	3.04
	$(11\bar{2}0)$	3.10	3.14	3.00	2.60
Ti	(0001)	3.30	3.11	3.16	3.22
	$(10\bar{1}0)$	3.14	3.03	2.97	2.98
	$(11\bar{2}0)$	2.86	2.59	2.63	2.94
Tc	(0001)	-0.59	-0.51	-0.51	-0.50
	$(10\bar{1}0)$	-0.76	-0.69	-0.69	-0.73
	$(11\bar{2}0)$	-0.95	-0.87	-0.88	-0.86
Sc	(0001)	4.20	3.89	3.87	3.54
	$(10\bar{1}0)$	3.95	3.45	3.46	3.45
	$(11\bar{2}0)$	3.49	3.10	3.13	2.78
Ru	(0001)	-1.41	-1.41	-1.40	-1.43
	$(10\bar{1}0)$	-1.32	-1.28	-1.28	-1.32
	$(11\bar{2}0)$	-1.29	-1.28	-1.26	-1.30
Re	(0001)	1.25	1.23	1.20	1.41
	$(10\bar{1}0)$	1.08	1.01	0.99	0.65
	$(11\bar{2}0)$	0.94	0.85	0.90	1.19
Os	(0001)	-0.40	-0.52	-0.42	-0.40
	$(10\bar{1}0)$	-0.38	-0.35	-0.35	-0.32
	$(11\bar{2}0)$	-0.25	-0.40	-0.28	-0.49
Hf	(0001)	2.99	2.88	2.85	2.82
	$(10\bar{1}0)$	2.77	2.74	2.67	2.71
	$(11\bar{2}0)$	2.30	2.23	2.29	2.40
Co	(0001)	-0.50	-0.52	-0.59	-1.00
	$(10\bar{1}0)$	-0.62	-0.66	-0.62	-1.17
	$(11\bar{2}0)$	-0.70	-0.75	-0.75	-0.46
Cd	(0001)	-8.59	-8.62	-8.76	-7.45
	$(10\bar{1}0)$	-8.52	-8.54	-8.68	-7.25
	$(11\bar{2}0)$	-8.35	-8.41	-8.55	-7.03
Rh	(001)	-1.53	-1.55	-1.52	-1.56
	(011)	-1.58	-1.58	-1.57	-1.59
	(111)	-1.66	-1.68	-1.64	-1.69
Pt	(001)	-2.05	-2.05	-2.02	-2.05
	(011)	-2.06	-2.05	-2.04	-2.07
	(111)	-2.15	-2.14	-2.18	-2.23
Pd	(001)	-1.74	-1.74	-1.73	-1.76
	(011)	-1.73	-1.72	-1.75	*a*
	(111)	-1.84	-1.85	-1.83	-1.90
	(001)	-1.37	-1.40	-1.40	-1.45

Ni	(011)	-1.21	-1.26	-1.27	-1.32
	(111)	-1.65	-1.66	-1.67	-1.74
Ir	(001)	-0.66	-0.65	-0.63	-0.41
	(011)	-0.66	-0.66	-0.64	-0.42
	(111)	-0.84	-0.99	-0.82	-0.70
Cu	(001)	-2.33	-2.30	-2.32	-2.37
	(011)	-2.32	-2.25	-2.27	-2.29
	(111)	-2.59	-2.54	-2.57	-2.59
Au	(001)	-3.15	-3.16	-3.23	-3.22
	(011)	-3.15	-3.18	-3.23	-3.24
	(111)	-3.35	-3.37	-3.42	-3.41
Ag	(001)	-3.77	-3.81	-3.92	-3.30
	(011)	-3.82	-3.86	-3.98	-3.30
	(111)	-3.98	-3.99	-4.10	-3.46
W	(001)	1.81	2.52	2.52	2.88
	(011)	1.17	1.92	1.86	1.98
	(111)	1.75	2.59	2.59	3.12
V	(001)	2.47	3.19	3.17	3.20
	(011)	3.09	3.74	3.72	3.76
	(111)	3.31	4.02	3.87	3.99
Ta	(001)	1.98	2.03	1.98	2.01
	(011)	2.94	2.97	2.88	2.22
	(111)	2.74	2.75	2.76	2.92
Nb	(001)	0.51	0.51	0.51	0.50
	(011)	0.93	0.92	0.93	0.94
	(111)	0.97	0.96	0.92	0.96
Mo	(001)	0.12	0.14	0.16	0.17
	(011)	-0.25	-0.26	-0.26	-0.25
	(111)	-0.12	-0.12	-0.11	-0.19
Fe	(001)	0.34	0.42	0.45	-8.06
	(011)	0.53	0.64	0.76	-0.11
	(111)	0.47	0.44	0.45	-1.55
Cr	(001)	-0.01	-0.03	0.02	-0.05
	(011)	-0.29	-0.28	-0.27	-0.25
	(111)	-0.18	-0.12	-0.14	-0.15

[a] in this particular case there were strong problems of electronic convergence, while trying to force a meta-GGA solution on a GGA optimized structure.

