Alkali cation specific adsorption onto fcc (111) transition metal electrodes – Supplementary Information

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Contents:

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

		$E_{C^*}^{DFT}$					
	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 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*}).

	M						
	Metal alone	H^+	Li^+	Na^+	K^+	Cs^+	Ba^{+2}
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

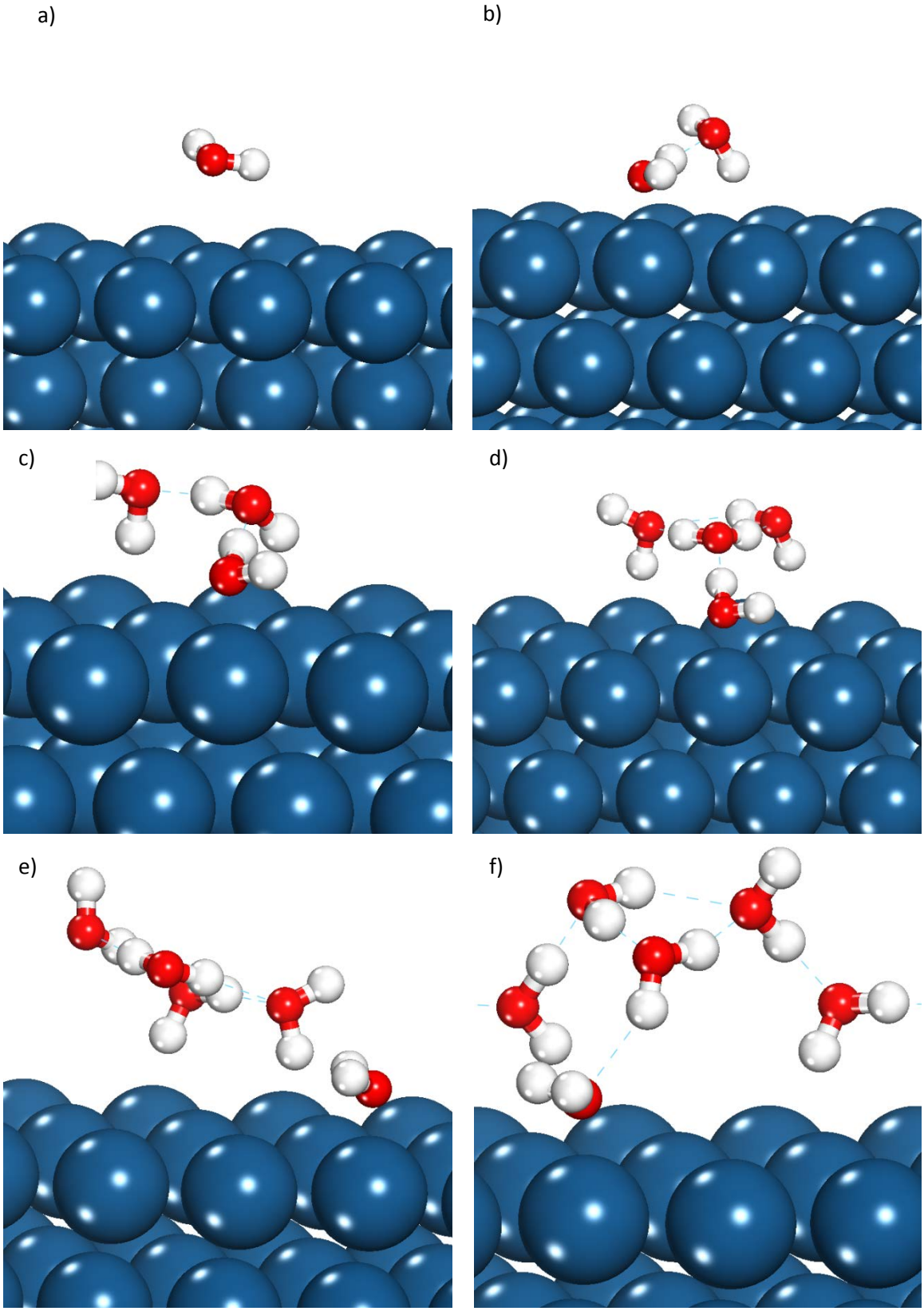
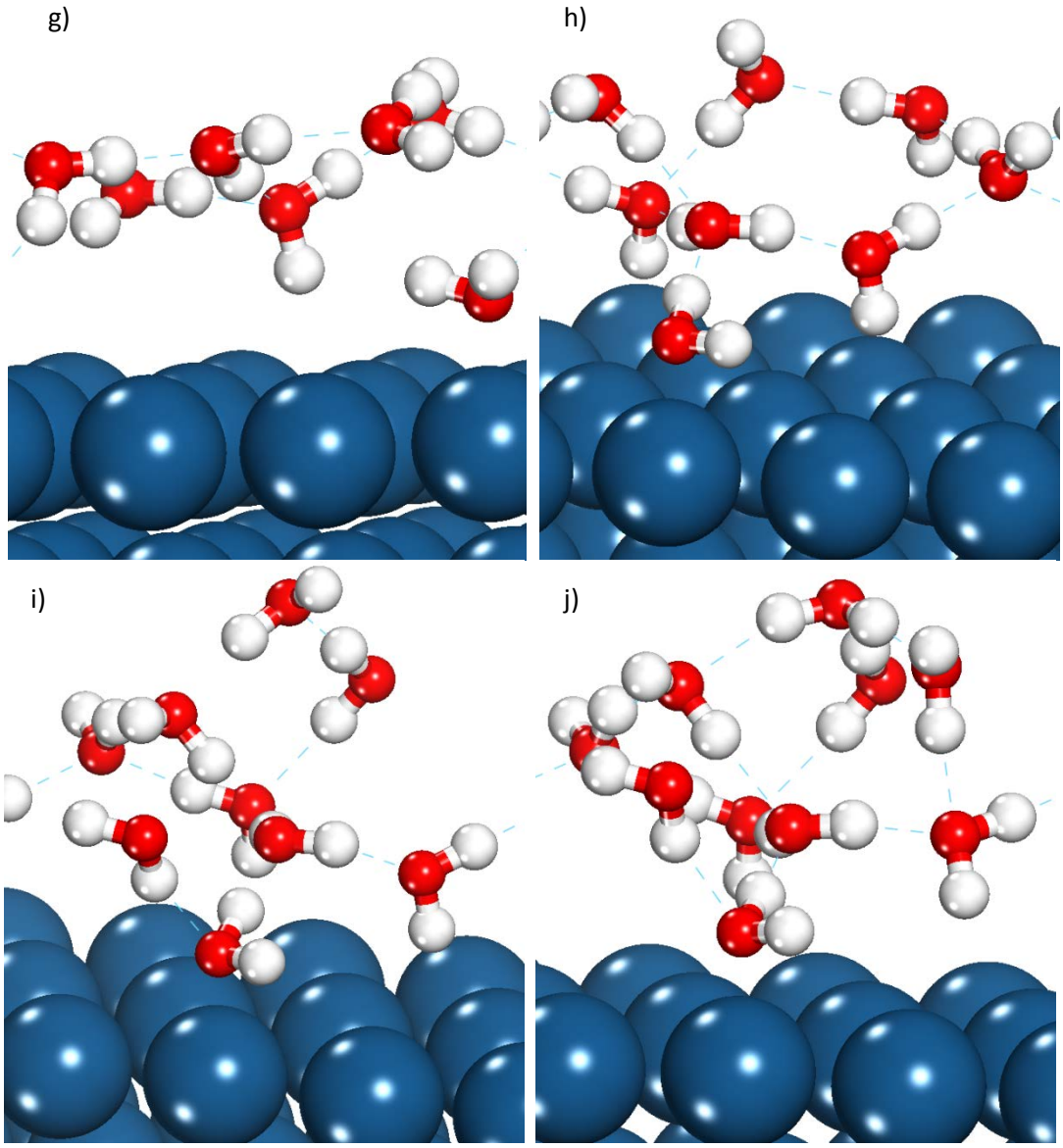


Figure S2: Relaxed solvated Pt(111) surface. a) 1 H_2O b) 2 H_2O c) 3 H_2O d) 4 H_2O e) 5 H_2O f) 6 H_2O g) 7 H_2O h) 8 H_2O i) 9 H_2O j) 