Abstract Submitted
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Ab initio simulation of hydrogen storage in BN systems [1]
STEPHEN SHEVLIN, Queen Mary, University of London, ZHENGXIAO GUO, Queen Mary, University of London — We model via first principles simulation hydrogen storage in boron nitride systems, such as h-BN sheets, the paradigm BN molecule borazine ($B_3N_3H_6$) and ammonia-borane (BNH_6). We found H_2 preferentially adsorbs on the perfect h-BN surface but strongly bound atomic hydrogen prefers to adsorb on vacancies, with consequences for hydrogen storage. The addition of TM (transition metal) atoms to boron nitride, to act as adsorbents for hydrogen, was investigated using borazine as a prototype system for h-BN. The binding of TM atoms (Sc, Ti, V etc.) to borazine was determined, with the variation in bonding intimately related to the electronic structure. The dopants were found to promote the binding of both hydrogen atoms and molecules to borazine, increasing binding energy by ∼300% and 1500%, respectively. Initially TM dihydrides form but as hydrogen concentration increases molecular hydrogen becomes preferred. Bound hydrogen is stable at room temperature and the maximum hydrogen capacity and kinematics of this prototype system will be presented. In addition, the dissociation of BNH_6 *in vacuo*, on the surface of MgH_2, and in the presence of TM catalysts is modeled.

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