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Density Functional Screening of Metal Hydride Reactions[1] KARL JOHNSON, University of Pittsburgh, SUDHAKAR ALAPATI, Carnegie Mellon University, BING DAI, University of Pittsburgh, KI-CHUL KIM, DAVID SHOLL, Georgia Institute of Technology — The on-board storage of hydrogen is one of the most vexing problems associated with the development of viable fuel cell vehicles. Hydrides of period 2 or 3 metals can store hydrogen at high gravimetric and volumetric densities. However, existing hydrides either have unacceptable thermodynamics or kinetics. New materials for hydrogen storage are therefore needed. We demonstrate how first principles density functional theory (DFT) can be used to screen potential candidate materials for hydrogen storage. We have used DFT calculations in conjunction with a free energy analysis to screen over a million reactions involving 212 known compounds. This approach has identified several interesting reaction schemes that have not yet been explored experimentally. We have computed the phonon density of states and used this information to predict the van't Hoff plots for some of the most promising candidate reactions identified though our modeling. We have also examined the thermodynamics of thin films and nanoparticles for selected metal hydrides by accounting for the surface energies of the films or nanoparticles.

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