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Ab-initio kinetics and thermodynamics studies of ammonia-borane for hydrogen storage[1] CAETANO R. MIRANDA, GERBRAND CEDER, Massachusetts Institute of Technology — Ammonia-borane (BH_3NH_3) is a promising chemical hydrogen storage material given its high gravimetry and volumetric properties. However, the ammonia-borane (AB) thermal hydrogen release is not very efficient, being mainly limited by the kinetics of hydrogenation. Using ab initio calculations, we have investigated the thermodynamics and kinetics of hydrogen release on AB by calculating the free energies of the H_2 release reactions for different possible decomposition products. Our results indicate that AB regeneration through the ammonia-borane polymeric and borazine-cyclotriborazane cycles is very unlikely due to the strong exothermic character of the reactions. The kinetics of hydrogen release is further investigated with the recently developed metadynamics method. This method allows us to calculate the multidimensional free energy surface of hydrogen release on AB. Our simulations reveal the atomistic mechanism of hydrogenation and provide the free energies barriers and transition states involved in inter and intramolecule H_2 release on AB.

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