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Figure S2: Relaxed solvated Pt(111)+H surface. a) 1 H_2O b) 2 H_2O c) 3 H_2O d) 4 H_2O e) 5 H_2O f) 6 H_2O g) 7 H_2O h) 8 H_2O i) 9 H_2O j) 10 H_2O

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Figure S4: Relaxed solvated Pt(111)+Ba surface. a) 1 H₂O b) 2 H₂O c) 3 H₂O d) 4 H₂O e) 5 H₂O f) 6 H₂O g) 7 H₂O h) 8 H₂O i) 9 H₂O j) 10 H₂O

		$E_{C^*}^{DFT}$					
	E_*^{DFT}	H⁺	Li⁺	Na⁺	K ⁺	Cs⁺	Ba ⁺²
Pt	-207.23	-210.92	-210.77	-210.27	-210.42	-210.59	-212.45
Pd	-177.80	-181.64	-181.05	-180.60	-180.71	-181.94	-182.75
Ni	-183.83	-185.04	-186.70	-186.29	-186.35	-186.54	-187.98
Au	-110.01	-112.48	-112.37	-111.94	-112.06	-112.25	-113.40
Ag	-91.86	-94.96	-94.24	-93.90	-93.94	-94.12	-94.78

Table S1: VASP energies (eV) for bare fcc(111) surfaces and single atoms adsorbed to fcc(111) surfaces.

Table S2: VASP gas phase cation energies and energy corrections used to calculate solution phase cation free energies at 300 K and 1M using equations 5 and 6. All values are in eV.

Cation	E _{dft}	TS _{TRANS}	ΔG_{SOLV}	G _{C+, aq}
H⁺	12.527	0.197	-11.411	1.378
Li⁺	5.344	0.414	-4.985	0.950
Na⁺	5.183	0.460	-3.887	0.901
K ⁺	4.347	0.481	-3.151	0.780
Cs⁺	3.874	0.528	-2.674	0.737
Ba ⁺²	15.388	0.529	-13.04	1.883

Table S3: Dipole moments (e⁻Å) for bare fcc(111) surfaces (μ_*) and surfaces with adsorbed atoms ((μ_{C*}).

	М						
	Metal	H⁺	Li⁺	Na⁺	K ⁺	Cs⁺	Ba ⁺²
	alone						
Pt	0.0166	0.000832	-0.567	-0.813	-1.06	-1.11	-1.19
Pd	0.00834	0.0172	-0.520	-0.733	-0.971	-0.997	-1.02
Ni	-0.0131	-0.0211	-0.506	-0.689	-0.906	-0.941	-0.891
Au	0.0279	0.0205	-0.549	-0.764	-1.03	-1.13	-1.18
Ag	0.0124	0.0295	-0.471	-0.635	-0.913	-1.02	-0.944

Table S4: Gas phase water properties at 300K (eV).

E _{DFT} ZPVE		TS _{VIB+ROT+TRANS}	U+PV	G
-14.272	0.5645	0.6733	0.1035	-14.278



Figure S2: Relaxed solvated Pt(111) surface. a) 1 H₂O b) 2 H₂O c) 3 H₂O d) 4 H₂O e) 5 H₂O f) 6 H₂O g) 7 H₂O h) 8 H₂O i) 9 H₂O j) 10 H₂O





Figure S2: Relaxed solvated Pt(111)+H surface. a) 1 H₂O b) 2 H₂O c) 3 H₂O d) 4 H₂O e) 5 H₂O f) 6 H₂O g) 7 H₂O h) 8 H₂O i) 9 H₂O j) 10 H₂O









 $\begin{array}{l} \textbf{Figure S3:} \ \ Relaxed \ solvated \ Pt(111) + Na \ surface. \ a) \ 1 \ H_2O \ b) \ 2 \ H_2O \ c) \ 3 \ H_2O \ d) \ 4 \ H_2O \ e) \ 5 \ H_2O \ f) \ 6 \ H_2O \ g) \ 7 \ H_2O \ h) \ 8 \ H_2O \ i) \ 9 \ H_2O \ j) \ 10 \ H_2O \ d) \ 4 \ H_2O \ b) \ 2 \ H_2O \ b) \ 2 \ H_2O \ c) \ 3 \ H_2O \ d) \ 4 \ H_2O \ e) \ 5 \ H_2O \ f) \ 6 \ H_2O \ g) \ 7 \ H_2O \ b) \ 2 \ H_2O \ b) \ 2 \ H_2O \ c) \ 3 \ H_2O \ d) \ 4 \ H_2O \ e) \ 5 \ H_2O \ f) \ 6 \ H_2O \ g) \ 7 \ H_2O \ b) \ 2 \ H_2O \ b) \ 2 \ H_2O \ b) \ 2 \ H_2O \ b) \ 4 \ H_2O \ e) \ 5 \ H_2O \ f) \ 6 \ H_2O \ g) \ 7 \ H_2O \ b) \ 7 \ H_2O \ b) \ 2 \ H_2O \ b) \ 4 \ H_2O \ b) \ 4 \ H_2O \ b) \ 5 \ H_2O \ b) \ 6 \ H_2O \ b) \ 7 \ H_2O \ b) \ 7 \ H_2O \ b) \ 6 \ H_2O \ b) \ 7 \ H_2O \ b) \ 6 \ H_2O \ b) \ 6 \ H_2O \ b) \ 7 \ H_2O \ b) \ 6 \ H_2O \ b) \ 7 \ H_2O \ b) \ 7 \ H_2O \ b) \ 6 \ H_2O \ b) \ 7 \ H_2O \ b) \ T_2O \ b) \ t) \ t) \ t) \ T_2O$





Figure S4: Relaxed solvated Pt(111)+Ba surface. a) 1 H₂O b) 2 H₂O c) 3 H₂O d) 4 H₂O e) 5 H₂O f) 6 H₂O g) 7 H₂O h) 8 H₂O i) 9 H₂O j) 10 H₂O

