Supporting Information

DFT+U Study of Properties of MoO_3 and Hydrogen Adsorption on MoO_3(010)

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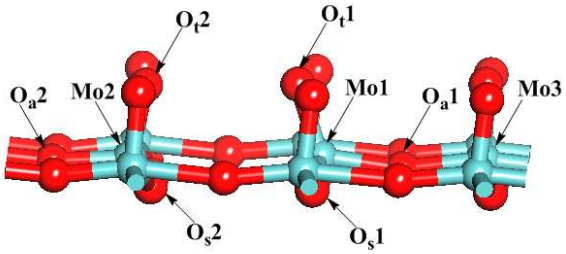
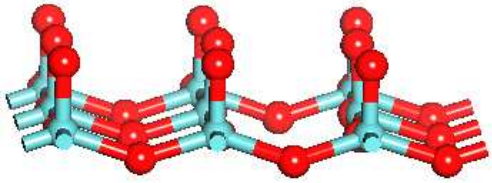
Table S1 The Mo-O bond length of MoO_3 (010) defect surface.

O_a defect		O_s defect	
Bond type	Bond length (Å)	Bond type	Bond length (Å)
Mo1-O_t1	1.73	Mo-O_t	1.72
Mo1-O_a1	1.88	Mo-O_a	1.80, 2.14
Mo3-O_a1	1.86	Mo-O_s	1.97,1.97
Mo1-O_s1	1.97		
Mo2-O_t2	1.71		
Mo2-O_a2	1.78		
Mo3-O_a2	2.04		
Mo2-O_s2	1.92		



(a)



(b)

Figure S1 The asymmetric(a) and symmetric(b) oxygen atom defective surface. Indigo spheres: Mo atoms, Red spheres: O atoms.

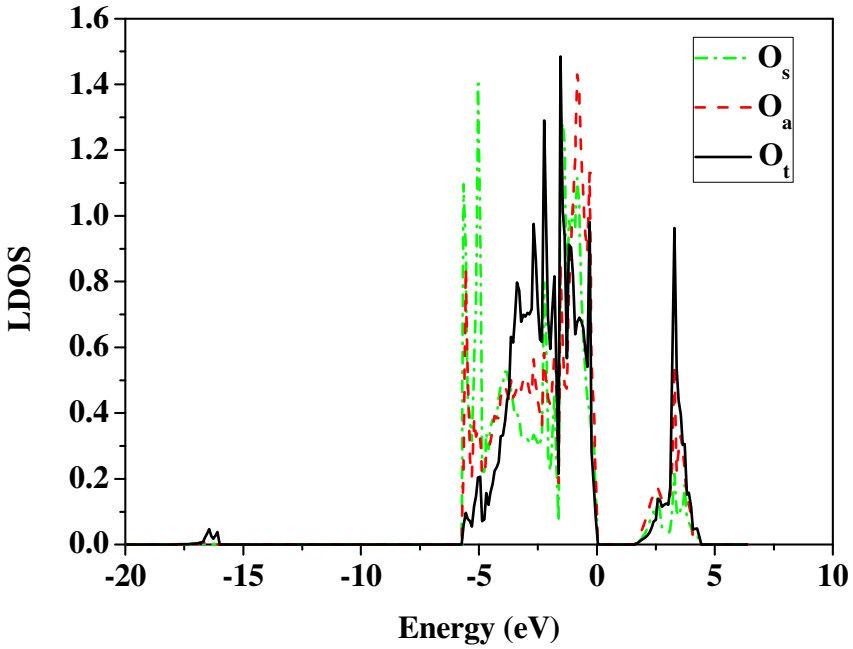


Figure S2 LDOS of three types of oxygen atoms in perfect surface.

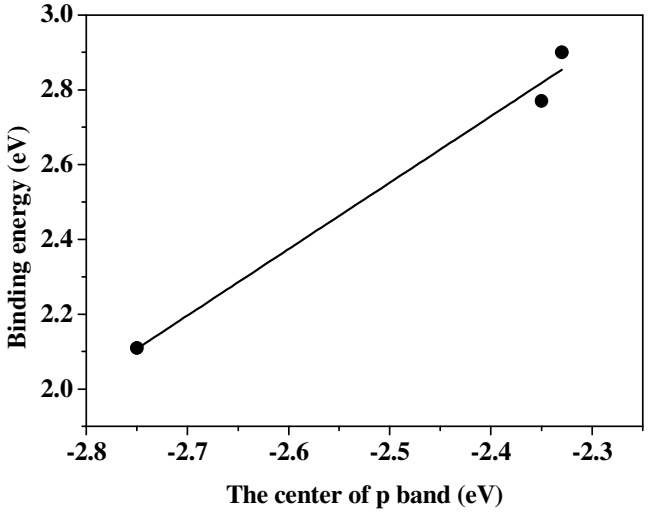


Figure S3 The binding energies of H binding on three types of oxygen atoms and the center of p band of these atoms in the MoO_3(010) surface.