Table S2. Calculated values of ε_d^W (eV) for all TMs surfaces by a set of density functionals optimized using PBE structure.

ε_d^W	surfaces	VWN	PBE_{sol}	RPBE	TPSS
Zr	(0001)	12.93	12.24	12.29	10.87
	$(10\bar{1}0)$	12.30	12.19	11.99	10.73
	$(11\bar{2}0)$	11.40	10.62	11.33	9.74
Zn	(0001)	-2.09	-2.00	-2.04	-2.33
	$(10\bar{1}0)$	-2.48	-2.39	-2.43	-1.94
	$(11\bar{2}0)$	-2.39	-2.31	-2.35	-2.66
Y	(0001)	12.96	12.36	12.09	10.10
	$(10\bar{1}0)$	12.10	12.06	11.20	10.26
	$(11\bar{2}0)$	10.70	10.67	10.17	8.48
Ti	(0001)	15.50	14.84	14.99	15.40
	$(10\bar{1}0)$	15.08	14.72	14.53	14.76
	$(11\bar{2}0)$	14.43	13.59	13.75	15.01
Tc	(0001)	5.01	6.12	6.10	6.69
	$(10\bar{1}0)$	4.27	5.40	5.32	5.27
	$(11\bar{2}0)$	4.47	5.57	5.34	5.72
Sc	(0001)	16.05	15.11	15.06	13.90
	$(10\bar{1}0)$	17.28	13.79	13.80	14.50
	$(11\bar{2}0)$	14.39	12.94	12.94	11.59
Ru	(0001)	4.79	4.91	4.82	4.62
	$(10\bar{1}0)$	4.58	5.02	4.83	4.61
	$(11\bar{2}0)$	5.02	5.09	5.07	5.01
Re	(0001)	14.52	14.39	14.22	14.63
	$(10\bar{1}0)$	13.90	13.61	13.50	11.48
	$(11\bar{2}0)$	14.44	14.08	14.25	14.41
Os	(0001)	12.07	11.59	12.02	12.10
	$(10\bar{1}0)$	11.75	11.99	12.01	11.37
	$(11\bar{2}0)$	12.43	12.00	12.49	11.52
Hf	(0001)	12.34	11.80	11.58	12.30
	$(10\bar{1}0)$	11.65	11.47	11.10	12.10
	$(11\bar{2}0)$	10.33	9.89	10.03	11.37
Co	(0001)	7.81	7.88	7.74	8.19
	$(10\bar{1}0)$	7.26	7.81	7.31	7.53
	$(11\bar{2}0)$	6.74	6.86	6.92	9.34
Cd	(0001)	-3.76	-3.78	-3.86	-3.02
	$(10\bar{1}0)$	-3.81	-3.83	-3.90	-2.25
	$(11\bar{2}0)$	-3.73	-3.77	-3.84	-2.98
Rh	(001)	4.95	4.56	4.89	4.36
	(011)	4.54	4.55	4.49	4.41
	(111)	3.79	3.64	3.85	3.68
Pt	(001)	4.07	4.03	4.13	3.99
	(011)	3.75	3.80	3.81	3.63
	(111)	3.76	3.87	2.89	3.50
Pd	(001)	1.56	1.56	1.50	1.67
	(011)	1.46	1.47	1.95	*a*
	(111)	1.51	1.50	1.44	2.03
Ni	(001)	4.97	5.80	5.83	4.69
	(011)	4.89	5.75	5.77	5.13