10 H_2O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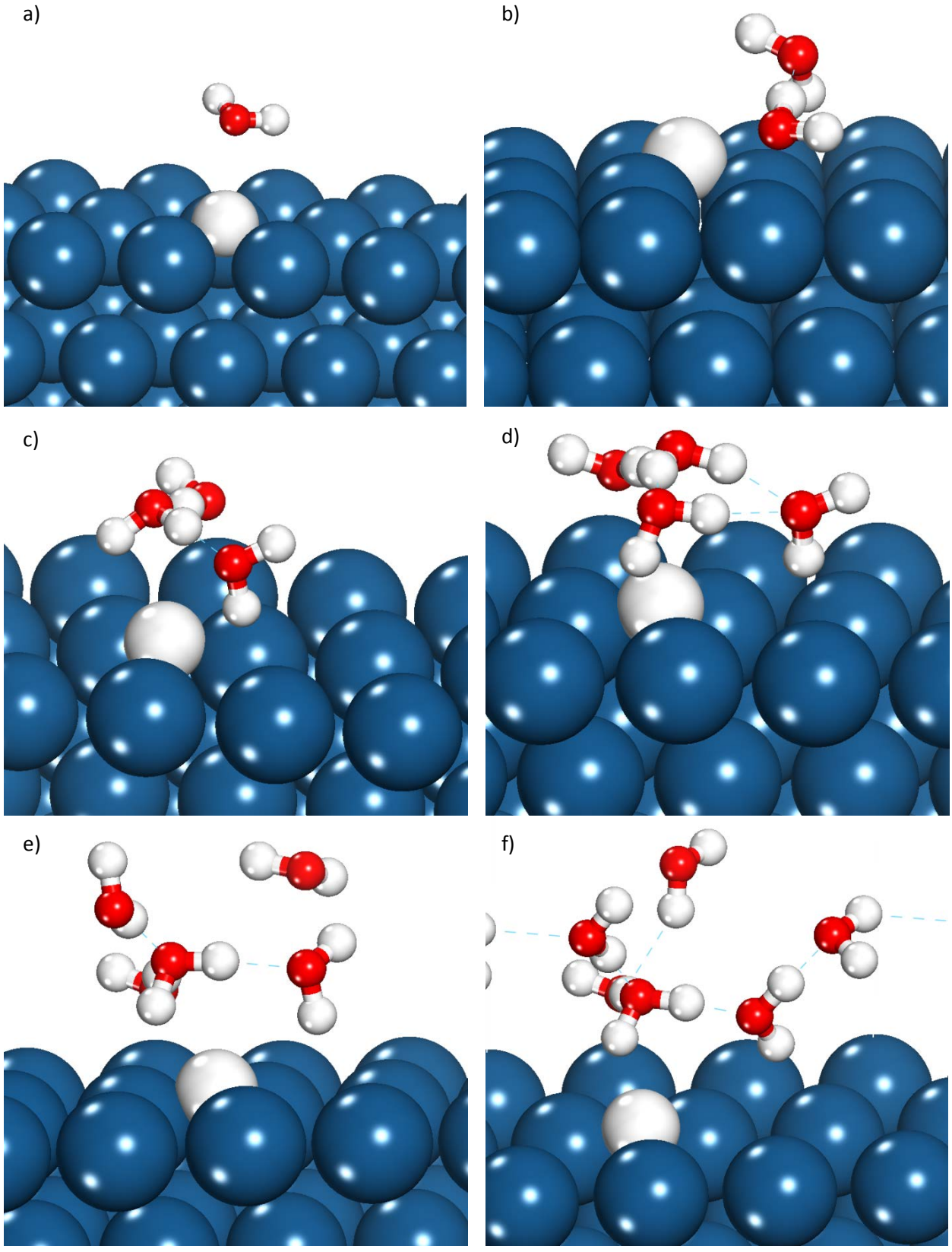
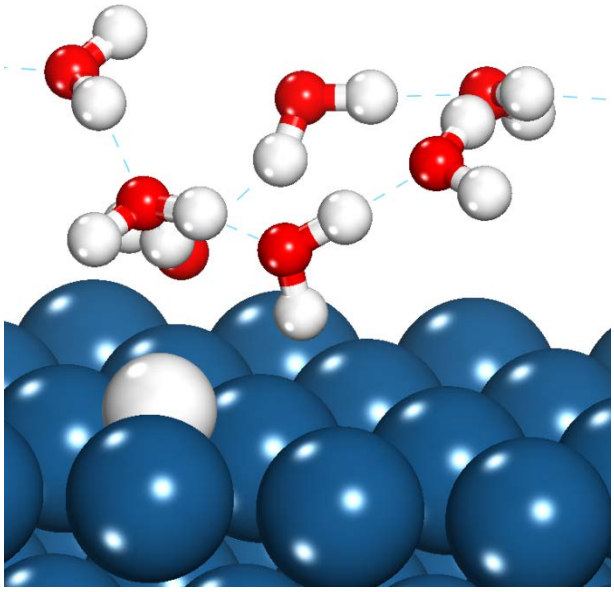


Figure S2: Relaxed solvated Pt(111)+H surface. a) 1 H_2O b) 2 H_2O c) 3 H_2O d) 4 H_2O