Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Supplementary Information

Water reduction on the facets of $Fe(OH)_2$: an experimental and DFT study

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This PDF file includes:

Figures S1 to S5 and Table S1 to S2

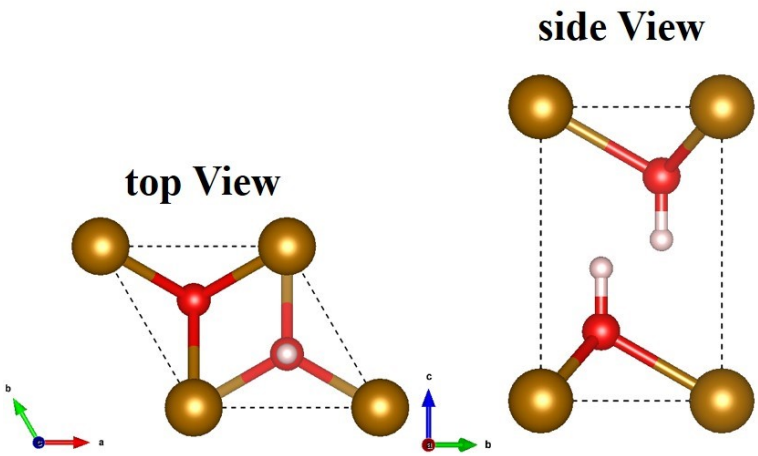

Fig. S1. DFT-optimized crystal structure of $Fe(OH)_2$; Fe = orange spheres, O= red spheres and H = white spheres.

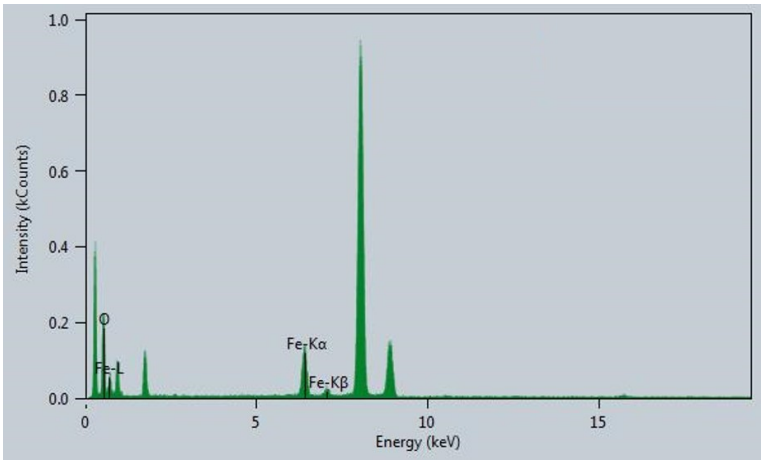

Fig. S2. The elemental spectroscopy of as-prepared $Fe(OH)_2$.

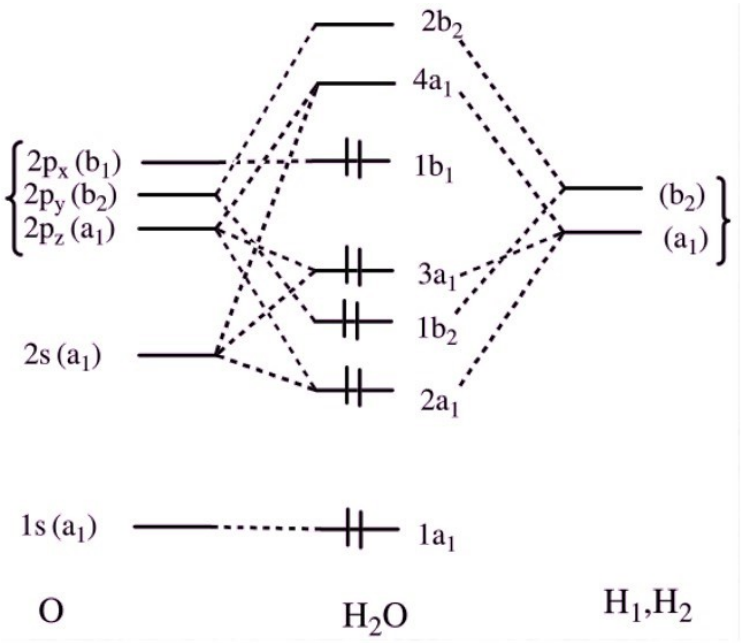

Fig. S3. The schematic diagram for molecular orbitals of free water molecule.

