Supplementary Information for

Modulation effect of S vacancy and Mo edge on the adsorption and dissociation behaviors of toxic gas (H_2S, SO_2) molecules on MoS_2 monolayer

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Figure S1. Spin-polarized band structures for (a) H_2S, (b) tilted structure, and (c) end-on structure of SO_2 adsorbed on MoS_2 with SV and (d) H_2S, (e) tilted structure, and (f) end-on structure of SO_2 adsorbed on Mo edge.

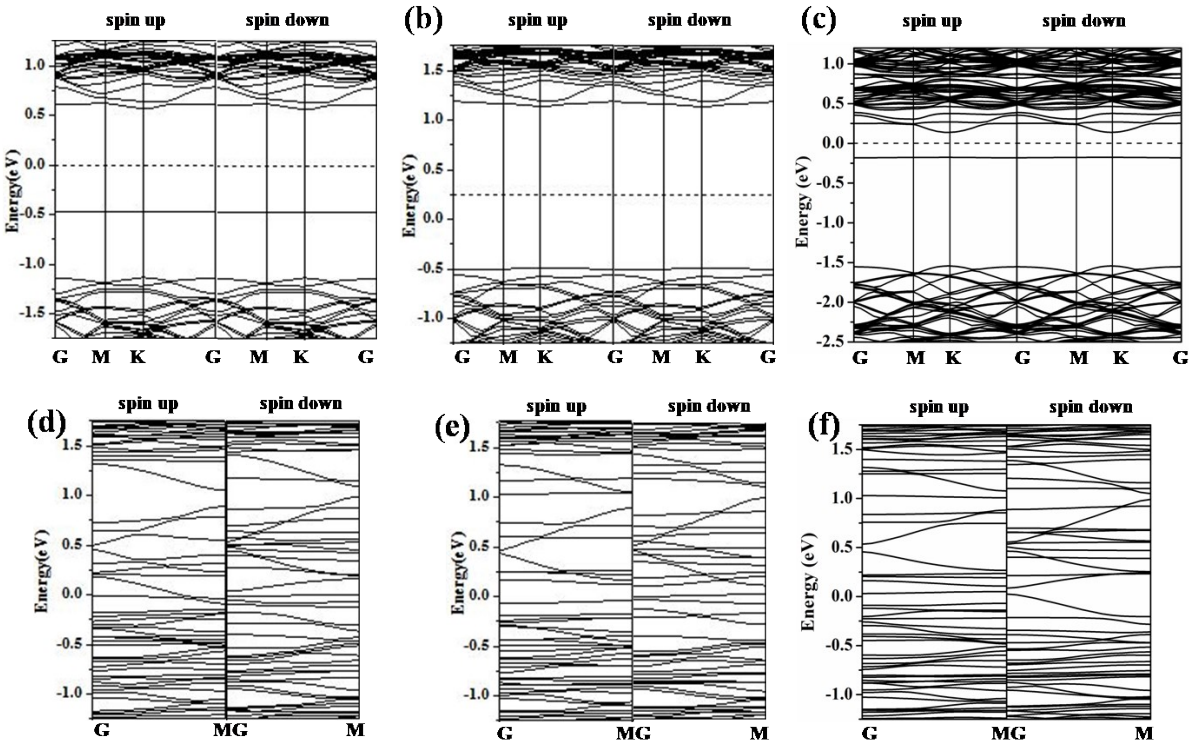

Figure S2. Calculted spin-polarized band structure and total density of states (TDOS) for the dissociated configuration of H_2S on MoS_2 with S vacancy.

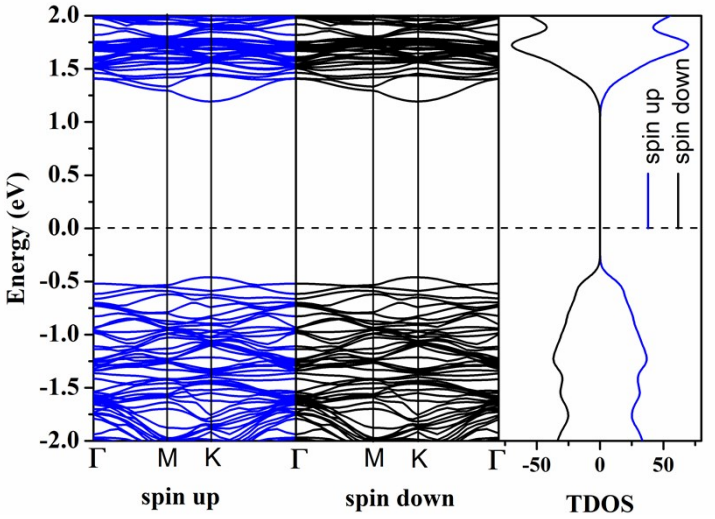

Figure S3. Top view (upper panel) and side view (lower panel) of optimized structure of O and S-O group adsorbed at Mo-50 edge, which is energetically unfavored by 1.25 eV related to the geometry of SO_2 molecule physisorbed at Mo-50 edge shown in Fig.4(b).

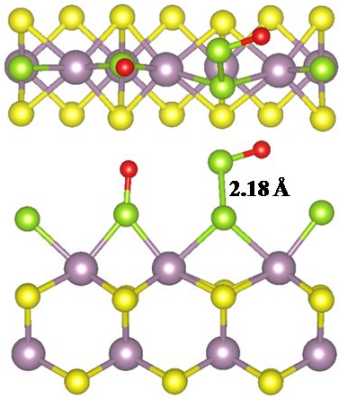

Figure S4. (a) Top view (upper panel) and side view (lower panel) of optimized structure of H-Mo-50 edge.

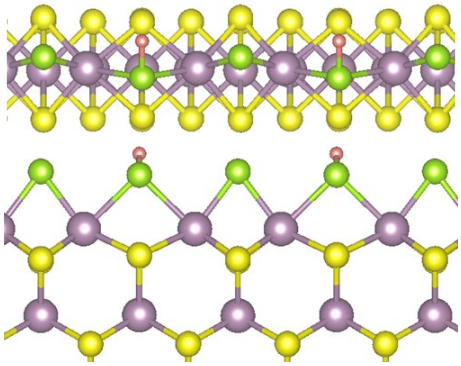

Table S1. Calculated formation energy (E_f) of single S vacancy of pristine MoS_2 ML and edge S vacancy of Mo-50 edge. The formation energy is calculated as $E_f = E_{SV} + V_S - E_0$, where E_{SV}, E_S and E_0 are calculated total energies for MoS_2 with SV or Mo-50 edge with edge SV, isolated S atom and clean MoS_2 ML or Mo-50 edge, respectively.

	MoS_2 ML	Mo-50 edge
E_f (eV)	6.65	5.01