First-principles calculations of covalently-bonded 3D networks of graphitic boron-nitride for hydrogen storage

SANGHOON LEE, Department of Physics, POSTECH, SEUNG-HOON JHI, Department of Physics and Division of Advanced Materials Science, POSTECH — Graphitic nanomaterials such as carbon nanotube (CNT) and covalently-bonded graphene (CBG) have attracted great attention due to their large surface area for high-capacity hydrogen storage. We carried out first-principles calculations based on density functional theory of covalently-bonded 3D networks of hexagonal boron nitride (hBN) layers and investigated the metal dispersion and subsequent hydrogen adsorption inside the networks. We performed a comparative analysis of stability, metal dispersion, and hydrogen sorption between graphene, CNT, hBN single layer, and 3D hBN networks.

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