e) 5 H_2O f) 6 H_2O g) 7 H_2O h) 8 H_2O i) 9 H_2O j) 10 H_2O

g)



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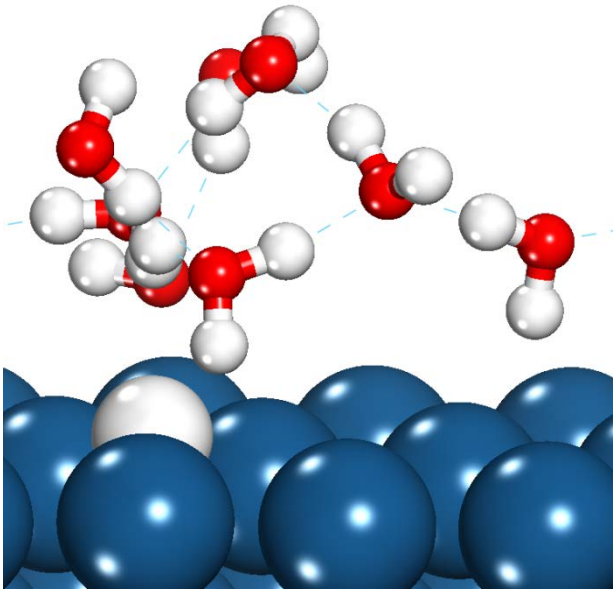

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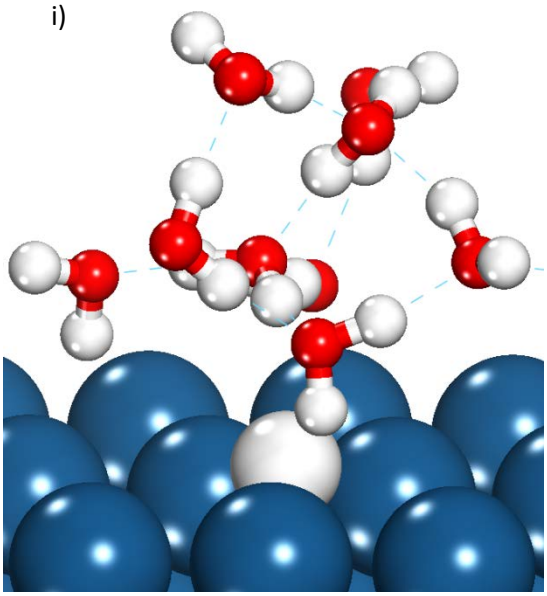

