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Title: I-V Characteristics of Doped Carbon Nanotubes

Name: Sakamoto, Shoichi

Affiliation: Seikei University

In this paper, we present electron transport properties in carbon nanotubes (CNTs) by {\it ab initio} density functional theory (DFT) method. Since a single-walled CNT becomes a metal or a semiconductor depending on its chirality, electronic devices, such as FETs and switching devices, can be made only by CNTs. The chiral indices (m,m), $(m,0)$, and (m,n) denote the armchair CNT (ACNT), the zigzag CNT (ZCNT), and the chiral CNT (CCNT), respectively. Experimentally, it has not been achieved yet to make the CCNT with specific chirality. So, making doped ACNTs and ZCNTs with various electronic properties is necessary for realizing the CNT nanodevices. As CNTs have high affinity for organic molecules, it is important to investigate electronic properties of the doped CNTs which covalently bond with other molecules or atoms. We calculate the properties of CNTs by using the Kleinman-Bylander (KB) pseudopotential and the Generalized Gradient Approximation (GGA). The CNT of diameter 1.0 to 1.4 nm and length 3.0 to 4.0 nm is put in a super cell, then the plane wave cutoff energy is adjusted to 350 Rydbergs with 256 k-points sampling in reciprocal space. The number of atoms in the CNT is about 300 to 600 and the structure is optimized energetically by the conjugate gradient (CG) method. Properties of electron transport through CNTs are evaluated by the non-equilibrium Green?s function methods. We show the current is quantized against the voltage for both metallic ACNTs and ZCNTs. In the comparison of $(8,8)$-CNT and $(15,0)$-CNT, the similar size of diameter, the current quantization is distorted from the low voltage region for the ACNT. As the impurity effect, for example, we also find that a doped oxygen on $(15,0)$-CNT slightly reduce the current. We try to explain the causes relating to electronic properties, the band structure, the density of state, and the transmission function, etc.