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

Ningning Yu, Lu Wang*, Min Li, Xiaotian Sun, Tingjun Hou, Youyong Li*

Functional Nano & Soft Materials Laboratory (FUNSOM), Soochow University, Suzhou, 215123 Jiangsu, China. Email: lwang22@suda.edu.cn and yyli@suda.edu.cn

**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.