

Abstract Submitted
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Improving ammonia borane as a hydrogen storage material with B-group substitutions¹ E. WELCHMAN, T. THONHAUSER, Wake Forest Univ — We present *ab initio* results for substitutions intended to lower the hydrogen desorption temperature of NH_3BH_3 (ammonia borane or AB), already a promising hydrogen storage material. Substitutions in the NH_3 group have previously been investigated with success; we propose a different route, instead performing substitutions in the BH_3 group. To keep gravimetric density high, we focus on the second period elements C, N, O, and F, all with higher electronegativities than H. We also investigate Cu and S as possible substituents. Results include hydrogen binding energies and kinetic barriers for the hydrogen release in the gas phase as well as the solid. Of the substituents studied, we identify Cu as the most promising substituent, which lowers the reaction barrier for the hydrogen release by 38% compared to pure AB and we estimate a new hydrogen desorption temperature between -10°C and 40°C .

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