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Predicting new multicomponent materials for hydrogen storage using first-principles calculations DILPUNEET AIDHY, CHRIS WOLVERTON, Northwestern University — Wide research has unraveled some very promising hydrogen storage materials such as metal borohydrides, amides and alanates. However, all of these materials are limited either thermodynamically or kinetically. The recent observation of mixing in these systems (e.g., borohydride-amide mixing in $Li_4(BH_4)(NH_2)_3$ [1] and metal mixing in $NaZn_2(BH_4)_3$) [2] has demonstrated the possibility of forming new multicomponent ordered compounds that may have desirable hydrogen storage properties. However, these multicomponent systems are largely unexplored. Here, we use density functional theory (DFT) along with Monte Carlo-based crystal structure prediction methods to search for new multicomponent hydrides. We find evidence for stable compounds in the $Mg(BH_4)_2/Mg(NH_2)_2$ system, which have not yet been observed. In addition, we also study a wide range of mixed metal borohydride systems, and find evidence of ordered stable structures such as $Li_2Na(BH_4)_3$. 1. F. E. Pinkerton, M. S. Meyer, G. P. Meisner and M. P. Balogh, J. Phys. Chem. B 110, 7967 (2006). 2. D. Ravnsbeak, Y. Filinchuk, Y. Cerenius, H. J. Jakobsen, F. Besenbacher, J. Skibsted and T. R. Jensen, Angew. Chem. 48, 6659 (2009).

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