	(111)	4.46	4.54	4.50	4.70
Ir	(001)	12.03	12.01	12.05	12.02
	(011)	12.00	12.01	12.02	12.01
	(111)	12.21	11.10	12.20	11.36
Cu	(001)	2.10	3.04	3.00	4.27
	(011)	2.03	2.96	2.92	4.27
	(111)	1.96	2.03	1.98	2.39
Au	(001)	1.28	1.26	1.16	1.10
	(011)	1.18	1.14	1.05	0.99
	(111)	1.20	1.16	1.08	1.02
Ag	(001)	-0.22	-0.27	-0.41	1.12
	(011)	-0.31	-0.37	-0.51	0.45
	(111)	-0.31	-0.33	-0.46	0.46
W	(001)	13.89	16.79	16.72	17.48
	(011)	12.15	15.28	15.05	15.06
	(111)	7.99	11.21	11.20	12.49
V	(001)	14.55	16.33	16.27	15.47
	(011)	16.02	17.28	17.23	17.14
	(111)	11.65	12.33	7.95	12.27
Ta	(001)	11.40	11.58	11.29	12.45
	(011)	13.89	13.95	13.54	13.73
	(111)	9.07	9.05	9.96	10.30
Nb	(001)	5.58	5.58	5.56	5.45
	(011)	6.44	6.35	6.35	6.33
	(111)	3.27	3.22	3.02	3.10
Mo	(001)	5.82	5.88	6.07	6.02
	(011)	5.26	5.15	5.14	5.08
	(111)	2.05	1.97	2.03	0.20
Fe	(001)	9.10	9.45	9.51	33.69
	(011)	9.92	10.20	10.40	12.97
	(111)	5.85	9.02	9.07	4.70
Cr	(001)	5.27	5.11	5.56	5.04
	(011)	5.60	5.31	5.33	6.24
	(111)	1.03	0.43	0.20	1.26

[a] in this particular case there were strong problems of electronic convergence, while trying to force a meta-GGA solution on a GGA optimized structure.

Table S3. Calculated values of ε_u (eV)density for all TMs surfaces by a set of density functionals optimized using PBE structure.

ε_u	surfaces	VWN	PBESOL	RPBE	TPSS
Zr	(0001)	3.53	4.62	4.85	5.08
	$(10\bar{1}0)$	2.93	0.63	9.59	5.52
	$(11\bar{2}0)$	4.96	2.61	2.84	2.31
Zn	(0001)	-6.96	-6.86	-6.90	-7.12
	$(10\bar{1}0)$	-6.62	-6.59	-6.81	-6.88
	$(11\bar{2}0)$	-6.79	-6.71	-6.75	-7.00
Y	(0001)	5.69	2.34	2.36	2.54
	$(10\bar{1}0)$	4.35	4.39	3.44	5.58
	$(11\bar{2}0)$	2.93	2.98	3.00	3.28
Ti	(0001)	3.46	2.96	3.34	3.31
	$(10\bar{1}0)$	3.28	3.30	3.28	2.63
	$(11\bar{2}0)$	2.06	2.08	-0.33	2.05
Tc	(0001)	3.09	-0.57	-0.58	3.14
	$(10\bar{1}0)$	2.92	2.14	2.13	1.63
	$(11\bar{2}0)$	1.43	2.42	0.95	-2.00
Sc	(0001)	3.24	3.87	3.70	3.84
	$(10\bar{1}0)$	2.87	2.79	2.80	3.74
	$(11\bar{2}0)$	2.32	2.50	2.38	2.39
Ru	(0001)	1.66	-4.04	1.53	1.73
	$(10\bar{1}0)$	0.88	-1.50	0.52	1.45
	$(11\bar{2}0)$	1.87	-3.20	1.58	0.45
Re	(0001)	6.32	-1.01	3.64	4.73
	$(10\bar{1}0)$	-0.23	2.10	-3.95	2.55
	$(11\bar{2}0)$	-2.76	2.28	-1.53	2.29
Os	(0001)	-3.71	2.15	2.52	2.41
	$(10\bar{1}0)$	-4.18	1.34	1.35	13.32
	$(11\bar{2}0)$	0.31	2.10	-0.10	0.15
Hf	(0001)	6.25	6.31	0.88	10.79
	$(10\bar{1}0)$	3.33	2.60	5.55	10.18
	$(11\bar{2}0)$	0.28	3.29	3.14	2.87
Co	(0001)	-2.35	-0.58	-2.17	-1.67
	$(10\bar{1}0)$	-0.97	-0.50	-3.42	-1.71
	$(11\bar{2}0)$	-0.32	-0.70	-1.52	-0.34
Cd	(0001)	-8.24	-8.28	-8.43	-6.99
	$(10\bar{1}0)$	-8.18	-8.21	-8.42	-6.75
	$(11\bar{2}0)$	-7.95	-8.00	-8.16	-6.63
Rh	(001)	0.80	0.99	-1.51	-0.35
	(011)	0.59	0.59	0.24	0.64
	(111)	-0.91	-3.67	-3.64	0.36
Pt	(001)	-0.85	-0.85	-0.85	0.15
	(011)	-1.41	0.09	0.09	0.09
	(111)	-0.19	-0.71	0.28	-3.71
Pd	(001)	-1.48	0.00	-0.08	-0.01
	(011)	0.00	-0.27	0.00	*a*
	(111)	-0.19	0.00	0.00	0.00
Ni	(001)	-1.99	-0.22	-0.24	-3.74
	(011)	-2.06	-0.32	-0.37	-0.57

