Table S-1. For each system, surface-surface separation distances (in Å) were selected to study the surface d-band center (referred to the Fermi level) and charge (in e), shown in parenthesis after the distance.

System:	d-band center (eV) and surface charge as a function of H (Å)	change d-band
Pt	**4.30Å** (-1.996;-0.043); **4.61Å** (-2.004;-0.047); **4.79Å** (-2.006;-0.045); **4.97Å** (-2.008;-0.046); **5.08Å** (-2.008;-0.046); **5.96Å** (-2.012;-0.045); **12.00Å** (-2.017;0.042)	very small
Ag/Pt	**3.88Å** (-3.834; 0.082); **4.10Å** (-3.848; 0.080); **4.23Å** (-3.843; 0.079); **5.66Å** (-3.836;0.082); **5.89Å** (-3.840; 0.081); **6.20Å** (-3.841;0.081); **12.00Å** (-3.842;0.082)	----
Au/Pt	**3.98Å** (-3.248; -0.0034); **4.12Å** (-3.248; -0.0025); **4.23Å** (-3.245; -0.0068); **5.48Å** (-3.252; -0.0043); **5.59Å** (-3.256; -0.0072); **6.18Å** (-3.255;-0.0022) ; **12.00Å** (-3.252;-0.0039)	----
Co/Pt	**3.82Å** (-1.207; 0.23); **3.92Å** (-1.207; 0.23); **4.07Å** (-1.207; 0.23); **4.80Å** (-1.441; 0.23); **5.31Å** (-1.441;0.23); **6.13Å** (-1.440; 0.23); **12.00Å** (-1.435;0.23)	large
Cu/Pt	**3.91Å** (-1.783; 0.16); **4.00Å** (-1.786; 0.16); **4.12Å** (-1.787; 0.16); **5.61Å** (-1.801; 0.16); **5.81Å** (-1.805; 0.16); **6.11Å** (-1.802; 0.16); **12.00Å** (-1.806;0.16)	small
Fe/Pt	**3.62Å** (0.844; 0.28); **3.77Å** (0.855; 0.28); **4.02Å** (0.854; 0.28); **5.64Å** (0.866; 0.29); **5.85Å** (0.864; 0.29); **6.14Å** (0.863; 0.29); **12.00Å** (0.870;0.29)	very small
Ir/Pt	**3.85Å** (-1.53; 0.0007); **3.95Å** (-1.541; -0.00025); **4.10Å** (-1.543; -0.00065); **5.62Å** (-1.554; 0.0017); **5.82Å** (-1.554; -0.0065); **6.13Å** (-1.554; -0.0057); **12.00Å** (-1.548;-0.0057)	very small
Ni/Pt	**3.80Å** (-1.169; 0.17); **3.95Å** (-1.171; 0.16); **4.10Å** (-1.173; 0.16); **5.50Å** (-1.174; 0.16); **5.81Å** (-1.175; 0.17); **6.10Å** (-1.175; 0.16); **12.00Å** (-1.177;0.16)	----
Pd/Pt	**3.81Å** (-1.539; 0.018); **4.00Å** (-1.55; 0.014); **4.12Å** (-1.556; 0.014); **5.11Å** (-1.712; 0.0092); **5.31Å** (-1.713; 0.014); **6.12Å** (-1.716; 0.011)	large
Re/Pt	**4.46Å** (-0.277;0.20); **4.80Å** (-0.241;0.20); **5.31Å** (-0.224;0.20); **6.42Å** (-0.223; 0.20); **6.62Å** (-0.193; 0.21); **6.93Å** (-0.227; 0.20) ; **12.00Å** (-0.251;0.20)	small
Ti/Pt	**4.51Å** (0.743; 0.47); **4.89Å** (0.749; 0.48); **5.48Å** (0.768; 0.48); **6.64Å** (0.557; 0.48); **6.85Å** (0.568; 0.48); **7.17Å** (0.04; 0.48) ; **12.00Å** (0.03;0.48)	large

Table S-2. For each system six H separations (in Å) were selected to show changes in the oxygen charge (Q, in e), the oxygen p-band center (in eV, relative to the Fermi level), and surface d-band center (in eV, relative to the Fermi level).

