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Discovery of Novel Hydrogen Storage Materials: An Atomic Scale Computational Approach

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136 DeBartolo Hall**

Professor Wolverton is a member of the International Commission C20 of IUPAP on Computation Physics and a member of the DOE/FreedomCAR Hydrogen Storage Technical Team. He received his Ph.D. in Physics from the University of California at Berkeley in 1993, and his B.S. degree in Physics from the University of Texas at Austin in 1987. He has been recognized for his many achievements and most recently received the USCAR Recognition Award and the Noah Greenberg Award from the American Musicological Society.



ABSTRACT

Practical hydrogen storage for mobile applications requires materials that exhibit high hydrogen densities, low decomposition temperatures, and fast kinetics for absorption and desorption. Unfortunately, no reversible materials are currently known that possess all of these attributes. Here we present an overview of our recent efforts aimed at developing a first-principles computational approach to the discovery of novel hydrogen storage materials. Such an approach requires several key capabilities to be effective: (i) Accurate prediction of decomposition thermodynamics, (ii) Prediction of crystal structures for unknown hydrides, and (iii) Prediction of preferred decomposition pathways. We present examples that illustrate each of these three capabilities: (i) prediction of hydriding enthalpies and free energies across a wide range of hydride materials, (ii) prediction of low-energy crystal structures for complex hydrides, [such as $\text{Ca}(\text{AlH}_4)_2$, CaAlH_5 , and Li_2NH], and (iii) predicted decomposition pathways for $\text{Li}_4\text{BN}_3\text{H}_{10}$ and destabilized systems based on combinations of LiBH_4 , $\text{Ca}(\text{BH}_4)_2$ and metal hydrides. For the destabilized systems, we propose a set of thermodynamic guidelines to help identify thermodynamically viable reactions. These capabilities have led to the prediction of several novel high-density hydrogen storage materials and reactions.

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