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Supporting Information: Oxygen Deficient α-MoO_3 with Promoted Adsorption and State-Quenching of H_2O for Gas Sensor: A DFT Study

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The formation energy of charged oxygen vacancies.

Table S1 The relative energies (ΔE_0) and electrostatic potential energy (E_{ep}) of the MoO_3 systems with oxygen vacancies in different valence calculated in PBE method, where the total energy of perfect MoO_3 is set to zero for comparison.

	0		**+1**		**+2**	
	ΔE_0 (eV)	E_{ep} (eV)	ΔE_0 (eV)	E_{ep} (eV)	ΔE_0 (eV)	E_{ep} (eV)
Perfect MoO_3	0	3.09	/	/	/	/
V_{Ot}-MoO_3	7.01	3.08	11.20	3.59	16.06	4.12
V_{Oa}-MoO_3	7.01	3.10	11.20	3.60	16.06	4.12
V_{Os}-MoO_3	9.16	3.08	13.32	3.59	17.41	4.12

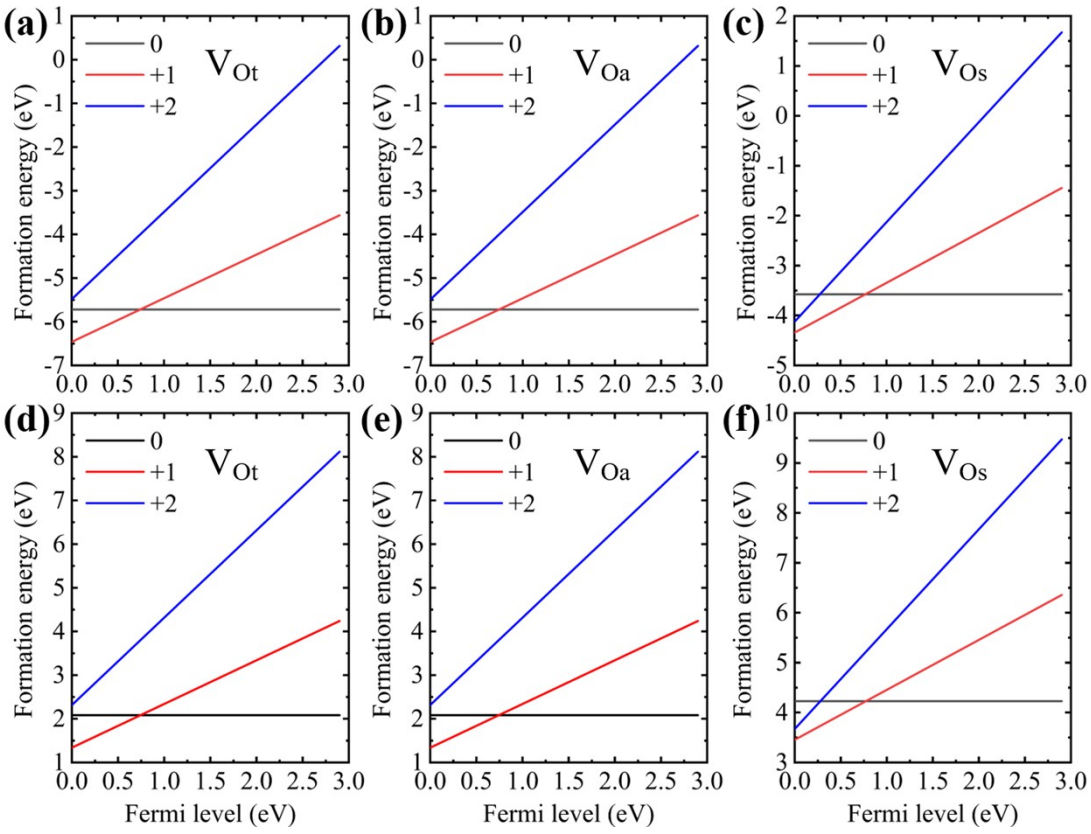

Fig. S1 Vacancy formation energies calculated in PBE method for the terminal, asymmetric, and symmetric O sites. The top row (a-c) refers to the O-poor environment and the bottom row (d-e) to the O-rich environment.

Comparison of V_{Ot}-MoO_3 and V_{Oa}-MoO_3.

