Supporting information for

Surface activation by electron scavenger metal nanorod adsorption on TiH_2, TiC, TiN, and Ti_2O_3

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Table S1. Information on thin and thick slab hydride models. Units: area in Å^2, cell height and slab thickness in Å, E_{surf} in meV/Å^2, and WF in eV.

Compound	Surface	Area	Cell height		Slab thickness		Number of atoms		E_{surf}		WF	
			Thin	Thick	Thin	Thick	Thin	Thick	Thin	Thick	Thin	Thick
HfH_2	(101)	9.5	29.5	29.5	16.1	18.8	18	21	101.6	101.7	3.86	3.84
LaH_3	(110)	21.4	29.2	29.2	15.6	17.5	32	36	55.5	56.6	2.05	2.04
NbH_2	(111)	8.9	28.8	31.4	15.7	18.3	18	21	88.0	86.8	4.35	4.42
ScH_2	(111)	9.7	30.0	30.0	16.4	19.1	18	21	65.3	65.4	3.50	3.56
TiH_2	(101)	8.3	27.7	30.3	15.1	17.7	18	21	99.5	99.6	4.30	4.29
V_2H	(111)	13.5	28.7	28.7	14.4	16.4	21	24	152.2	152.6	4.46	4.45
VH_2	(111)	11.5	29.7	32.7	17.8	20.8	18	21	58.4	60.0	3.02	3.07
YH_3	(001)	33.9	39.0	45.5	22.8	29.3	84	108	42.4	43.1	4.55	4.55
ZrH_2	(101)	9.8	27.3	32.8	16.4	19.1	18	21	97.0	97.3	3.89	3.86

Table S2. Information on thin and thick slab carbide models. Units: area in Å^2, cell height and slab thickness in Å, E_{surf} in meV/Å^2, and WF in eV.

Compound	Surface	Area	Cell height		Slab thickness		Number of atoms		E_{surf}		WF	
			Thin	Thick	Thin	Thick	Thin	Thick	Thin	Thick	Thin	Thick
HfC	(110)	10.6	30.0	30.0	16.1	18.4	14	16	122.2	121.2	4.36	4.29
La_2C_3	(100)	75.7	30.5	30.5	15.2	17.4	70	80	71.7	71.3	2.40	2.34
LaC_2	(110)	18.0	27.5	27.5	13.7	16.5	15	18	39.5	39.4	2.53	2.51
Nb_2C	$(10\bar{1}1)$	17.6	28.5	28.5	14.2	16.6	18	21	157.8	157.4	4.40	4.39
NbC	(100)	10.0	29.1	29.1	15.7	17.9	14	16	100.2	100.1	3.82	3.86
Sc_2C	(0001)	9.4	32.9	32.9	16.5	22.0	9	12	66.0	65.6	3.74	3.74
Ta_2C	$(10\bar{1}1)$	17.3	28.2	28.2	14.1	16.5	18	21	175.6	175.4	4.51	4.51
TaC	(100)	9.9	28.9	28.9	15.5	17.8	14	16	112.2	110.7	3.70	3.80
TiC	(100)	9.3	28.0	28.0	15.1	17.2	14	16	116.2	115.5	4.66	4.61
V_2C	(111)	44.3	31.7	34.5	17.3	20.1	72	84	194.4	193.9	3.66	3.66
Y_2C	(0001)	11.0	36.5	36.5	18.2	24.3	9	12	51.5	51.3	3.64	3.65
YC_2	(110)	15.8	28.2	28.2	15.4	17.9	18	21	44.4	43.2	2.72	2.69
ZrC	(100)	10.9	28.0	28.0	14.0	16.4	12	14	110.3	110.4	4.21	4.17

Table S3. Information on thin and thick slab nitride models. Units: area in Å^2, cell height and slab thickness in Å, E_{surf} in meV/Å^2, and WF in eV.

