I-M Electronic Properties of Nanostructured Materials

I-M-1 Electronic Structure of K-Doped Carbon Nanotubes

MIYAKE, Takashi[1]; SAITO, Susumu[2]
([1]Tokyo Inst. Tech.; [2]IMS and Tokyo Inst. Tech.)

[submitted]

Alkali-metal doping is expected to provide a means of controlling electronic properties of carbon nanotubes. Previous band structure calculations support the charge-transfer picture in both K and Li doping. However, more systematic analysis is desirable, since transport properties of nanotubes are sensitive to their size and chirality. We study the effect of K doping inside a few zigzag nanotubes by using density functional method. We find that the effect depends on the diameter significantly, and it is not described fully by the simple charge-transfer picture. In particular, in the (10,0) and (12,0) tube, which are possible to produce macroscopic amount, the nearly free electron (NFE) state of the nanotube is pulled down by hybridization with the K 4s state, and crosses the Fermi level. We will discuss the influence on transport properties from the spatial distribution of the NFE state.

I-M-2 Geometries, Electronic Properties, and Energetics of Isolated Single Walled Carbon Nanotubes

KANAMITSU, Kenjiro[1]; SAITO, Susumu[2]
([1]Tokyo Inst. Tech.; [2]IMS and Tokyo Inst. Tech.)

[submitted]

Using the density-functional electronic-structure calculations, we study so-called zig-zag carbon nanotubes. From the complete geometry optimization, it is found that two kinds of bond lengths are considerably different from each other. They possess strong tube-diameter dependence. In addition, changes of the electronic band structure upon the geometry relaxation from the uniform bond-length tube are found to be sizable. Also the electronic properties and energetics obtained are discussed in detail.