System	H	E_{ad}	Q (O)	p-band center for O	d-band surface center	System	H	E_{ad}	Q (O)	p-band center for O	d-band surface center
Ag/Pt	4.31	0.56	-0.53	-8.67	-2.13	Ir/Pt	4.09	-2.94	-0.71	-7.44	-2.45
	4.48	0.15	-0.54	-8.40	-2.11		4.23	-3.31	-0.74	-7.28	-2.44
	4.67	-0.12	-0.54	-8.12	-2.08		4.53	-3.77	-0.73	-6.98	-2.42
	5.23	0.25	-0.60	-1.28	-1.99		5.40	-4.11	-0.73	-6.52	-2.40
	5.88	0.014	-0.27	-5.61	-2.04		5.76	-0.12	-0.25	-5.61	-2.65
	6.21	0.020	-0.19	-7.15	-2.04		6.12	-0.04	-0.19	-6.61	-2.67
Au/Pt	4.41	2.01	-0.42	-6.84	-2.17	Ni/Pt	4.00	-4.38	-0.83	-5.74	-2.54
	4.59	1.54	-0.43	-9.07	-2.15		4.18	-4.70	-0.82	-5.65	-2.54
	4.80	1.16	-0.43	-8.74	-2.12		4.46	-5.00	-0.81	-5.52	-2.53
	4.97	1.45	-0.57	-1.46	-2.08		5.23	-5.28	-0.84	-5.30	-2.52
	5.61	0.70	-0.17	-5.79	-2.04		5.64	-0.57	-0.43	-5.58	-2.55
	6.26	0.26	-0.08	-7.60	-2.05		6.04	-0.34	-0.16	-6.51	-2.59
Co/Pt	4.01	-4.91	-0.95	-5.22	-2.55	Pd/Pt	4.18	-0.96	-0.61	-6.17	-2.16
	4.17	-5.16	-0.93	-5.18	-2.56		4.34	-1.37	-0.60	-5.99	-2.15
	4.48	-5.48	-0.94	-5.10	-2.57		4.58	-1.73	-0.61	-5.71	-2.14
	5.40	-5.86	-0.96	-4.97	-2.58		4.93	-2.00	-0.65	-5.59	-2.11
	5.78	-5.90	-0.96	-4.98	-2.57		5.20	-0.56	-0.29	-5.59	-2.06
	6.04	-0.39	-0.23	-5.91	-2.67		6.12	-0.10	-0.06	-7.05	-2.10
Cu/Pt	4.04	-2.57	-0.87	-4.88	-2.18	Re/Pt	4.39	-6.40	-0.89	-6.19	-2.89
	4.21	-2.77	-0.88	-4.78	-2.39		4.56	-6.85	-0.92	-5.97	-2.88
	4.49	-3.03	-0.86	-4.65	-2.39		5.32	-7.27	-0.92	-5.72	-2.87
	5.47	-3.33	-0.90	-4.46	-2.38		6.12	-7.30	-0.93	-5.67	-2.87
	5.77	-0.23	-0.38	-5.46	-2.13		6.63	0.17	-0.13	-6.96	-3.04
	6.10	-0.13	-0.29	-7.09	-2.14		6.94	0.15	-0.01	-7.32	-3.05
Fe/Pt	4.11	-5.50	-0.98	-5.45	-2.56	Ti/Pt	4.75	-10.7	-1.07	-5.40	-2.66
	4.27	-5.93	-1.00	-5.27	-2.56		5.00	-11.1	-1.06	-5.34	-2.66
	4.56	-6.40	-1.00	-5.23	-2.55		5.51	-11.4	-1.08	-5.25	-2.65
	5.31	-6.86	-1.01	-5.03	-2.54		6.35	-11.5	-1.09	-5.23	-2.66
	5.64	-6.90	-1.02	-5.02	-2.55		6.66	-0.72	-0.36	-5.62	-2.70
	6.00	-0.60	-0.41	-5.90	-2.50		6.95	-0.17	-0.27	-5.87	-2.70

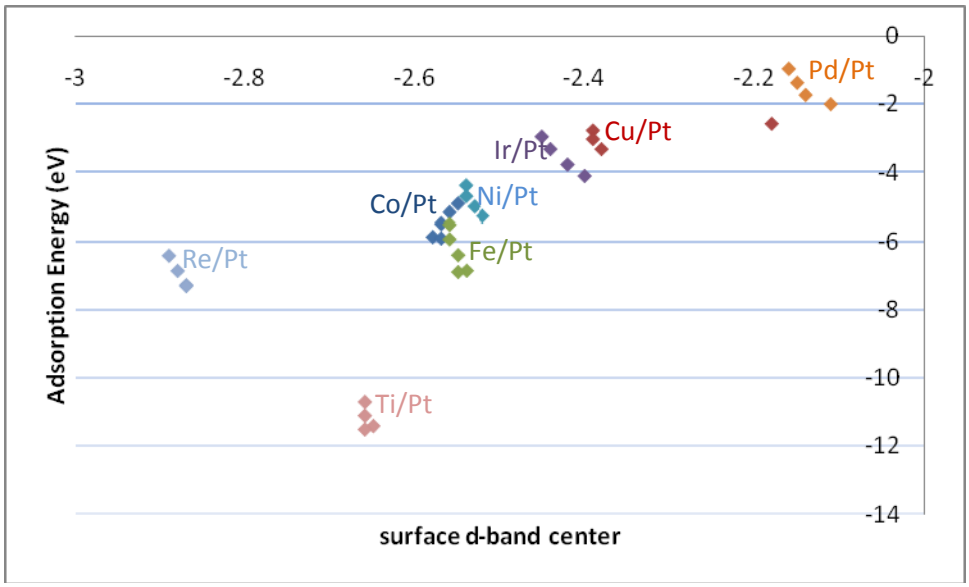

Figure S1. Surface d-band center as a function of adsorption energy defined as the energy gain or lost by taking both Oxygen atoms from the surface and forming molecular Oxygen in the gas phase.

Table S-3. Surface charges (in e), and d-band center (in eV) at the value of H indicated in parenthesis.

System	surface charge	d-band surface	System	surface charge	d-band surface
Ti	0.48	0.77 (5.48Å)	Fe	0.28	0.85 (4.02Å)
Co	0.23	-1.21 (4.07Å)	Ni	0.16	-1.17 (4.10Å)
Cu	0.16	-1.79 (4.12Å)			
Pd	0.014	-1.56 (4.12Å)	Ag	0.079	-3.84 (4.23Å)
Re	0.20	-0.22 (5.31Å)	Ir	-0.00065	-1.54 (4.10Å)
Pt	-0.045	-2.006 (4.79Å)	Au	-0.0068	-3.24 (4.23Å)