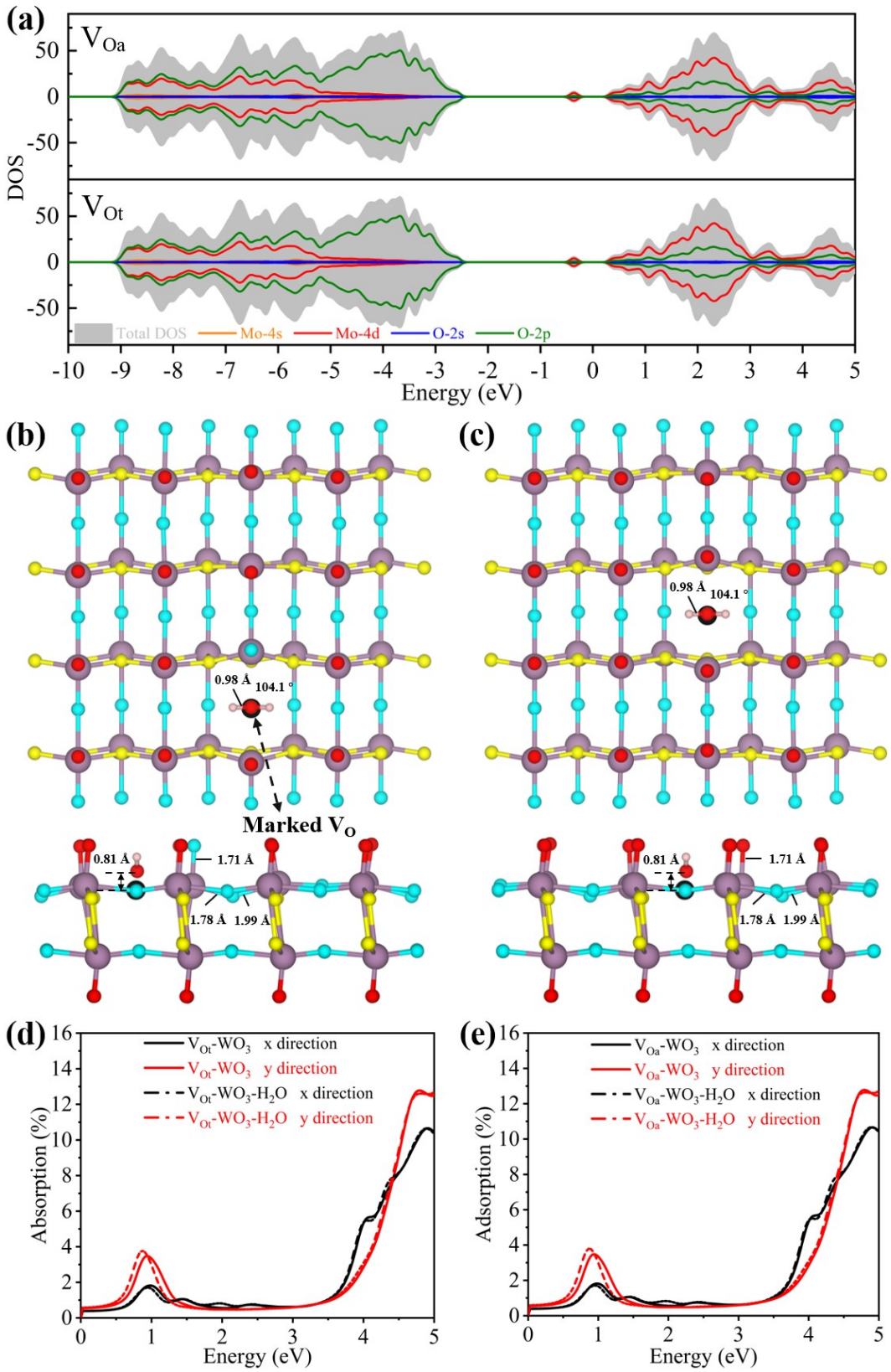

Fig. S2 PDOS (a) of V_{Ot}-MoO_3 and V_{Oa}-MoO_3 systems, and adsorption structures (b and c), and absorption spectra (d and e) with the uptake of water.

Adsorption of H_2O molecule on different sites.