Compound	Surface	Area	Cell height		Slab thickness		Number of atoms		E_{surf}		WF	
			Thin	Thick	Thin	Thick	Thin	Thick	Thin	Thick	Thin	Thick
HfN	(100)	10.1	29.2	29.2	15.7	18.0	14	16	110.2	107.4	2.35	2.36
LaN	(100)	13.8	28.9	28.9	15.7	18.4	12	14	32.5	34.3	2.88	2.82
Nb_2N	$(11\bar{2}\bar{2})$	66.6	29.0	29.0	14.5	16.3	72	81	177.0	176.9	3.59	3.59
Nb_4N_3	(100)	37.9	28.5	28.5	15.4	17.6	49	56	111.0	111.0	3.27	3.27
NbN	$(11\bar{2}0)$	14.7	28.0	28.0	14.8	16.2	20	22	198.7	198.9	4.20	4.20
NbN	$(11\bar{2}2)$	21.1	27.8	27.8	15.4	16.5	30	32	196.5	196.5	3.06	3.06
ScN	(100)	9.9	29.0	29.0	15.6	17.8	14	16	86.3	86.4	3.61	3.62
Ta_2N	$(11\bar{2}\bar{2})$	65.6	28.7	28.7	14.4	16.2	72	81	193.6	193.7	3.76	3.75
Ti_2N	(110)	20.9	31.3	34.7	17.4	20.8	30	36	164.7	164.5	3.61	3.61
TiN	(100)	8.9	29.5	29.5	14.8	16.9	14	16	96.0	95.4	3.01	3.03
VN	(100)	8.3	28.6	28.6	14.3	16.3	14	16	62.5	52.2	4.00	4.07
YN	(100)	11.8	29.1	29.1	14.6	17.0	12	14	70.1	70.0	3.23	3.24
ZrN	(100)	10.4	29.6	29.6	15.9	18.2	14	16	100.1	97.7	2.37	2.37

Table S4. Information on thin and thick slab oxide models. Units: area in Å^2, cell height and slab thickness in Å, E_{surf} in meV/Å^2, and WF in eV.

Compound	Surface	Area	Cell height		Slab thickness		Number of atoms		E_{surf}		WF	
			Thin	Thick	Thin	Thick	Thin	Thick	Thin	Thick	Thin	Thick
HfO_2	$(11\bar{1})$	43.2	28.2	31.3	15.7	18.8	60	72	68.9	67.3	6.33	6.35
α-La_2O_3	(111)	220.2	29.3	32.5	16.3	19.5	200	240	40.0	39.3	4.51	4.52
β-La_2O_3	(0001)	13.2	36.2	42.2	24.1	30.2	20	25	41.6	40.1	5.27	5.24
β-La_2O_3	$(10\bar{1}1)$	27.0	32.5	35.4	17.7	20.7	30	35	39.6	38.8	4.68	4.68
Nb_2O_5	(111)	51.3	30.1	33.5	16.7	20.1	70	84	37.6	36.3	7.13	7.11
NbO	(110)	25.2	29.8	32.8	16.9	19.9	34	40	138.8	137.5	3.75	3.73
NbO	(211)	43.6	27.6	31.0	16.1	17.8	56	62	139.3	139.4	3.83	3.84
NbO_2	(110)	20.4	31.6	35.1	17.5	21.0	30	36	53.4	48.8	4.25	4.33
ScO	(100)	9.7	28.6	28.6	15.4	17.6	14	16	58.7	57.6	2.00	1.97
Sc_2O_3	(111)	165.1	31	33.8	16.9	19.7	240	280	60.0	58.7	5.95	5.96
Ta_2O_5	(111)	50.4	29.9	33.2	16.6	19.9	70	84	46.6	44.9	6.92	6.87
Ti_3O	$(10\bar{1}0)$	47.7	30.9	35.3	17.6	22.0	64	80	143.3	142.4	3.21	3.21
Ti_2O	$(10\bar{1}\bar{1})$	15.8	29.2	29.2	15.7	18.0	21	24	109.1	108.2	3.58	3.57
Ti_3O_2	$(11\bar{2}3)$	48.6	29.3	31.5	15.8	18.0	70	80	108.3	107.5	3.66	3.67
Ti_2O_3	$(01\bar{1}2)$	27.8	33.4	37.1	18.5	22.3	50	60	64.8	62.6	3.26	3.26
Rutile-TiO_2	(110)	19.2	29.4	32.6	16.3	19.6	30	36	37.9	29.5	7.19	7.25
Anatase-TiO_2	(101)	19.5	31.8	35.3	17.6	21.2	30	36	31.7	30.1	7.25	7.25
V_2O_5	(001)	41.2	29.4	33.7	16.8	21.0	56	70	0.2	-1.3	8.40	8.33
Y_2O_3	(111)	192.4	27.4	30.4	15.2	18.3	200	240	57.8	56.7	5.27	5.23
ZrO_2	$(11\bar{1})$	44.2	28.5	31.6	15.8	19.0	60	72	59.8	58.2	6.38	6.34

Table S5. Information on thin and thick slab sulfide models. Units: area in Å^2, cell height and slab thickness in Å, E_{surf} in meV/Å^2, and WF in eV.

