Electronic Supplementary Material (ESI) for Nanoscale.
This journal is © The Royal Society of Chemistry 2014

Strain Engineering of Selective Chemical Adsorption on Monolayer MoS_2

Liangzhi Kou [a,*], Aijun Du [b], Changfeng Chen[c] and Thomas Frauenheim[a]

[a] Bremen Center for Computational Materials Science, University of Bremen, Am Falturm 1, 28359 Bremen, Germany

[b] School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology, Brisbane, QLD 4001, Australia

[c] Department of Physics and Astronomy and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada, 89154, United States

*Corresponding author: kouliangzhi@gmail.com

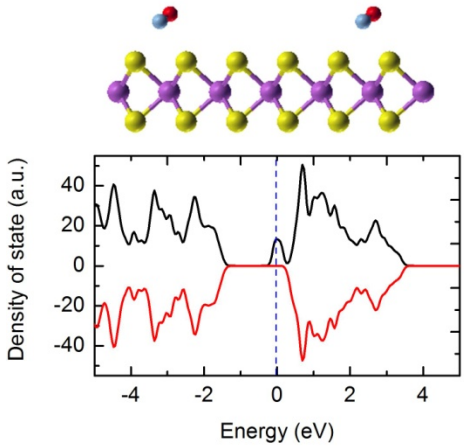

Figure S1. Top: structural model of the 4×4 MoS_2 with 2 NO adsorption; Bottom: the calculated electronic density of states, which shows that half-metallicity is preserved.

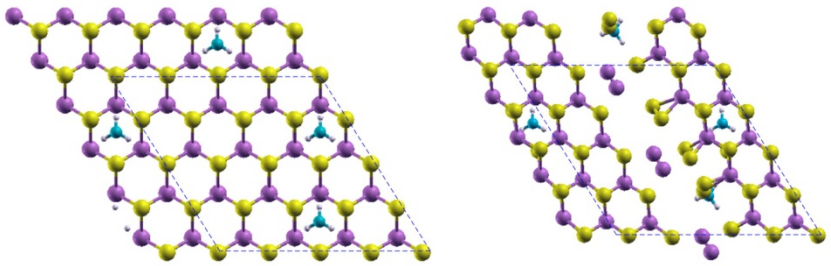

Figure S2. Structural breaking with the adsorption of two ammonia molecules, and the dashed frame denotes the studied supercell.

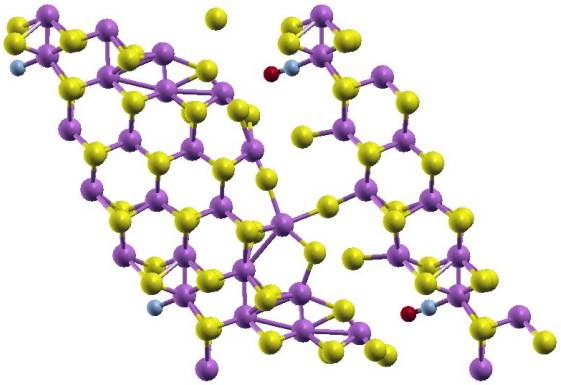

Figure S3. Relaxed structure of NO adsorbed MoS_2 under 18% strain.

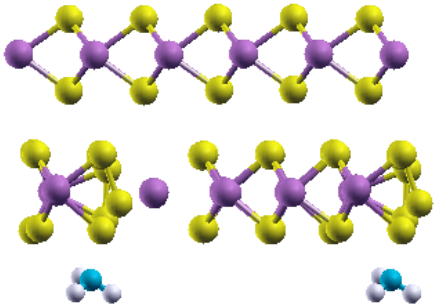

Figure S4. The structure of bilayer MoS_2 with NH_3 adsorption under 12.5% strain.