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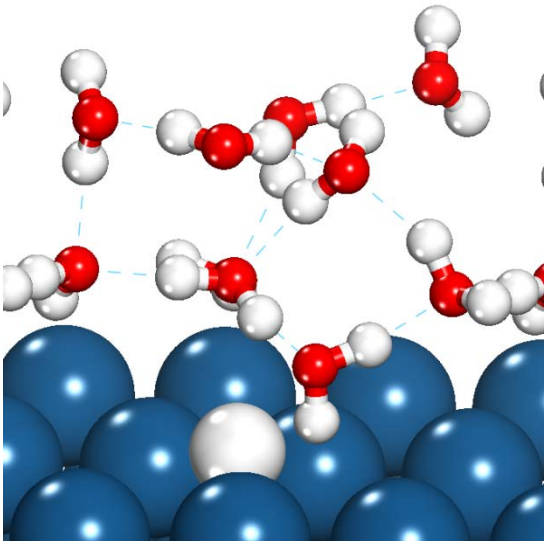


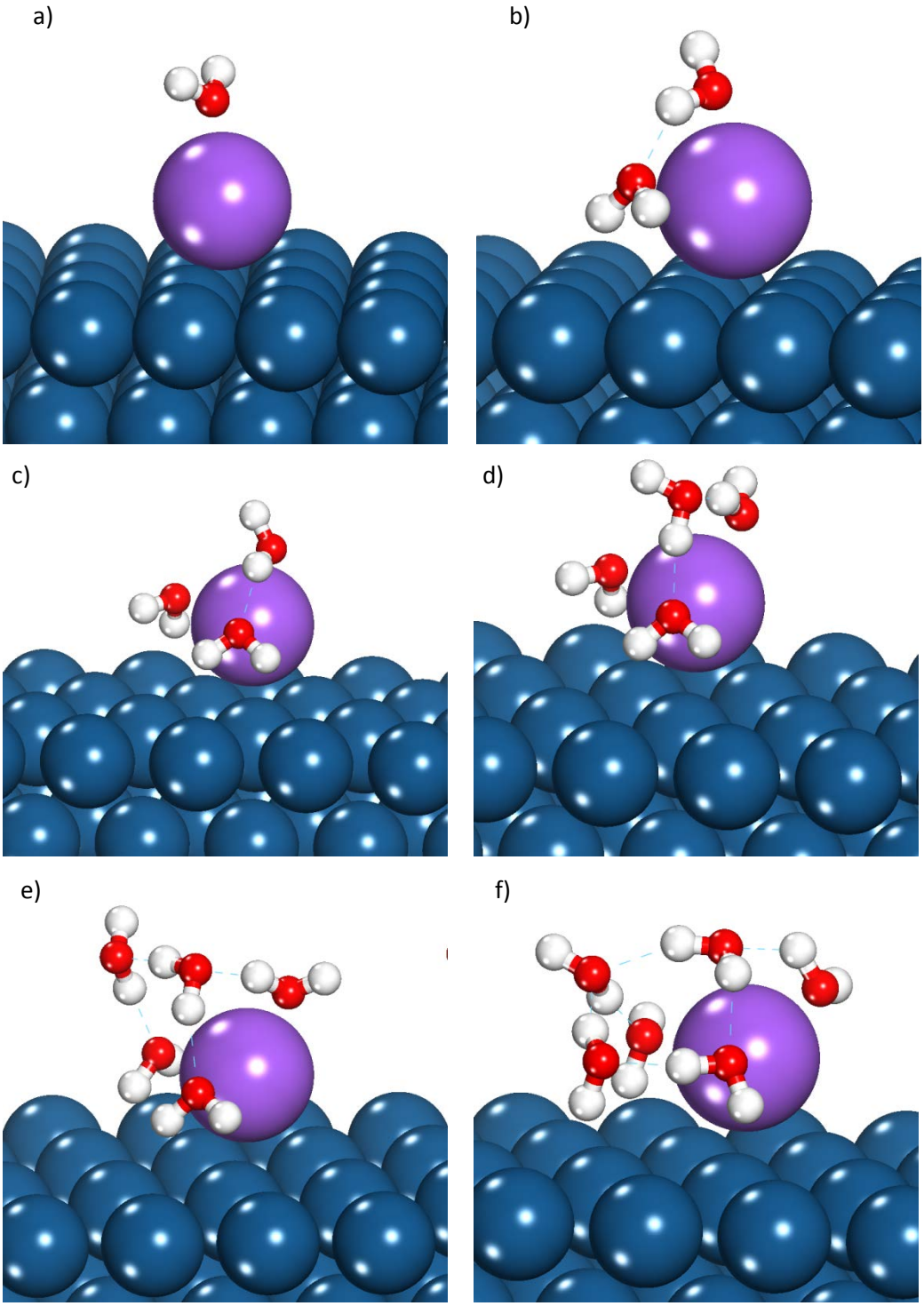
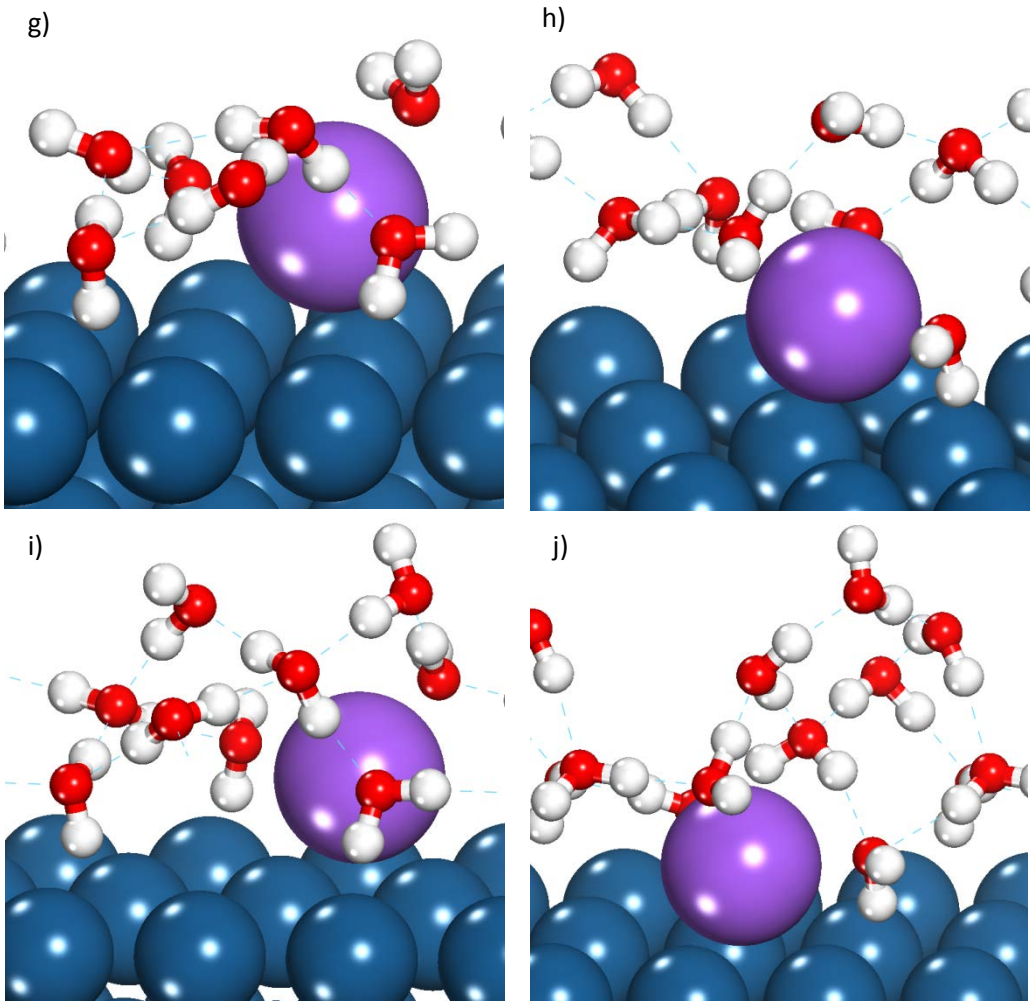