Compound	Surface	Area	Cell height		Slab thickness		Number of atoms		E_{surf}		WF	
			Thin	Thick	Thin	Thick	Thin	Thick	Thin	Thick	Thin	Thick
Hf_2S	(0001)	9.6	58.3	70.0	40.8	52.5	21	27	154.5	154.5	4.38	4.39
HfS_2	(0001)	11.1	35.7	35.7	17.8	23.8	9	12	1.6	1.5	6.00	5.98
HfS_3	(001)	18.0	54.0	63.0	36.0	45.0	32	40	1.8	1.8	5.62	5.56
LaS	(100)	16.8	29.0	29.0	14.5	17.4	10	12	39.4	40.0	2.28	2.16
Nb_3S_4	$(12\bar{3}0)$	85.0	28.2	31.3	15.7	18.8	70	84	64.3	69.2	5.04	4.92
NbS_3	$(10\bar{1})$	49.0	54.7	63.8	36.4	45.6	96	120	2.6	2.6	5.01	5.01
ScS	(100)	13.2	28.3	28.3	15.4	18.0	12	14	40	41.7	2.96	2.95
TiS	$(10\bar{1}0)$	20.6	30.6	33.4	16.7	19.5	24	28	81.8	82.2	4.04	4.03
TiS_2	(0001)	9.7	39.3	45.0	22.5	28.1	12	15	3.6	3.6	5.84	5.84
TiS_3	(001)	16.5	52.7	61.4	35.1	43.9	32	40	2.2	2.2	5.26	5.26
V_3S	(110)	59.8	39.0	45.5	26.0	32.5	128	160	118.3	118.1	3.46	3.46
V_5S_4	(110)	19.5	37.6	43.8	25.1	31.3	36	45	63.7	63.4	3.67	3.68
VS	(101)	25.7	28.4	32.5	16.2	20.3	32	40	58.4	58.4	4.13	4.13
VS_4	$(11\bar{1})$	73.2	39.9	45.6	22.8	28.5	80	100	2.0	2.0	4.33	4.32
VS_4	(010)	80.4	36.3	41.5	20.8	26.0	80	100	2.1	2.0	4.18	4.16
YS	(100)	14.9	27.3	27.3	13.6	16.4	10	12	39.5	40.1	2.46	2.37
Y_5S_7	$(10\bar{1})$	55.6	33.3	38.1	19.0	23.8	48	60	57.2	57.5	3.85	3.82
ZrS	(001)	12.8	37.9	43.3	21.7	27.1	16	20	25.7	25.8	3.43	3.41
ZrS_2	(0001)	11.4	35.4	35.4	17.7	23.6	9	12	1.9	1.9	6.02	6.02
ZrS_3	(001)	18.3	54.0	63.0	36.0	45.0	32	40	1.9	1.9	5.61	5.64

Table S6. Comparison of calculated (PBEsol) and experimentally obtained work functions of elementary metals. The unit is eV. The experimental values are from Derry et al., Journal of Vacuum Science & Technology A 33, 060801 (2015). The mean error is -0.12 eV. The experimental value for Ru shown with * is for the (100) surface in Table I of Derry et al. However, this value appears to be for the (001) surface based on individual values cited in Table II of Derry et al.

Metal	Crystal	Surface	Calculation	Experiment	Difference
Al	fcc	(111)	4.06	4.32±0.05	-0.26
Zn	hcp	(0001)	4.31		
Ag	fcc	(111)	4.56	4.53±0.07	0.03
Co	hcp	$(1\bar{1}00)$	4.84		
Fe	bcc	(110)	4.93	5.07±0.04	-0.14
Cu	fcc	(111)	4.94	4.90±0.02	0.04
Re	hcp	(0001)	5.07		
Ru	hcp	(0001)	5.13	5.40±0.11*	-0.27
Ni	fcc	(111)	5.22	5.24±0.07	-0.02
Au	fcc	(111)	5.28	5.33±0.06	-0.05
Rh	fcc	(111)	5.29	5.46±0.09	-0.17
Pd	fcc	(111)	5.38	5.67±0.12	-0.29
Ir	fcc	(111)	5.64	5.78±0.04	-0.14
Pt	fcc	(111)	5.84	5.91±0.08	-0.07

Table S7. E_{Hvac}, E_{bulk}, and WF for hydrides plotted in Fig. 6.

	E_{Hvac}(eV/defect)	E_{bulk} (eV/atom)	WF (eV)
ScH_2	1.45	-0.75	3.54
YH_2	1.45	-0.79	3.02
LaH_2	1.39	-0.68	2.66
TiH_2	1.50	-0.58	4.29
ZrH_2	1.60	-0.67	3.89
HfH_2	1.51	-0.60	3.85
VH_2	1.44	-0.30	4.70
NbH_2	1.51	-0.33	4.42
TaH_2	1.32	-0.19	4.25

Table S8. E_{Cvac}, E_{bulk}, and WF for carbides plotted in Fig. 6.

