



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 AlH_4^- groups. We discovered that this complex played important roles in hydrogen release/uptake from TM-doped NaAlH_4 . 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 LiBH_4 and found that both the local complex structure and the effect of doped Ti are different from that in NaAlH_4 .

Host:
Dr. Xiao Cheng Zeng
Department of
Chemistry

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548 Hamilton Hall: 3:15-4:15 pm
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