Figure S3: Relaxed solvated Pt(111)+Na surface. a) 1 H_2O b) 2 H_2O c) 3 H_2O d) 4 H_2O e) 5 H_2O f) 6 H_2O g) 7 H_2O h) 8 H_2O i) 9 H_2O j) 10 H_2O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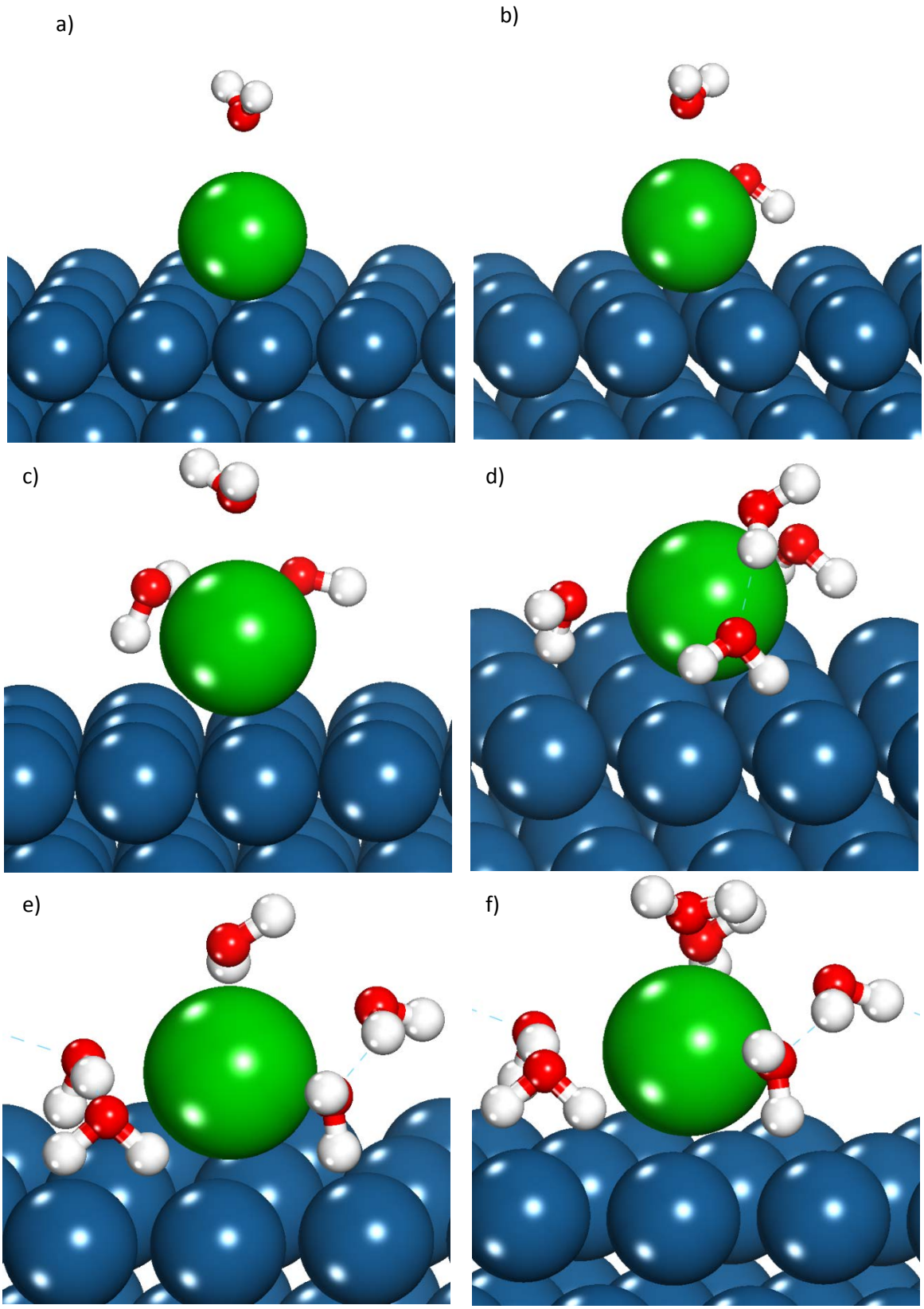
