Electronic structures of boron-doped single-walled carbon nanotube

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Since the discovery of the superconductivity in boron-doped diamond [1], the carrier doping, especially boron doping in carbon materials attracts much attentions. For the carbon nanotube, however, the effect of boron doping as well as the possibility of the superconductivity [2] have not been well understood yet. Thus, we systematically study the boron-doped single-walled zigzag carbon nanotube using density functional theory to explore the basic properties of boron-doped nanotubes.

From the total energies of isolated boron-doped carbon nanotubes obtained after the geometrical optimization, it is found that the energy cost of substitutional boron doping is smaller for thin nanotubes. Furthermore, the energy cost exhibits a clear periodicity in the case of zigzag nanotubes as shown in Fig. 1.

For the (10,0) nanotube, which is a moderate-gap semiconductor, we calculated the doping rate dependence of the electron structure and found that the boron-doped nanotube has the hole-doped valence band within our calculated boron concentrations (0.8-2.5at.%). However, the Fermi level is already off the peak of the density of states. We speculate that the low boron concentration is sufficient to realize the high Fermi-level density of states and the superconductivity in boron-doped nanotube, which is in sharp contrast to the boron-doped diamond. We also discuss the effect of the intertube interaction on the electronic structure of crystalline bundles.

References:

[1] E.A. Ekimov et al., Nature **428** 542 (2004).
[2] I. Takesue et al., Phys. Rev. Lett. **96** 057001 (2006).

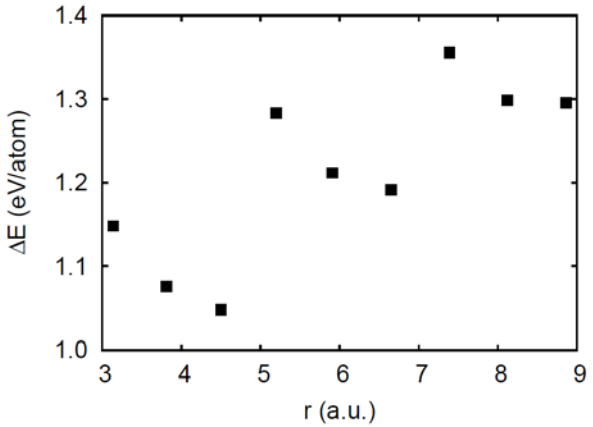

Fig 1 Formation energy of B-doped zigzag carbon nanotube, (n,0) for n=4-12, as a function of nanotube radius.