Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Cohesion Energetics of Carbon Allotropes: Quantum Monte Carlo Study HYEONDEOK SHIN, SINABRO KANG, JAHYUN KOO, HOONKYUNG LEE, School of Physics, Konkuk University, KOREA, JEONGNIM KIM, Materials Science and Technology Division and Computer Science and Mathematics Division, Oak Ridge National Laboratory, YONGKYUNG KWON, School of Physics, Konkuk University, KOREA — We have performed quantum Monte Carlo calculations to study the cohesion energetics of carbon allotropes, including sp^3-bonded diamond, sp^2-bonded graphene, sp-sp^2 hybridized graphynes, and sp-bonded carbyne. The computed cohesive energies of diamond and graphene are found to be in excellent agreement with the corresponding values determined experimentally for diamond and graphite, respectively, when the zero-point energies, along with the interlayer binding in the case of graphite, are included. We have also found that the cohesive energy of graphyne decreases systematically as the ratio of sp-bonded carbon atoms increases. The cohesive energy of γ-graphyne, the most energetically-stable graphyne, turns out to be 6.766(6) eV/atom, which is smaller than that of graphene by 0.698(12) eV/atom. Experimental difficulty in synthesizing graphynes could be explained by their significantly smaller cohesive energies. Finally we conclude that the cohesive energy of a newly-proposed two-dimensional carbon network can be accurately estimated with the carbon-carbon bond energies determined from the cohesive energies of graphene and three different graphynes.

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Date submitted: 08 Nov 2013 Electronic form version 1.4