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### **Computational Study of Metal Hydride Destabilization**

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The safe and efficient on-board storage of hydrogen in fuel cell vehicles is one of the major road-blocks for utilization of hydrogen in transportation. This talk will illustrate the use quantum molecular modeling techniques for investigating atomic-level details of hydrogen storage in new materials. Metal hydrides of period 2 and 3 materials have high volumetric and gravimetric hydrogen storage capacities. However, these materials typically have very high heats of reaction, meaning that high temperatures are required to dissociate the hydrides. Likewise, hydrogenation reactions evolve very large quantities of energy, making thermal management during refueling a impractical. Recent experimental work has focused on chemical destabilization of metal hydrides as a means of decreasing the heats of reaction. We have carried out quantum mechanical calculations, using the electronic density functional theory (DFT) formalism, for various metal hydride systems. The heats of reaction for over 300 different reactions have been computed. We have compared our calculations with experimental and tabulated data where available and find reasonable agreement. Our calculations demonstrate the utility of DFT for screening reactions and for identifying promising materials for further computational and experimental studies. We have also studied the hydration of  $\text{Mg}_2\text{Si}$ , a destabilized hydride of  $\text{MgH}_2$ . Experiments have failed to hydrogenate this material in the laboratory under high pressures of  $\text{H}_2$ . We examine adsorption of  $\text{H}_2$  and dissociation on the  $\text{Mg}_2\text{Si}(110)$  surface to see if kinetic limitations are responsible for the failure to observe hydrogenation of this material.