	E_{Cvac}(eV/defect)	E_{bulk} (eV/atom)	WF (eV)
TiC	0.69	-0.85	4.66
ZrC	0.71	-0.92	4.17
HfC	1.09	-1.03	4.36
VC	-0.43	-0.48	4.36
NbC	-0.24	-0.54	3.82
TaC	0.35	-0.66	3.99

Table S9. E_{Nvac}, E_{bulk}, and WF for nitrides plotted in Fig. 6.

	E_{Nvac}(eV/defect)	E_{bulk} (eV/atom)	WF (eV)
ScN	2.86	-2.13	3.61
YN	2.70	-1.89	3.24
LaN	1.29	-1.41	2.82
TiN	2.83	-1.89	3.01
ZrN	3.49	-1.97	2.37
HfN	3.83	-2.01	2.35
VN	1.15	-1.16	4.00
NbN	1.31	-1.07	3.35
TaN	1.62	-1.08	3.09

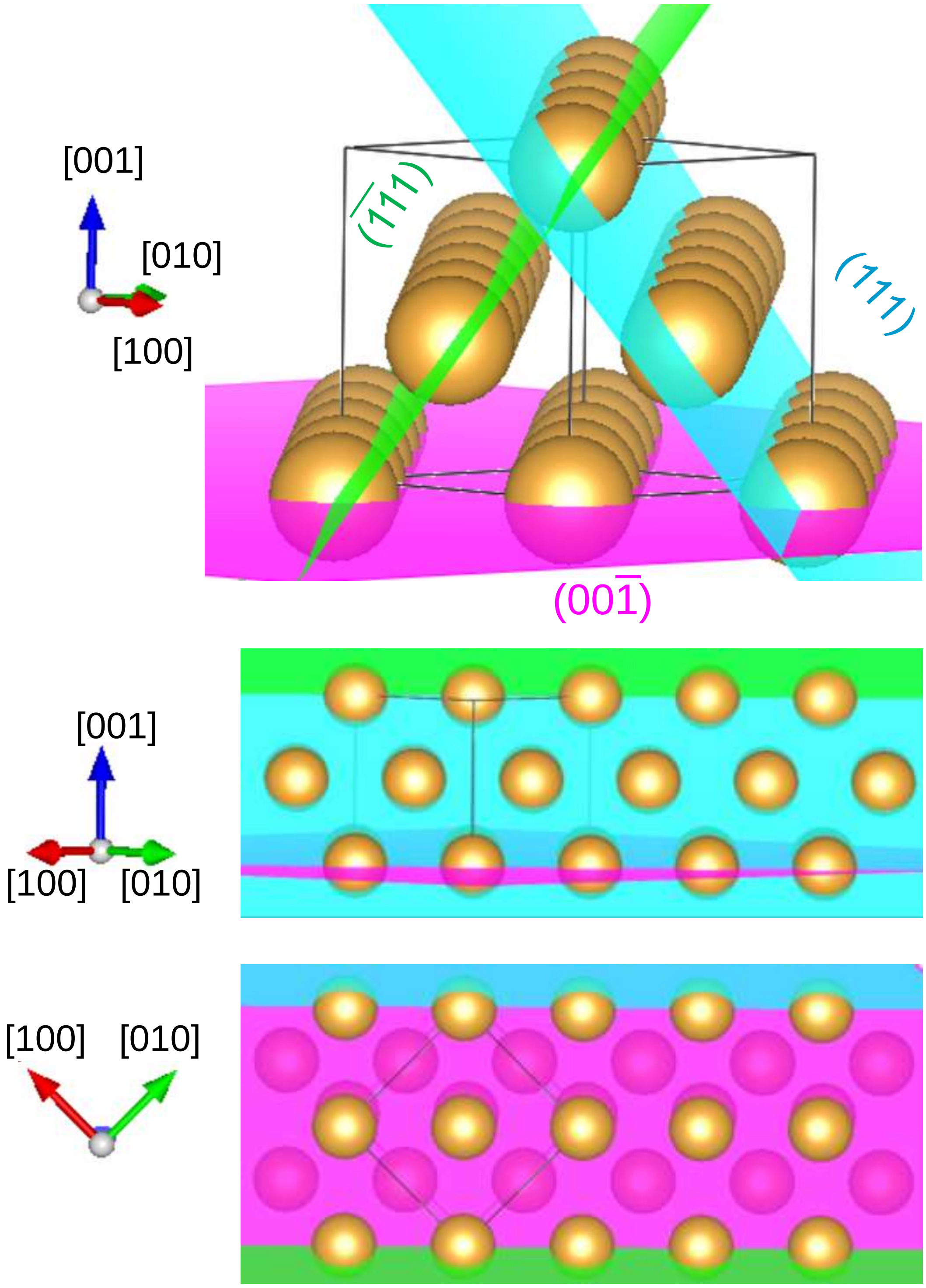

Fig. S1. Nanorod of a face-centered cubic metal viewed from three directions.

