Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Exfoliation of graphene flake from SiC substrate using hydrogen injection; a first-principle study BORA LEE, SEUNGWU HAN, Ewha Womans University, YONG-SUNG KIM, Korea Research Institute of Standards and Science — Recently there is an immense interest in studying graphene for investigating its unique electronic properties as well as practical applications to nanoscale devices. Up to now there are two methods to obtain graphene layers. The first one is a mechanical method in which the single graphene sheet is split off the bulk graphite crystals using adhesives. The other method is graphitization of SiC surfaces by annealing at elevated temperatures. Even though the latter approach can provide a graphene layer in a more controlled way, the exfoliation of the graphene layer still poses a big challenge. In this presentation, based on the first-principles results, we propose a novel exfoliation method using hydrogen. As a model system, the 6H-SiC(0001) 4×4 cell is used, which corresponds to the 3×3 graphene cell. We calculate the binding energy of single hydrogen atom in various places; above and below graphene surface and inside the first SiC layer. The binding energies of hydrogen are calculated for different coverages. It is found that at high coverages, the hydrogen atoms prefer to bind below the graphene surface, cutting the graphene-SiC bonds. This means that the graphene can be exfoliated in the hydrogen-rich environment. The detailed analysis including the electronic structures will be presented.

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Date submitted: 20 Nov 2008 Electronic form version 1.4