

Abstract Submitted
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Thermodynamic guidelines for the prediction of hydrogen storage reactions and their application to destabilized hydride mixtures¹ DONALD SIEGEL, Ford Motor Company, C. WOLVERTON, Northwestern University, V. OZOLINS, University of California at Los Angeles — We propose a set of thermodynamic guidelines aimed at facilitating more robust screening of hydrogen storage reactions. The utility of the guidelines is illustrated by reassessing the validity of reactions recently proposed in the literature and through vetting a list of more than 20 candidate reactions based on destabilized LiBH_4 and $\text{Ca}(\text{BH}_4)_2$ borohydrides. Our analysis reveals several reactions having both favorable thermodynamics and relatively high hydrogen densities (ranging from 5–9 wt % H_2 and 85–100 g H_2/l), and demonstrates that chemical intuition alone is not sufficient to identify valid reaction pathways.

¹D. J. Siegel et al, Phys. Rev. B **76**, 134102 (2007)

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