H2 Activation by Lewis Acid Lewis Base Molecular Complexes: From Hydrogen Storage to Molecular Catalysis

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We have been investigating the chemical and physical properties of ammonium borohydride and ammonia borane to gain fundamental insight into the interactions between protonic and hydridic hydrogen in the pedagogical Lewis acid/base pair.

[NH4][BH4] <=> H3NBH3 + H2

Using a combination of experimental thermochemistry, spectroscopy, and kinetics with computational modeling approaches we have developed an understanding of how to optimize the reactivity of these materials to permit development of novel solutions to energy storage for fuel cell power applications - however, we are now interested in a larger context - using ambiphilic complexes to activate small molecules in catalytic transformations. In the first part of this presentation an overview of the structure and dynamics of ammonia borane, the diammoniate of diborane and ammonium borohydride will be described to provide a baseline for understanding the reactivity of hydrogen activation in simple Lewis acid/base pair complexes. The second part of the presentation will provide an account of new efforts to understand approaches to modify the structure/reactivity relationships to tune the thermodynamics of hydrogen activation in Lewis acid/base complexes with a goal towards catalytic hydrogenation.