Supporting information

Water dissociation on clean and potassium pre-adsorbed transition metals: A systematic theoretical study

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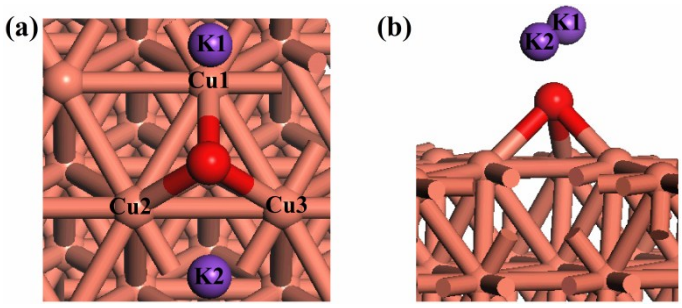

Fig. S1 Top (left) and side (right) views of optimized structures of K_2O adsorption on Cu(111) surface. The light red, purple and red balls represent the Cu, K and O atoms, respectively.

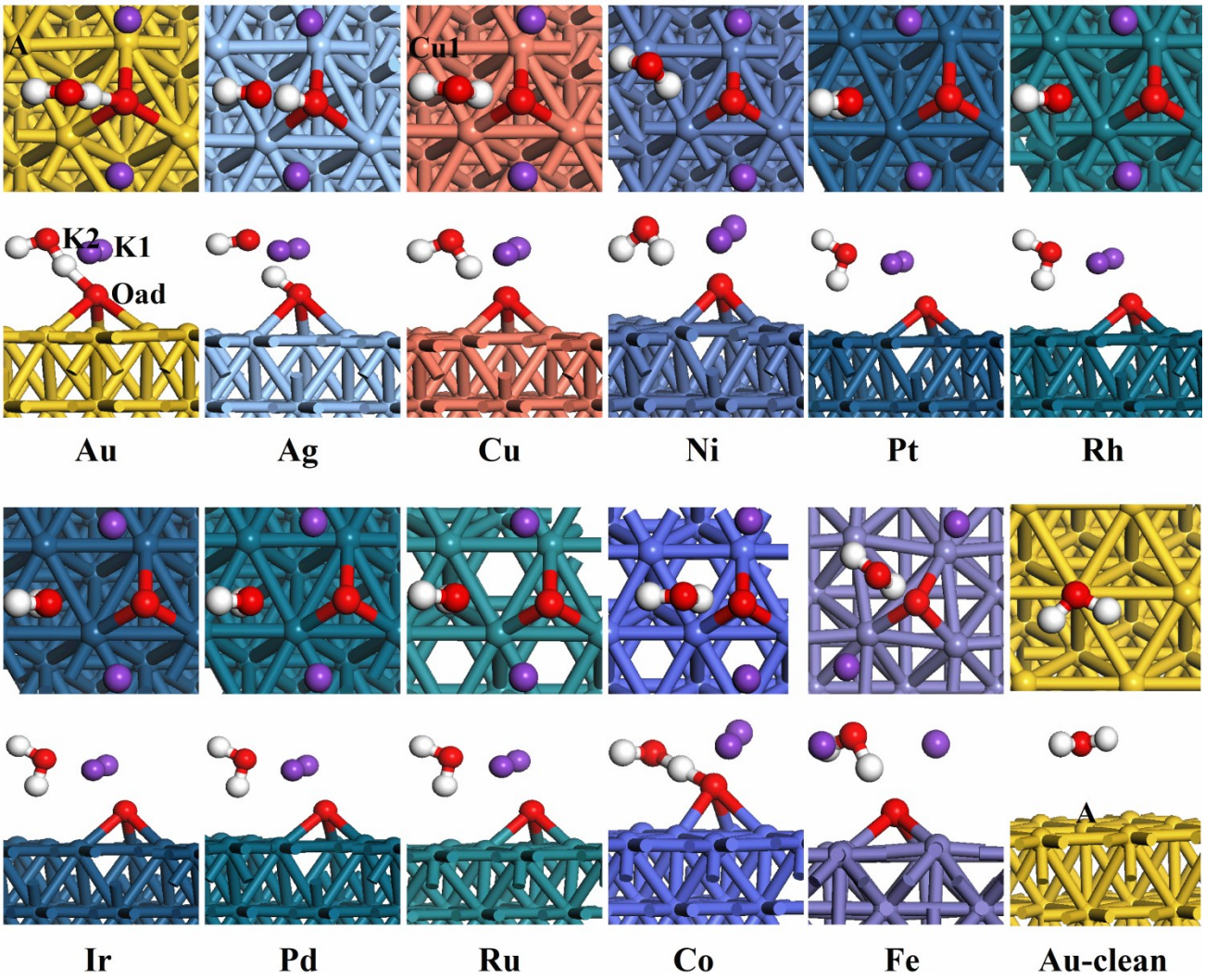

Fig. S2 Top and side view of optimized structures for H_2O adsorption on various metal surfaces. The purple, red and white balls represent the K, O and H atoms, respectively.

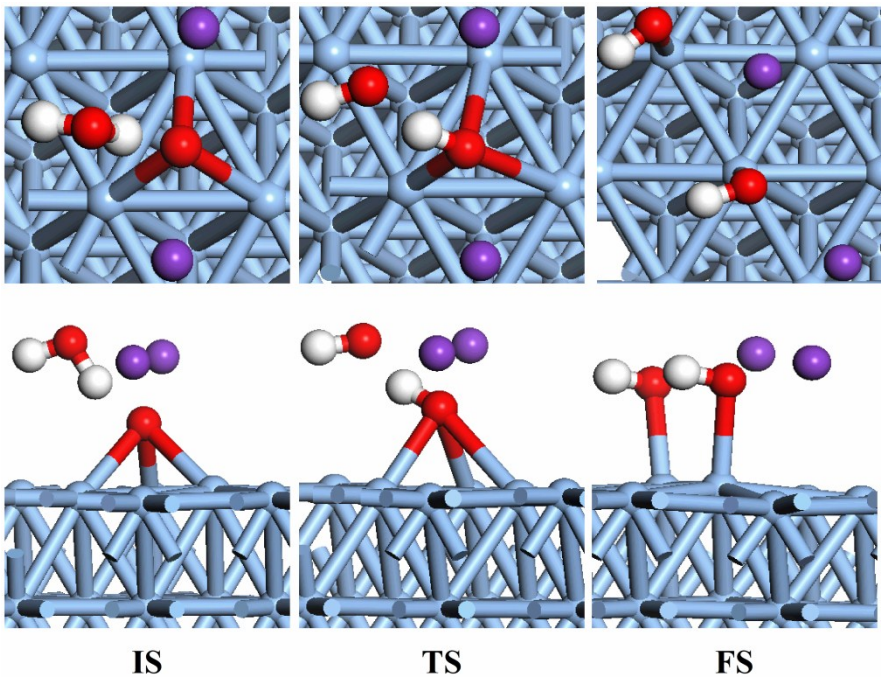

