HYDROGEN STORAGE ISSUES IN A NEW HYDROGEN ECONOMY

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The limited supply of fossil fuels, its adverse effect on the environment, and growing worldwide demand for energy has necessitated the search for new and clean sources of energy. The possibility of using hydrogen to meet this growing energy need has rekindled interest in the study of safe, efficient, and economical storage of hydrogen. Unfortunately, the current methods for storing hydrogen as a compressed gas or liquid do not meet the industry requirements. An alternate method for hydrogen storage involves metal hydrides. The conventional intermetallic hydrides store hydrogen at interstitial sites and are reversible at around room temperature. However, the relative weight of stored hydrogen in these materials is rather low (1 – 3 wt %) and do not meet the requirement of the transportation industry (~10 wt %). A novel approach for hydrogen storage is to combine the favorable kinetics and thermodynamics of conventional metal hydrides with that of the large hydrogen storing capacity of organic molecules such as CH_4. Although alanates, with the chemical composition $[M^{n+} (AlH_4)^{n-}$, M= Li, Na, K, Mg], belong to this class, the desorption temperature of hydrogen in these materials is rather high. It was recently discovered that doping of Ti-based catalyst in $NaAlH_4$ can significantly lower the hydrogen desorption temperature, but why and how Ti accomplishes this task remains a mystery. Using first principles calculations, we will provide a molecular level understanding of the role of Ti in lowering the hydrogen desorption temperature in $NaAlH_4$ and $LiBH_4$. It is hoped that the understanding gained here can be useful in designing better catalysts as well as hosts for hydrogen storage.