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

Supporting Information

More Accurately Depicting Adsorption Energy on Transition Metal using Work Function as One Additional Descriptor

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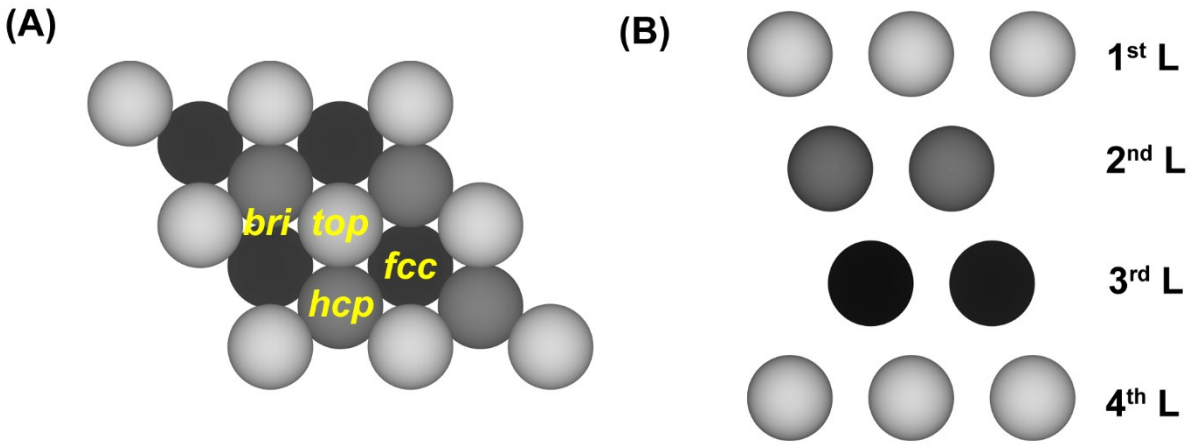

Figure S1. (A) Different adsorption sites on transition metal (111) surface. (B) Side view of the transition metal surface model.

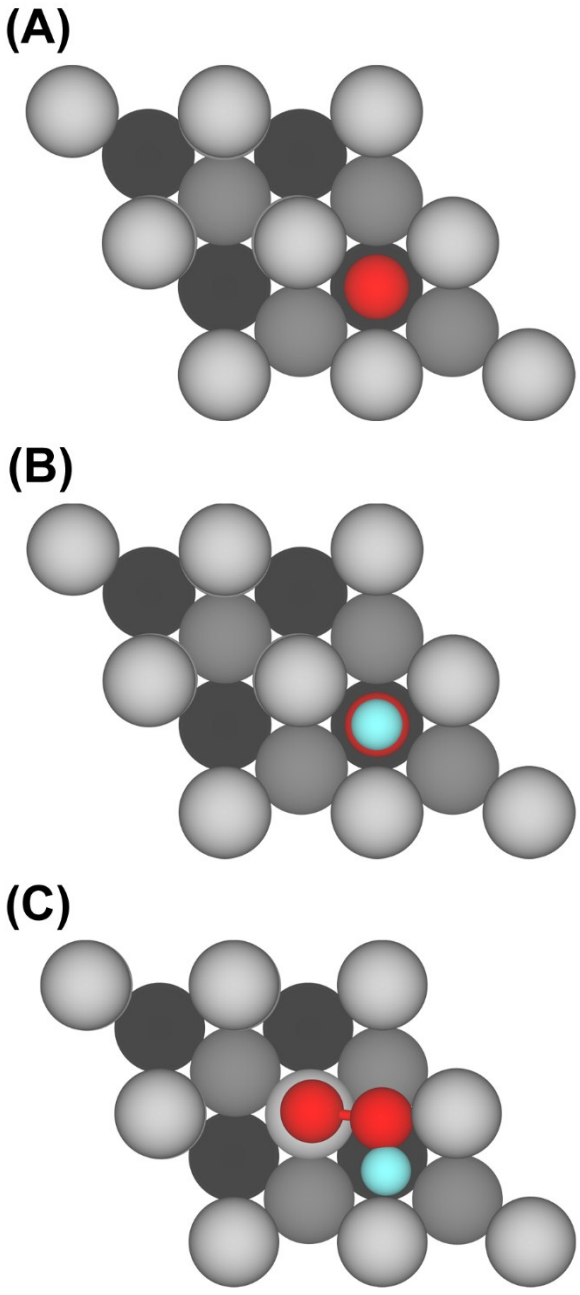

Figure S2. Top view of adsorption model of (A) O, (B) OH, (C) OOH species on transition metal (111) surface. (●: oxygen, ●: hydrogen)

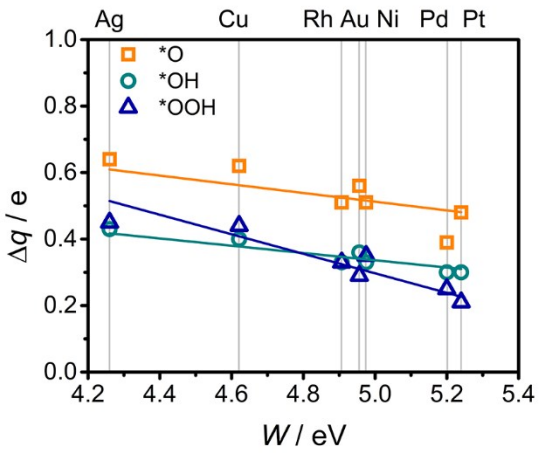

Figure S3. *Δq*–*W* plots and linear correlation for O, OH and OOH adsorption to transition metal (111) surface.

