Supporting information

Stability of Pt near surface alloys under electrochemical conditions: a model study

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Results

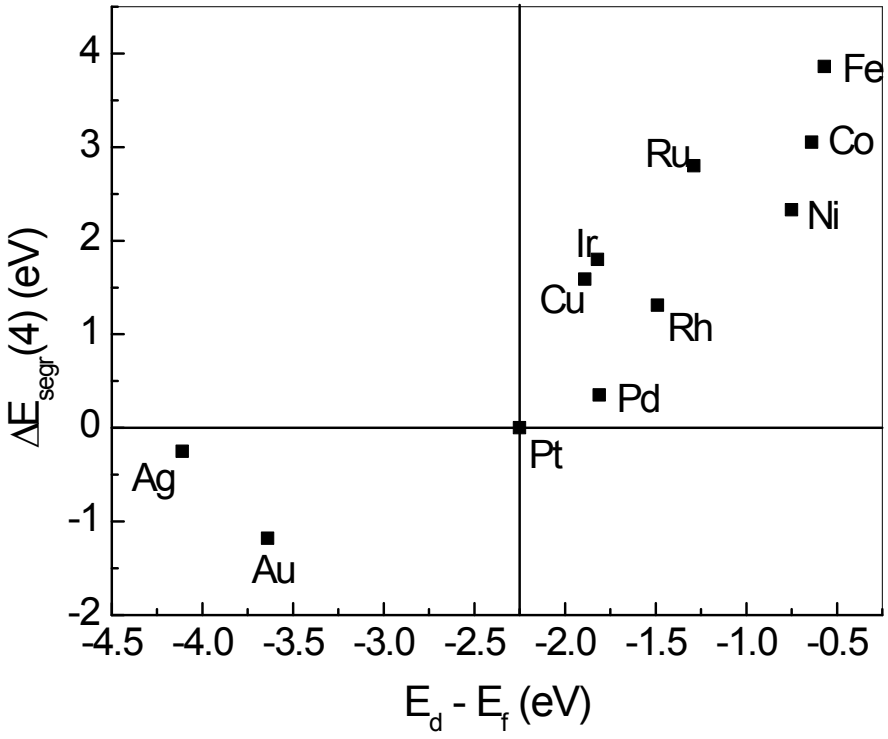

Figure S1 Correlation between the calculated $^{\Delta E_{segr}(4)}$ for $Pt_{ML}/M_{ML}/Pt(111)$ NSAs under vacuum conditions and the d-band center of M on the surface of $M_{ML}/Pt(111)$. The d-band center was cited from Ref (40).

Table S1 Segregation energies (eV) for various NSAs under vacuum conditions

M	ΔE_{segr} (1)	ΔE_{segr} (2)	ΔE_{segr} (3)	ΔE_{segr} (4)
Fe	0.65	1.68	2.21	3.86
Co	0.69	1.48	1.97	3.05
Ni	0.63	1.32	1.69	2.33
Cu	0.5	0.93	1.26	1.59
Ru	0.51	1.06	1.83	2.8
Rh	0.23	0.58	0.95	1.31
Pd	0.07	0.17	0.26	0.35
Ag	0.24	-0.01	0.09	-0.25
Os	0.74	1.19	2.05	2.89
Ir	0.54	0.82	1.39	1.80
Pt	0	0	0	0
Au	-0.09	-0.46	-0.68	-1.18

Table S2 Segregation energies (eV) for various NSAs in $HClO_4$ solution

M	ΔE_{segr} (1)	ΔE_{segr} (2)	ΔE_{segr} (3)
Fe	0.38	0.64	-0-0
Co	0.28	0.32	0.67
Ni	0.16	0.20	0.45
Cu	-0.01	-0.08	0.02
Ru	0.33	0.57	0.89
Rh	-0.03	-0.07	-0.06
Pd	-0.08	-0.18	-0.20
Os	0.55	0.77	1.48
Ir	0.26	0.31	0.78
Pt	0	0	0

Table S3 Segregation energies (eV) for various NSAs in H_2SO_4 solution

M	ΔE_{segr} (1)	ΔE_{segr} (2)	ΔE_{segr} (3)
Fe	-0.04	0.04	0.05
Co	-0.04	-0.18	-0.06
Ni	-0.01	-0.10	0.01
Cu	-0.28	-0.29	-0.31
Ru	0.08	0.05	0.09
Rh	-0.13	-0.19	-0.18
Pd	-0.04	-0.03	-0.02
Os	0.32	0.50	0.42
Ir	0.21	0.32	0.29
Pt	0	0	0

Table S4 Segregation energies (eV) for various NSAs in H_3PO_4 solution

M	ΔE_{segr} (1)	ΔE_{segr} (2)	ΔE_{segr} (3)
Fe	-0.36	-0.52	-0.76
Co	-0.23	-0.52	-0.57
Ni	-0.08	-0.23	-0.20
Cu	-0.09	-0.09	-0.45
Ru	-0.26	-0.48	-0.59
Rh	-0.13	-0.17	-0.16
Pd	0.03	0.04	0.13
Os	-0.06	-0.37	-0.53
Ir	0.11	0	-0.01
Pt	0	0	0

Table S5 Segregation energies (eV) for various NSAs in alkaline solution

M	ΔE_{segr} (1)	ΔE_{segr} (2)	ΔE_{segr} (3)
Fe	0.15	0.80	0.81
Co	0.08	0.44	0.32
Ni	0.16	0.49	0.04
Cu	-0.10	0.21	-0.11
Ru	-0.05	0.33	0.70
Rh	0.04	0.02	0
Pd	0.20	0.08	-0.15
Os	-0.04	0.53	1.27
Ir	0.08	0.30	1.03
Pt	0	0	0

Table S6 Segregation energies (eV) for various NSAs in interaction with *O

M	ΔE_{segr} (1)	ΔE_{segr} (2)	ΔE_{segr} (3)
Fe	-0.30	-0.52	-0.60
Co	-0.28	-0.68	-0.59
Ni	-0.09	-0.45	-0.43
Cu	0.10	0.048	0.18
Ru	-0.26	-0.40	-0.48
Rh	-0.06	-0.26	-0.22
Pd	-0.01	-0.11	-0.06
Os	-0.62	-0.25	-0.34
Ir	0.20	0.29	0.29
Pt	0	0	0

Table S7 Segregation energies (eV) for various NSAs in interaction with *OOH

M	ΔE_{segr} (1)	ΔE_{segr} (2)
Fe	0.20	-1.32
Co	0.10	-1.14
Ni	0.27	0.64
Cu	0.22	0.86
Ru	-0.02	-1.58
Rh	-0.02	0
Pd	0.14	0.17
Os	-1.70	-2.05
Ir	0.08	-0.87
Pt	0	0