Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

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.

SangHoon Lee
Department of Physics, POSTECH

Date submitted: 27 Nov 2011 Electronic form version 1.4