Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Computational Study of hydrogen storage characteristics of the Covalent-Bonded Graphites. NOEJUNG PARK, Dankook University, Seoul, Korea, SEUNG-HOON JHI, KYUBONG KIM, Pohang University of Science and Technology, Korea, SUKLYUN HONG, Sejong University, Seoul, Korea — We perform electronic structure calculations to investigate hydrogen-storage characteristics of the solid carbon structures which consist of covalent-bonded graphenes. First, we show that some regular or irregular combinations of $\boldsymbol{sp}^2$-and $\boldsymbol{sp}^3$-bonded carbon atoms lead to very stable porous carbon structures, which is designated as the covalent-bonded graphites (CBGs). Using the density-functional calculation and the Møller-Plesset perturbation method we show that the H_2 molecular bindings in CBGs are stronger than those on the isolated graphene by about 20%. We also suggest the CBGs with appropriate pore sizes can be utilized as framework structures for dispersing metal atoms. Energetics show that the Ti atoms are likely to be adsorbed at vertex sites of the CBGs. The hydrogen adsorption properties on metal atoms dispersed inside the CBGs are also presented.

Noejung Park
Dankook University

Date submitted: 04 Dec 2006 Electronic form version 1.4