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

Supporting Information

Oxygen assisted H_2O partial dissociation on the Copper: A model study

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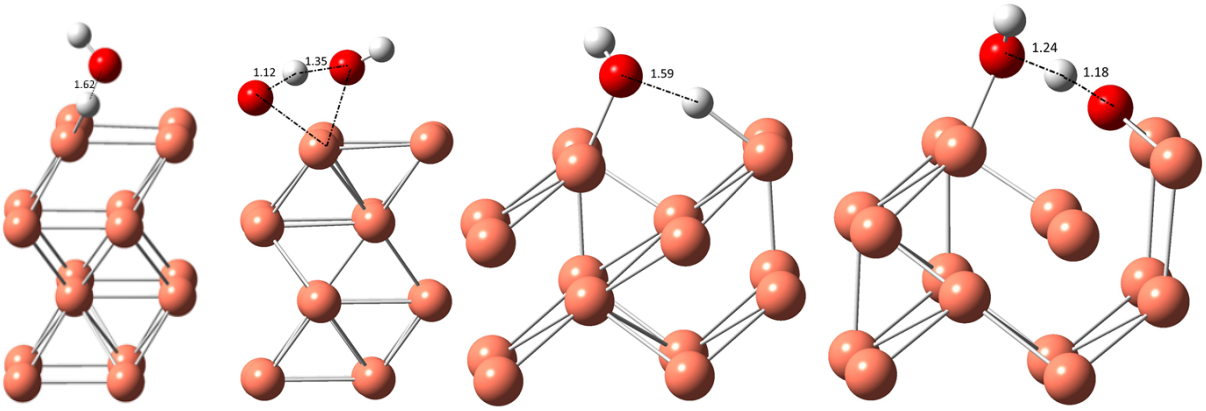
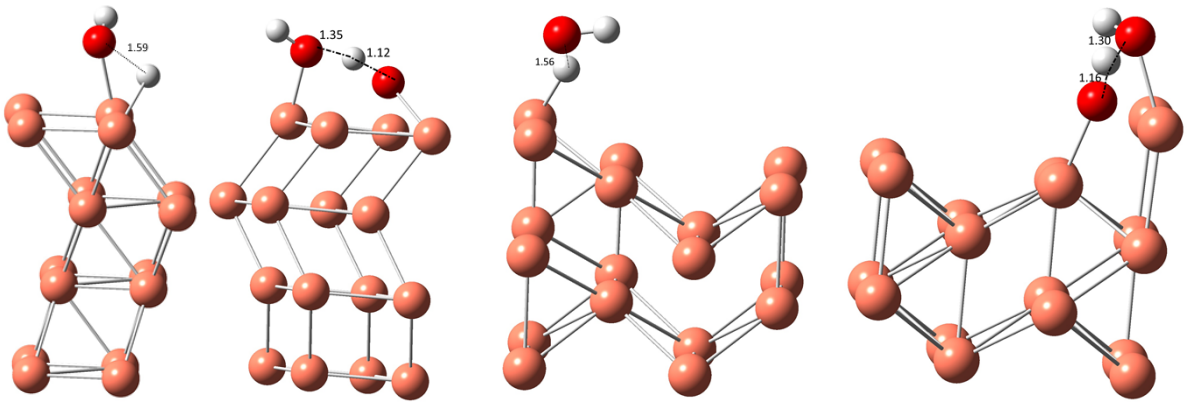
Table S1 Energy decomposition of the adsorption energy of H_2O on clean and oxygen-preadsorbed Cu surfaces (eV).

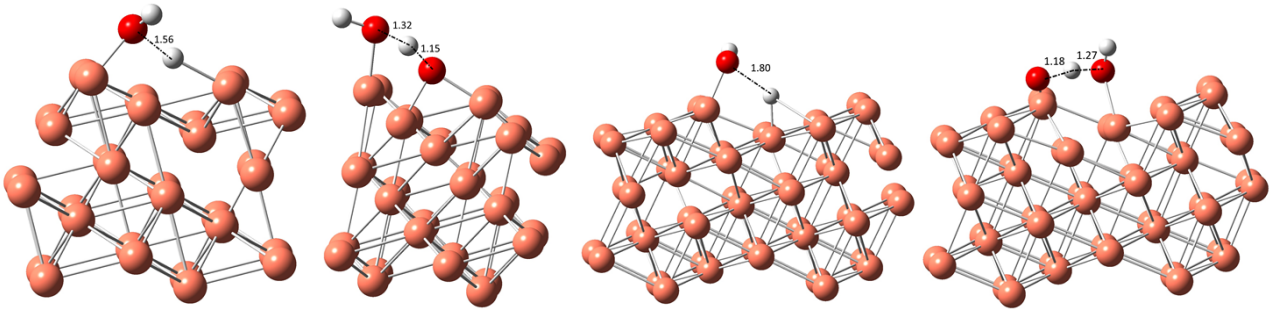
	M				O/M			
	E_{ad}	$E_{Substract}^{Def}$	$E_{H_2O}^{Def}$	E_{int}	E_{ad}	$E_{Substract}^{Def}$	$E_{H_2O}^{Def}$	E_{int}
(111)	-0.22	0.09	0.00	-0.31	-0.65	0.12	0.13	-0.80
(110)	-0.38	0.06	0.00	-0.44	-0.90	0.15	0.17	-1.22
(110)-(1x2)	-0.29	0.11	0.01	-0.41	-0.35	0.15	0.02	-0.52



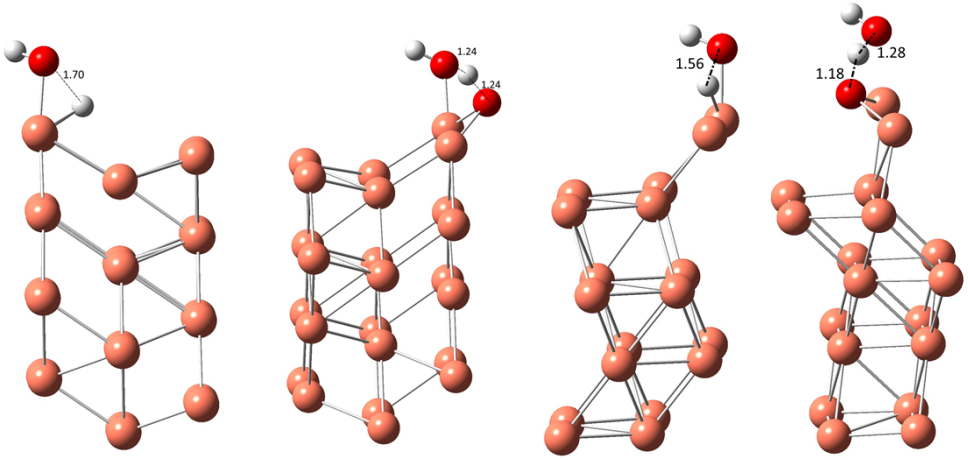
(100) (110)

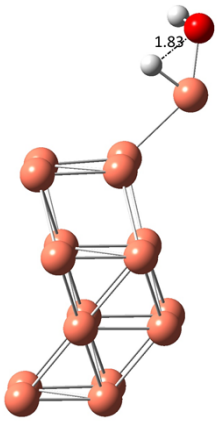


(111) (110)-(1x2)



(210) (310)





(211) Ad-row Ad-atom

Figure S1 The transition states (TSs) of H_2O partial dissociation on clean and oxygen-preadsorbed copper surfaces.