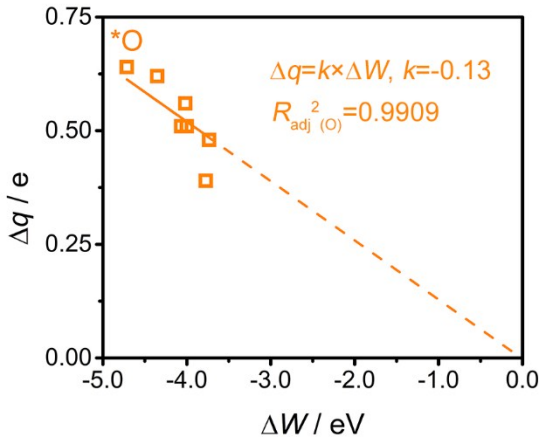

Figure S4. A proportional correlation between *Δq* and *ΔW* for O adsorption to transition metals.

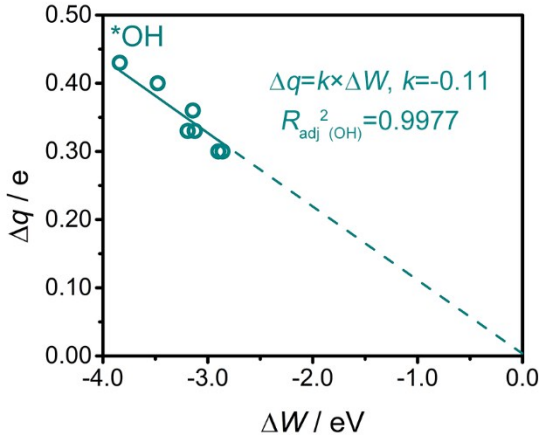

Figure S5. A proportional correlation between *Δq* and *ΔW* for OH adsorption to transition metals.

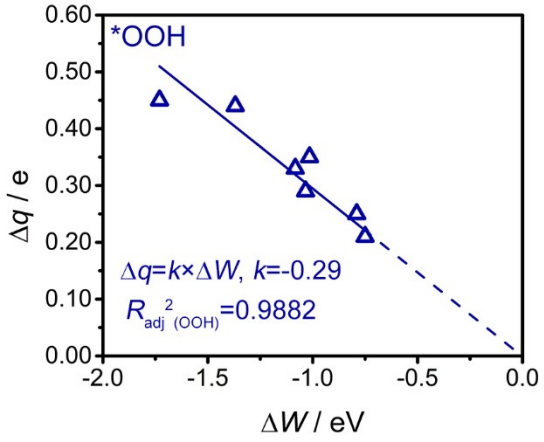

Figure S6. A proportional correlation between *Δq* and *ΔW* for OOH adsorption to transition metals.

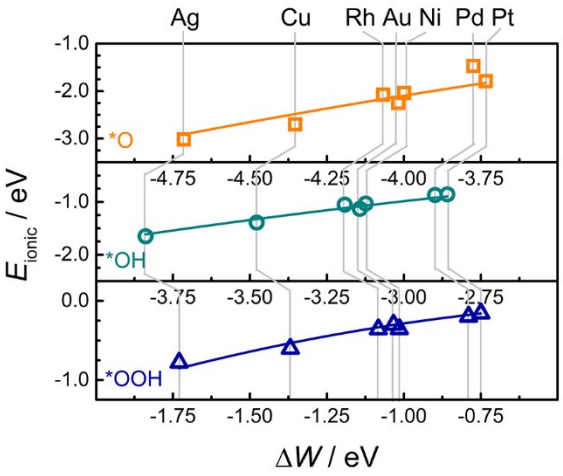

Figure S7. The E_{ionic}–ΔW correlation for O, OH and OOH adsorption to transition metals.

Table S1. DFT calculated ε_d, W and adsorption energies.

	ε_d /	W / eV	E_{ads}(O) / eV	E_{ads}(OH) / eV	E_{ads}(OOH) / eV
Au(111)	-3.55	4.96	-0.62	-2.47	-1.00
Cu(111)	-2.60	4.62	-2.25	-3.58	-2.05
Pd(111)	-2.17	5.20	-1.88	-3.04	-1.72
Pt(111)	-2.78	5.24	-1.58	-2.49	-1.56
Rh(111)	-2.47	4.91	-2.45	-3.59	-2.25
Ag(111)	-4.27	4.26	-1.05	-3.28	-1.72
Ni(111)	-1.66	4.98	-3.08	-3.75	-2.20

Table S2. Fitting results of the E_{ionic}–W and the $E_{covalent}$–ε_d relation.

		O	OH	OOH
E_{ionic}–W	k	-0.13	-0.11	-0.29
	W_0	8.97	8.10	5.99
	R_{adj}^2	0.8524	0.9647	0.9497
$E_{covalent}$–ε_d	slope	-1.23	-0.48	-0.43
	intercept	-3.08	-3.36	-2.59
	R_{adj}^2	0.9357	0.5893	0.6747

Table S3. Fitting results of the E_{ads}–(ε_d, W) model and E_{ads}–ε_d model.

	O	OH	OOH
z_0	-2.29	-2.36	-2.83
a	-1.19	-0.70	-0.60
k	-0.17	-0.26	-0.47
W_0	8.97	8.10	5.99
R_{adj}^2	0.9059	0.9053	0.7142
$R_{adj}^2(E_{ads}–\varepsilon_d)$*	0.6865	0.0116	0.2096

* $R_{adj}^2(E_{ads}–\varepsilon_d)$ values are for the E_{ads}–ε_d linear fitting correlation.