	(111)	-2.23	-2.28	-1.92	3.38
Ir	(001)	-0.42	-0.35	-0.35	-0.33
	(011)	-0.08	-0.09	-0.09	-3.18
	(111)	1.55	0.55	1.55	1.17
Cu	(001)	-1.43	-1.30	-1.33	-1.35
	(011)	-2.43	-1.27	-1.30	-1.24
	(111)	-1.76	-1.70	-1.74	-1.62
Au	(001)	-1.84	-1.89	-3.11	-1.94
	(011)	-1.64	-1.71	-1.78	-2.80
	(111)	-2.02	-3.87	-3.91	-3.88
Ag	(001)	-2.86	-3.59	-4.18	-2.07
	(011)	-2.80	-2.84	-4.67	-2.16
	(111)	-4.69	-2.99	-3.11	-2.35
W	(001)	-2.51	3.26	-2.16	-2.57
	(011)	3.87	7.95	2.83	-1.52
	(111)	-1.35	-1.33	-4.54	-3.95
V	(001)	2.63	3.27	3.25	0.52
	(011)	3.04	3.50	3.47	3.48
	(111)	1.90	11.63	0.00	0.00
Ta	(001)	4.38	4.60	4.63	4.35
	(011)	7.65	5.05	5.40	4.72
	(111)	4.44	0.46	0.47	5.12
Nb	(001)	0.57	0.58	0.59	0.57
	(011)	4.27	4.54	3.37	3.43
	(111)	2.19	-0.62	0.71	4.34
Mo	(001)	-0.21	-0.21	-2.79	-0.24
	(011)	2.70	2.31	2.70	2.79
	(111)	0.39	1.84	3.42	-2.76
Fe	(001)	-2.18	-2.35	-2.40	-71.90
	(011)	-2.67	0.22	0.23	-15.52
	(111)	-2.98	-1.02	-1.78	2.33
Cr	(001)	1.45	1.24	1.47	1.42
	(011)	2.83	1.42	1.99	1.78
	(111)	-0.82	-0.83	-1.46	-0.79

[a] in this particular case there were strong problems of electronic convergence, while trying to force a meta-GGA solution on a GGA optimized structure.

Table S4. Bulk-truncated surface and bulk calculations of ε_d at PBE level. All values are given in eV.

hcp				
ε_d	Bulk	(0001)	$(10\bar{1}0)$	$(11\bar{2}0)$
Cd	-9.16	-8.70	-8.57	-8.57
Co	-0.33	-0.45	-0.63	-0.66
Hf	3.07	2.60	2.47	2.36
Os	-0.80	-0.39	-0.37	-0.21
Re	1.02	0.85	0.96	0.75
Ru	-1.73	-1.29	-1.20	-1.19
Sc	4.18	3.24	3.58	3.19
Tc	-0.65	-0.57	-0.65	-0.65
Ti	2.96	2.82	2.65	2.64
Y	4.78	3.48	3.51	2.88
Zn	-7.69	-7.18	-7.10	-7.11
Zr	3.18	2.78	2.76	2.47
fcc				
ε_d	Bulk	(001)	(011)	(111)
Ag	-4.39	-3.84	-3.83	-4.03
Au	-3.83	-3.19	-3.04	-3.40
Cu	-2.86	-2.26	-2.20	-2.55
Ir	-1.52	-0.58	-0.47	-0.91
Ni	-0.64	-1.35	-1.14	-1.66
Pd	-2.42	-1.70	-1.56	-1.83
Pt	-2.73	-1.95	-1.77	-2.20
Rh	-2.19	-1.43	-1.38	-1.59
bcc				
ε_d	Bulk	(001)	(011)	(111)
Cr	-0.48	-0.09	-0.29	0.00
Fe	0.53	0.47	0.55	0.30
Mo	-0.41	0.06	-0.26	0.04
Nb	1.23	0.41	0.88	0.74
Ta	2.97	1.65	3.03	2.10
V	3.88	2.65	3.28	2.90
W	1.94	1.91	1.78	1.78