

Abstract Submitted
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Hydrogen clathrates of ammonia borane MACIEJ GUTOWSKI, ALEXANDER ABRAMOV, Chemistry-School of EPS, Heriot-Watt University — The concept of hierarchical hydrogen storage is illustrated by clathrates built from ammonia borane (AB) and loaded with molecular hydrogen. These new materials would have two levels of hydrogen storage: (i) physisorbed H₂ and (ii) hydrogen chemically bound in AB. The advantages of these materials would be: (i) fast kinetics and (ii) high hydrogen density. We developed a construction principle for clathrates of AB and performed electronic structure calculations for isolated cages and for periodic structures. Hydrogen capacity of the most stable periodic structure (cuntruncated cubic honeycomb) is estimated to be 21 wt%, 19 wt% chemically bound in AB and 2 wt% of H₂ physisorbed in cages of AB. We developed a statistical model of clathrate phase equilibria that is based on calculated guest-host interactions, entropy of guest molecules in spherical cages, and corrections for non-ideality of gases. Application of the model to known hydrates showed quantitative agreement between experimental and theoretical data. We predicted stability of hydrogen clathrates of ammonia borane at ambient pressure and T=77 K. Further stabilization by formation of double clathrates and semi-clathrates will be discussed.

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