

Molybdenum Disulfide as a Highly Efficient Absorbent for Non-polar Gases

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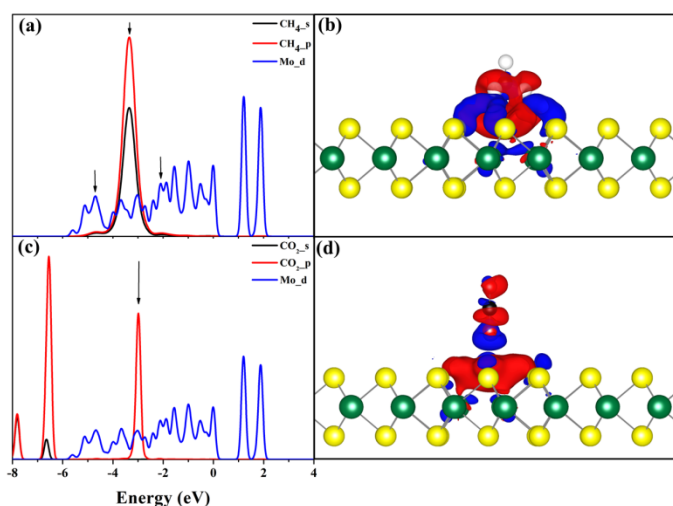


FIG. S1. The projected density of states (PDOS) for the d orbital of Mo and the s and p orbitals of (a) CH_4 and (c) CO_2 ; (b) and (d) are the deformation density for CH_4 and CO_2 adsorbed on MoS_2 layer with S-DV defect. The increase and decrease of the electron density are colored in red and blue, respectively.

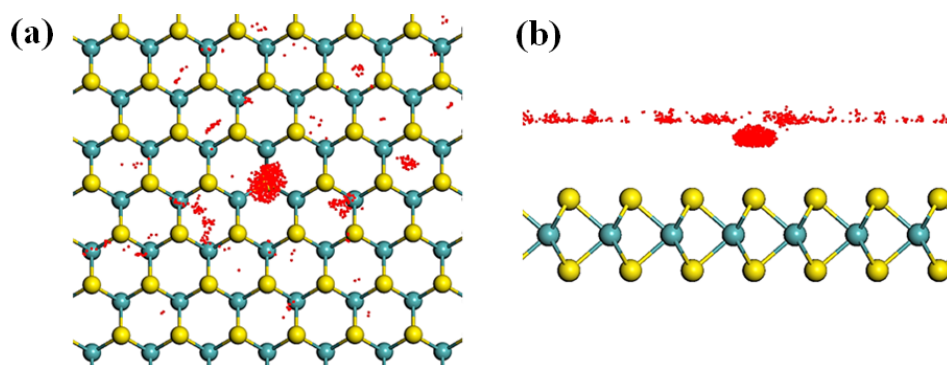


FIG. S2. (a) and (b) are the top view and side view of adsorption density distribution for CO_2 molecules on MoS_2 with S-SV defect at 80 bar.