Abstract Submitted
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Theoretical characterization of the NHxBHx compounds[1] MACIEJ GUTOWSKI, Pacific Northwest National Laboratory — The NH_xBH_x (x=1-4) compounds display favorable gravimetric and volumetric properties of hydrogen storage. Molecular species have been characterized using highly correlated electronic structure methods. Extended systems (polymers, solids) have been characterized at the density functional level of theory with a Perdew-Wang exchange correlation functional. The results demonstrate unique cohesive properties resulting from dihydrogen intermolecular bonds between protic and hydridic hydrogens of NH and BH, respectively. The kinetic and thermodynamic parameters for hydrogen release and uptake will be discussed.

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