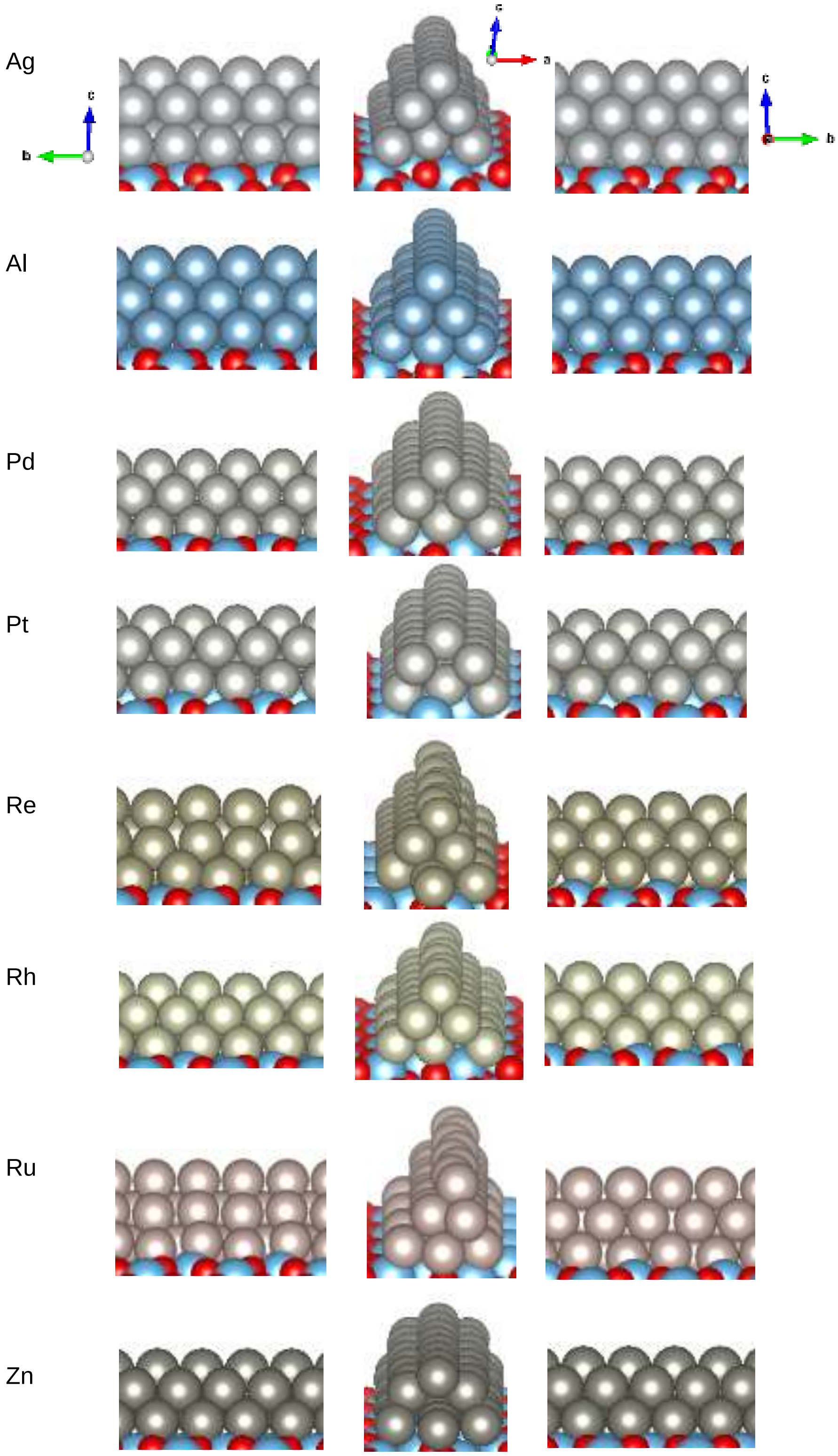

Fig. S2. Adsorption of a nanorod of a face-centered cubic metal on the Ti_2O_3 $(01\bar{1}2)$ surface, as viewed from three directions.