Fig. S3 Top and side view of the initial (IS), transition (TS) and final state (FS) for H_2O dissociation on K2O-pre-adsorbed Ag(111) surface. The blue, purple, red and white balls represent the Ag, K, O and H atoms, respectively.

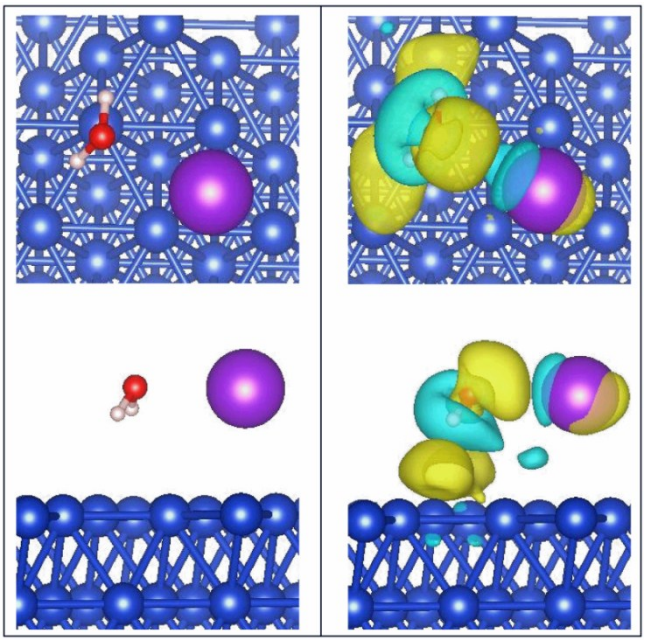

Fig. S4 (a) Top and side views of stable H_2O adsorption structures on K-pre-adsorbed Cu(111) surface and (b) Charge density difference map for H_2O adsorption on K-pre-adsorbed Cu(111) surface. (blue: Cu; red: O; white: H; Purple: K). The yellow and cyan isosurfaces stand for the accumulation of electron density and the depletion of electron density, respectively.

