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Role of defects in the adsorption of small molecules on single-layer hexagonal boron nitride[1] TAO JIANG, TAKAT B. RAWAL, DUY LE, TALAT S. RAHMAN, Universtiy of Central Florida — In this work, we have investigated the adsorption of small molecules (CO, CO_2, H_2) on single-layer hexagonal boron nitride (h-BN) with point defects employing *ab initio* density functional theory (DFT) with incorporation of non-local van der Waals functional. We find that N vacancy (V_N) and N substituted by B (B_N) facilitate the adsorption of CO and CO_2 molecules on h-BN. CO molecularly chemisorbs on h-BN with these defects with adsorption energy of -1.01 eV and -2.56 eV, whereas CO_2 molecularly chemisorbs with adsorption energy of -1.66 eV and -0.094 eV. In contrast H_2 does not chemisorb on these defects. We will analyze the geometric and electronic structure of these systems to establish the rationale for the differences in behavior for these adsorbates. We will also present results of the phonon dispersion of the systems, and discuss the vibrational modes of those adsorbed molecules. These results provide atomistic understanding of the physical processes involved in, occurring at the reaction sites, the conversion of synthetic gases into higher alcohols as observed in recent experiments [1]. [1] R. Blair, and L. Tetrad, private communication (2016)

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