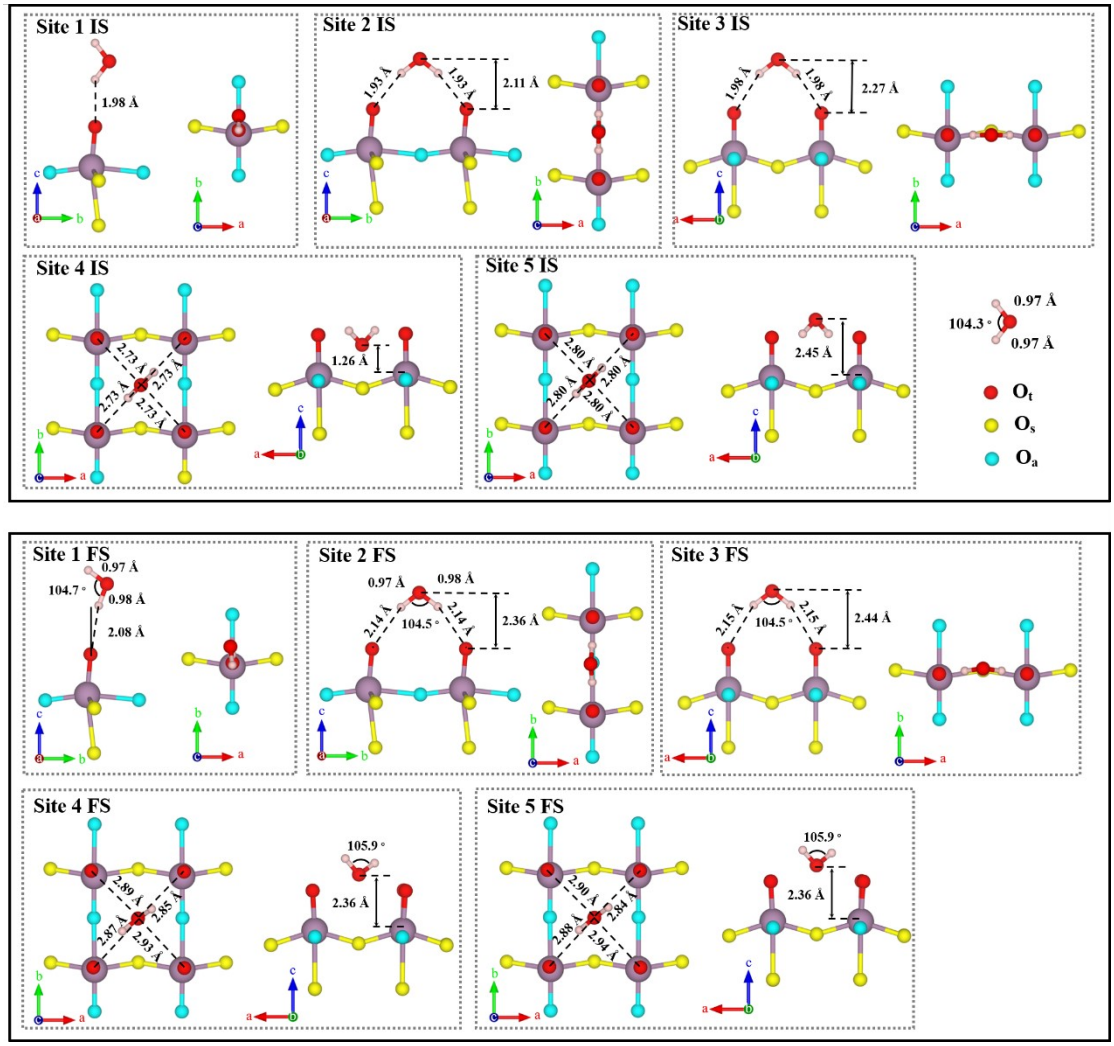

Fig. S3 The five adsorption sites of H_2O on perfect MoO_3 and the corresponding initial (top panel) and final (bottom panel) structures.

Table S2 The adsorption energies of the perfect-MoO_3 with different adsorption sites.

	Site 1	Site 2	Site 3	Site 4	Site 5
E_{ads} (eV)	-0.11	-0.16	0.15	-0.30	-0.30