Table S1 Adsorption energies and geometry parameters of K_2O on different metal surfaces

	E_{ads}	d_{O-M1}	d_{O-M2}	d_{O-M3}	d_{O-M4}	d_{O-K1}	d_{O-K2}	d_{K1-M}	d_{K2-M}
Au	-2.92	2.450	2.292	2.289	-	2.553	2.519	2.846	2.770
Ag	-2.63	2.389	2.323	2.317	-	2.496	2.479	2.919	2.841
Cu	-3.47	2.052	2.026	2.026	-	2.541	2.491	2.911	2.920
Ni	-4.45	1.898	1.889	1.890	-	2.667	2.600	2.739	2.707
Pt	-4.29	2.146	2.133	2.134	-	3.038	2.626	2.805	2.785
Rh	-4.64	2.089	2.107	2.106	-	2.758	2.572	2.848	2.863
Ir	-4.49	2.138	2.151	2.151	-	2.826	2.582	2.938	2.942
Pd	-4.38	2.102	2.099	2.097	-	2.761	2.611	2.817	2.804
Ru	-5.04	2.096	2.105	2.103	-	2.770	2.621	2.997	2.984
Co	-4.51	1.958	1.957	1.957	-	2.634	2.570	2.986	2.973
Fe	-4.32	2.158	2.100	2.11	2.104	2.930	2.892	2.886	2.875

Table S2 Bader charges of O and K atoms at ISs for various clean, K-pre-adsorbed and K_2O-pre-adsorbed metal surfaces

	K_2O/M			K/M[44]		clean[44]
metal	O/e	K1/e	K2/e	O/e	K/e	O/e
Au	-2.10	0.86	0.85	-2.04	0.88	-1.97
Ag	-1.78	0.85	0.85	-2.07	0.85	-1.99
Cu	-2.12	0.81	0.81	-2.09	0.85	-1.98
Ni	-2.14	0.80	0.80	-2.10	0.90	-1.98
Pt	-2.08	0.84	0.84	-2.04	0.87	-1.92
Rh	-2.12	0.82	0.82	-2.08	0.85	-1.94
Ir	-2.09	0.83	0.83	-2.05	0.86	-1.93
Pd	-2.10	0.82	0.82	-2.07	0.86	-1.95
Ru	-2.13	0.82	0.82	-2.09	0.85	-1.99
Co	-2.11	0.79	0.79	-2.11	0.84	-1.99
Fe	-2.12	0.79	0.80	-2.13	0.82	-2.03

Table S3 Bader charges of OH and H atoms at TSs for various clean, K-pre-adsorbed and K_2O-pre-adsorbed metal surfaces[a]

	Au	Ag	Cu	Ni	Pt	Rh	Ir	Pd	Ru	Co	Fe
OH/e	-0.4	-0.5	-0.47	-0.45	-0.37	-0.4	-0.39	-0.38	-0.48	-0.45	-0.52
H/e	+0.11	-0.02	-0.01	0	+0.18	+0.14	+0.14	+0.13	+0.04	-0.01	0
K/OH/e	-0.59	-0.63	-0.62	-0.59	-0.5	-0.55	-0.54	-0.53	-0.59	-0.60	-0.64

K/H/e	+0.12	+0.08	0	+0.08	+0.23	+0.15	+0.20	+0.13	+0.06	+0.04	+0.03
K_2O/OH/e	-0.72	-	-0.75	-0.77	-1.07	-0.69	-1.05	-0.63	-1.1	-0.75	-1.14
K_2O/H/e	+1	-	+0.6	+0.61	+1	+0.61	+1	+1	+1	+0.61	+1

[a] The Bader charges of OH and H atoms at TSs for various clean, K-pre-adsorbed metal surfaces stem from our previous results.[43]