Computational studies on Transition Metal Based Multidecker Complexes as Hydrogen Storage Materials

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***Abstract*—**A good number of multidecker transition metal complexes have been studied for their hydrogen storage ability. Herein, we report a comparative study on multidecker complexes of $VTi(C_6H_6)_3$, $Sc_2(C_6H_6)_3$, and $Sc_2(C_5H_5)_2(C_6H_6)$ using density functional theory at PBEPBE functional and 6-31G (d,p) basis set level of theory. The three complexes show hydrogen adsorption capacity in a range of 2.94 to 5.28 wt%, with an average binding energy of 0.65 to 0.92 eV/H_2. Trends in adsorption energies, Gibbs free energy changes and energy gaps indicate the adsorption of H_2 molecules on these multidecker complexes is thermodynamically and kinetically favorable.

Keywords: Multidecker complexes; Reactivity descriptors; Physisorption.