

Abstract Submitted  
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**Computational search for hydrogen storage materials: accuracy and alloys**<sup>1</sup> LUCAS WAGNER, Massachusetts Institute of Technology, ERIC MAJZOUB, University of Missouri-Saint Louis, MARK ALLENDORF, Sandia National Labs, JEFFREY GROSSMAN, Massachusetts Institute of Technology — Metal hydride materials are among the strongest contenders for hydrogen storage, offering good weight and volume density. The main reason that these materials are not used now is that it is very challenging to find a material that is both light enough and has the proper binding to allow for easy absorption/desorption near room temperature. We will evaluate two routes to controlling the binding energy: particle size and alloy composition using the highly accurate quantum Monte Carlo method. We find that traditional methods of calculating the binding energy such as the Wulff construction and density functional theory should be applied with caution, as they can lead to misleading results. We will also report on the prospects for finding a sweet spot of size and alloy composition that has the correct binding energy for hydrogen storage applications.

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