A Coupled Cluster Approach to Computationally Design an Acid Catalyst for Viable Release of H2 from BN Nanotubes

Lisa Roy[1]

[1]Institute of Chemical Technology

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Abstract

Catalytic removal of H2 from boron-nitride (BN) based nanomaterials at ambient conditions is of paramount importance in order to develop light-weight hydrogen storage media. Herein, the DLPNO- CCSD(T) technique is used for calculating accurate relative energies and activation barriers of Brønsted acid-initiated removal of H2 from hydrogenated BN nanotubes (HBNNTs) with several in silico designed catalysts. Three crucial steps are identified in the mechanism: 1st H2 release, catalyst regeneration via proton transfer and 2nd H2 release to ensure feasibility of the dehydrogenation proposal. Our computational studies reveal that sulfonic acids with appropriate electron withdrawing substituents can facilitate dehydrogenation of HBNNT at a low free energetic cost ([?]G++ = 17 kcal mol-1). Importantly, these findings illustrate reversibility of hydrogen stored in BN nanomaterials at room conditions and raises hope for a sustainable chemical hydrogen storage strategy.

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