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Hydrogen uptake and the 18-electron rule KIRAN BOGGAVARAPU, ANIL KANDALAM, PURU JENA, Virginia Commonwealth University — Hydrogen is considered to be an ideal energy carrier in the foreseeable future; however, the key problem is its storage. Solid state materials capable of storing hydrogen with high gravimetric (9 wt %) and volumetric density (70 g/L) operating under ambient thermodynamic conditions and exhibiting fast hydrogen sorption kinetics are of practical importance. It is clear that the storage material should consist of light elements such as Li, B, and C etc. Hydrides of these elements are too strongly bound to be easily desorbed. Attempts were made to deposit light weight transition metals on carbon surfaces such as fullerenes, nanotubes etc., however, they tend to cluster together reducing hydrogen uptake dramatically. One way to achieve high storage is to functionalize simple organic molecules such as C_4H_4 , C_5H_5 etc. with light weight metals such as Sc and Ti. In this presentation, we will discuss based on DFT computations, the dependence of hydrogen uptake on the nature of substrate, the desorption energies, and the nature of bonding.

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