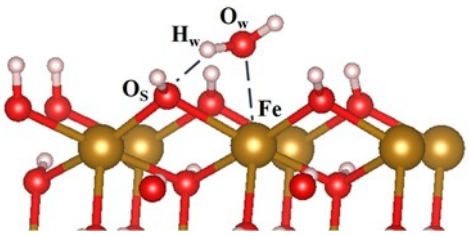

Fig. S4. The DFT-optimized atomic configurations of two atom pairs for COHP and ICOHP calculation, when H_2O was adsorbed on (100) facet of $Fe(OH)_2$.

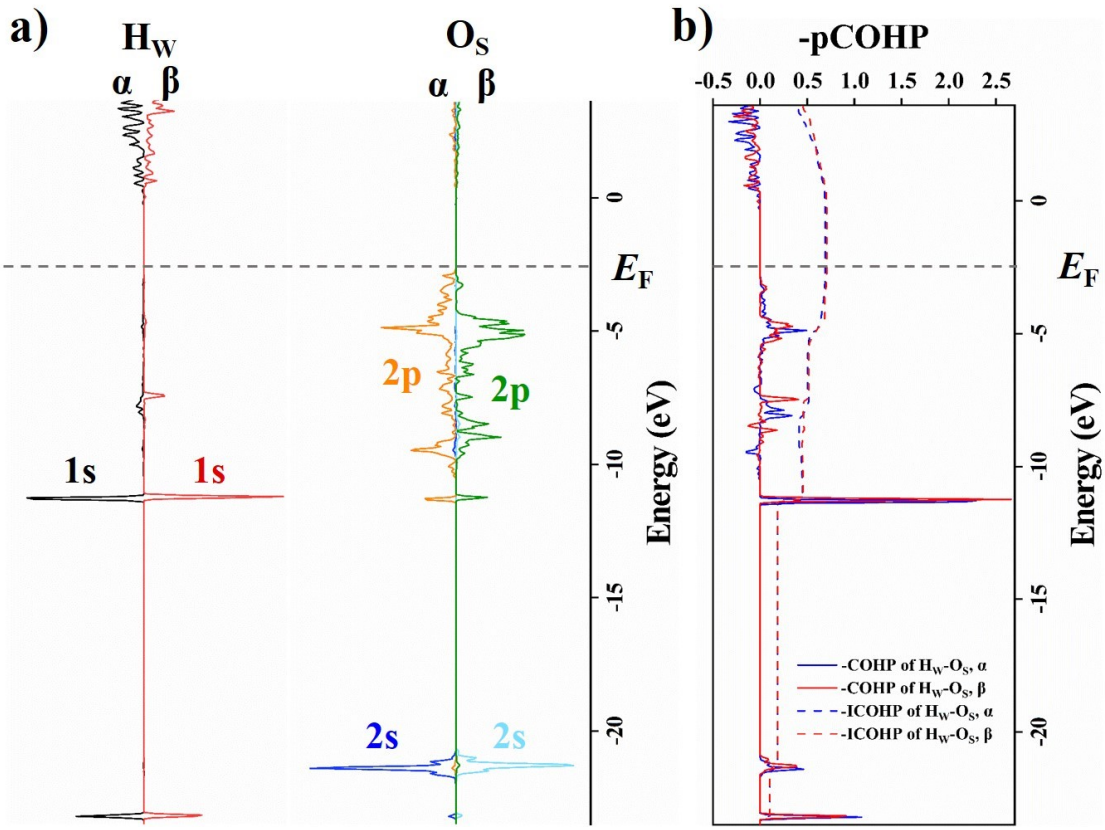

Fig. S5. Projected electronic densities of states (pDOS) of 1s orbital of H_W, 2s and 2p orbitals of O_S on $Fe(OH)_2$ (100) facet after H_2O adsorption. b) The crystal orbital hamilton population (COHP) and integrated COHP (ICOHP) density between H_W and O_S. α = spin up and β = spin down.

Table S1. The comparison of H_2O morphology before and after adsorbed on different facets of $Fe(OH)_2$.

Facet	(100)	(101)	(102)	Free water molecule
Angel/^{o}	105.7	104.9	105.4	104.5
O-H_1/Å	1.015	0.994	0.976	0.973
O-H_2/Å	0.973	0.975	0.974	0.973

Table S2. The Bader charge of free H_2O molecule and after adsorbed on different surfaces of $Fe(OH)_2$.

Sample	Bader charge (electrons)			
	H_1	H_2	O	Total
(100)	0.33	0.26	7.43	8.02
(101)	0.33	0.32	7.34	7.99
(102)	0.34	0.36	7.28	7.98
Free H_2O molecule	0.33	0.31	7.36	8.00