Co-sponsored with the Department of Chemistry

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Effect of Doped Transition Metals on Hydrogen Interaction in Complex Hydrides

Developing a practical hydrogen storage material based on light complex metal hydrides requires a detailed understanding of the intrinsic hydrogen-metal bond strength and the effect of local reaction environment. In this talk, I will discuss the results of our DFT study of the transition metal (TM)-doped complex hydrides. In particular, we predicted that the doped transition metal form a surface interstitial complex structure with three neighboring AlH4- groups. We discovered that this complex played important roles in hydrogen release/uptake from TM-doped NaAlH4. Our analysis demonstrated that the early TMs are more effective to reduce the hydrogen desorption energy as well as activate the H—H bond than the late TMs. The hydrogen release/uptake process can be viewed as an exchange of σ-bond ligands (H—H for Al—H) by TM on the basis of the complex through a metathesis process involving σ-bonds. The balanced ability of accepting electrons in and backdonating electrons from the d orbitals of the early TMs made them ideal candidates as catalysts for hydrogen release/uptake. We extended the analysis to Ti-doped LiBH4 and found that both the local complex structure and the effect of doped Ti are different from that in NaAlH4.

Monday, March 7, 2011
548 Hamilton Hall: 3:15-4:15 pm
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