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Suppressing diborane production during the hydrogen release in metal borohydrides: The example of doped $Al(BH_4)_3$[1] DAVID HARRISON, TIMO THONHAUSER, Wake Forest University — Aluminum borohydride ($Al(BH_4)_3$) is an example of a promising hydrogen storage material with exceptional hydrogen densities by weight and volume and a low hydrogen desorption temperature. But, unfortunately its production of diborane (B_2H_6) gases upon heating restricts its practical use. To elucidate this issue, we investigate the properties of a number of metal borohydrides with the same problem and find that the electronegativity of the metal cation is not the best descriptor of diborane production. We show that, instead, the closely related formation enthalpy is a much better descriptor and we find that diborane production is an exponential function thereof. We conclude that diborane production is sufficiently suppressed for formation enthalpies of -80 kJ/mol BH_4 or lower, providing specific design guidelines to tune existing metal borohydrides or synthesize new ones. We then use first-principles methods to study the stabilizing effects of Sc alloying in $Al(BH_4)_3$, predicting that with sufficient alloying diborane can be fully suppressed. We conclude that stabilizing $Al(BH_4)_3$ and similar borohydrides via alloying or other means is a promising route to suppress diborane production and thus develop viable hydrogen storage materials.

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