Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Strain effect on electronic properties of low-dimensional γ-graphyne : first principles study HYEONSU LEE, SEOUNG-HUN KANG, SORA PARK, CHANG-SUN LEE, YOUNG-KYUN KWON, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University — Using first-principles calculations, we study the interplay between structural and electronic properties of γ-graphyne nanotubes (γGNTs) consisting of hexagonal carbon rings and acetylenic linkages. We first identify the equilibrium structures of various γGNTs classified in terms of chirality: $(n, 0)$ denotes an armchair-type tube, whereas (n, n) does a zigzag-type, in contrast with CNTs. Then their Young's moduli are calcuated to be a few hundreds in GPa, which are smaller than those of CNTs. We verify that all γGNTs are intrinsic semicondutors with energy gap ($\lesssim$ 1.22 eV) decreasing with tube diameter. It is, however, found that axial strain can significantly modifies the electronic structures of semiconducting γGNTs. Very intriguingly, even semiconductor-metal transition occurs under compressive strain: all armchair γGNTs, exept for (3,0) γGNT with small diameter, become metallic, while only some types of zigzag γGNTs metallic under compression. To explain the origin of such electronic structure modifications, we examine the effect of structural change on the band structures of two-dimensional γ-graphyne sheet under strains and match them with the band structure of γGNTs using the zone-folding scheme.

Young-Kyun Kwon
Department of Physics and Research Institute for Basic Sciences,
Kyung Hee University

Date submitted: 15 Nov 2013 Electronic form version 1.4