Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

The effect of hetero-structure material MoS_2-TiO_2(110) on CO and NO adsorption: insights from *ab-initio* calculations[1] TAKAT RAWAL, DUY LE, TALAT RAHMAN, University of Central Florida — Using first-principles simulation based on the density functional theory, we show the effect of substrate on the adsorption of small gas molecules (CO and NO) on molybdenum disulfide (MoS_2) by investigating the adsorption on bare MoS_2 and on MoS_2-TiO_2(110) systems. First, our results show that MoS_2 binds to the rutile TiO_2 surface by forming bonds between unsaturated edge sulfur atoms of MoS_2 with both bridge oxygen atoms and five-fold titanium atoms of TiO_2. Second, results from structural optimizations show that CO prefers to adsorb on $(\bar{1}010)$ edge (S-edge) of bare MoS_2 but on $(10\bar{1}0)$ edge (Mo-edge) of MoS_2 when coupled to the TiO_2(110) surface. Third, results from Bader analysis indicate a very small difference in charge transfer (i.e. 0.01e) to CO molecule from these two systems. We also present detailed analysis of the electronic density of states and the charge density of adsorbate-substrate systems to explain the effect of substrates on the adsorption of CO. We compare and contrast the adsorption characteristics of NO with those of CO on these surfaces.

[1]Work supported in part by DOE grant DE FG02-07ER15842.

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Date submitted: 14 Nov 2013 Electronic form version 1.4