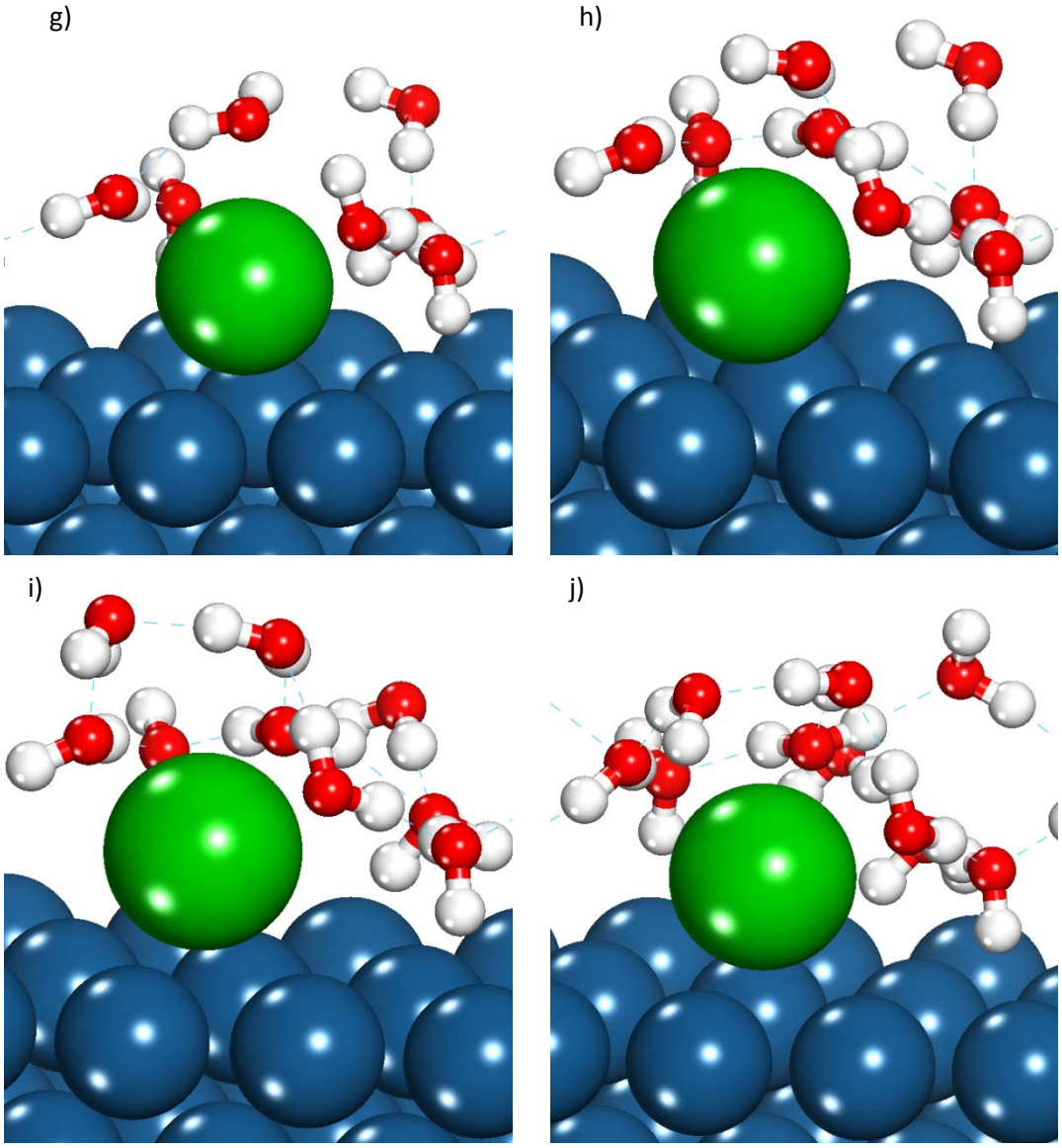


Figure S4: Relaxed solvated Pt(111)+Ba surface. a) 1 H_2O b) 2 H_2O c) 3 H_2O d) 4 H_2O e) 5 H_2O f) 6 H_2O g) 7 H_2O h) 8 H_2O i) 9 H_2O j) 10 H_2O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