

Electronic Properties of Carbon Nanotubes under the Electric Field

Ayaka Yamanaka and Susumu Okada

Graduate School of Pure and Applied Sciences, University of Tsukuba
Tennodai, Tsukuba 305-8577, Japan

Phone: +81-29-853-5600 (ext. 8233) E-mail: ayamanaka@comas.frsc.tsukuba.ac.jp

1. Introduction

In these two decades, carbon nanotubes have attracted a great deal of attention in both pure and applied sciences due to its unique structural and electronic properties [1]. They have tubular structure with nanometer diameter and micrometer length, and are metal and semiconductor depending on the atomic arrangement along the circumference. These fascinating features open the possibility of fabricating superior nanometer-scale electronic devices in the next generation [2, 3], in which nanotubes are key constituent units by forming hybrid structures with conventional materials. Indeed, it has been demonstrated that the individual semiconducting carbon nanotubes can work as field-effect transistors (FETs) in which nanotubes form hybrid structures with insulating substrates and metal electrodes. In the FET, nanotube is attached to the source/drain electrodes, and is put onto the insulating substrates covering gate electrodes. Electronic structure of carbon nanotube is modulated by forming such as hybrid structures. Furthermore, since the electric field is essential for operating and functionalizing the electronic devices, nanotubes feel external electric field not only in normal but also parallel to the tube axis. Therefore, it is necessary to understand the fundamental behavior of carbon nanotubes under the electric field. In particular, it has been still uncertain that the correlation between geometric and electronic structures of nanotubes under electric field.

In this work, we aim to theoretically investigate the electronic properties of carbon nanotubes under the electric field by performing the first-principle total-energy calculations based on the density functional theory. In particular, we unravel the interplay between the atomic arrangement of nanotube and electronic properties under the parallel electric field. Our calculations show that electrostatic potential in nanotube strongly depends on the atomic arrangement of the nanotube indicating that the screening effect on the external field is non-uniform inside the nanotube.

2. Method and Model

All calculations are performed in the framework of density functional theory [4, 5] using the Simulation Tool for Atom TEchnology (STATE) [6]. For the exchange correlation energy among electrons, we use the local density approximation (LDA) with the functional form Perdew-Zunger [7, 8]. An ultrasoft pseudopotential generated using the Vanderbilt scheme is adopted to describe the

electron-ion interaction [9]. The valence wave functions and charge density are expanded in terms of the plane waves of which cutoff energy is 25 Ry and 225 Ry, respectively. To simulate nanotubes under the electric field, we perform calculations for finite-length (5,5) and (9,0) nanotubes whose edges are capped by a hemisphere of C₆₀. Accordingly, the finite-length nanotubes are modeled by the fullerenes molecules with five-fold symmetry and three fold symmetry axes parallel to tube axis for armchair and zigzag nanotubes, respectively. Here, we consider C₈₀, C₉₀, C₁₀₀, C₁₁₀, C₁₂₀, and C₁₃₀ for the capped (5,5) nanotubes and C₇₈, C₉₆, C₁₁₄, and C₁₃₂ for the capped (9,0) nanotubes. We adopt the effective screening medium method to solve the Poisson equation including the external electric field [10]. The applied electric field is parallel to the nanotube axis between two metal electrodes situated above and below the topmost and the bottommost atoms of nanotubes, respectively, with 8 angstrom vacuum regions (see Fig. 1). Atomic structures are fully optimized under zero electric fields. In the calculations under the condition of a finite electric field of 0.25 V/angstrom, the geometries are fixed to those under the condition of a zero electric field.

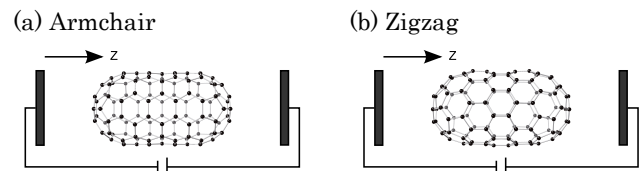


Fig. 1 Structural model of capped carbon nanotubes under parallel electric field. Dark shaded rectangles denote the metal electrode simulated by ESM.

3. Results

Figure 2 shows the averaged electrostatic potential of carbon nanotubes on the plane normal to the direction of the external electric field. For all cases, as shown in figures, gradient of the potential is shallower than that for the vacuum region indicating that the nanotubes could screen the external field. However, the potential has finite gradient so that the nanotubes do not perfectly screen the field. By taking the ratio of potential gradient in the nanotube region to that in the vacuum regions, we estimate the dielectric constant of the capped nanotubes. The constant is proportional to the tube length. The calculated values are $\epsilon_r = 2.8895l + 2.5746$ where l is the length of armchair nanotubes and $\epsilon_r = 4.0099l - 10.616$ where l is the length of zigzag nanotubes.

Furthermore, for the carbon nanotubes longer than 13 angstrom, we found that the dielectric constant of zigzag nanotube is larger than that of the armchair nanotube with the same length.

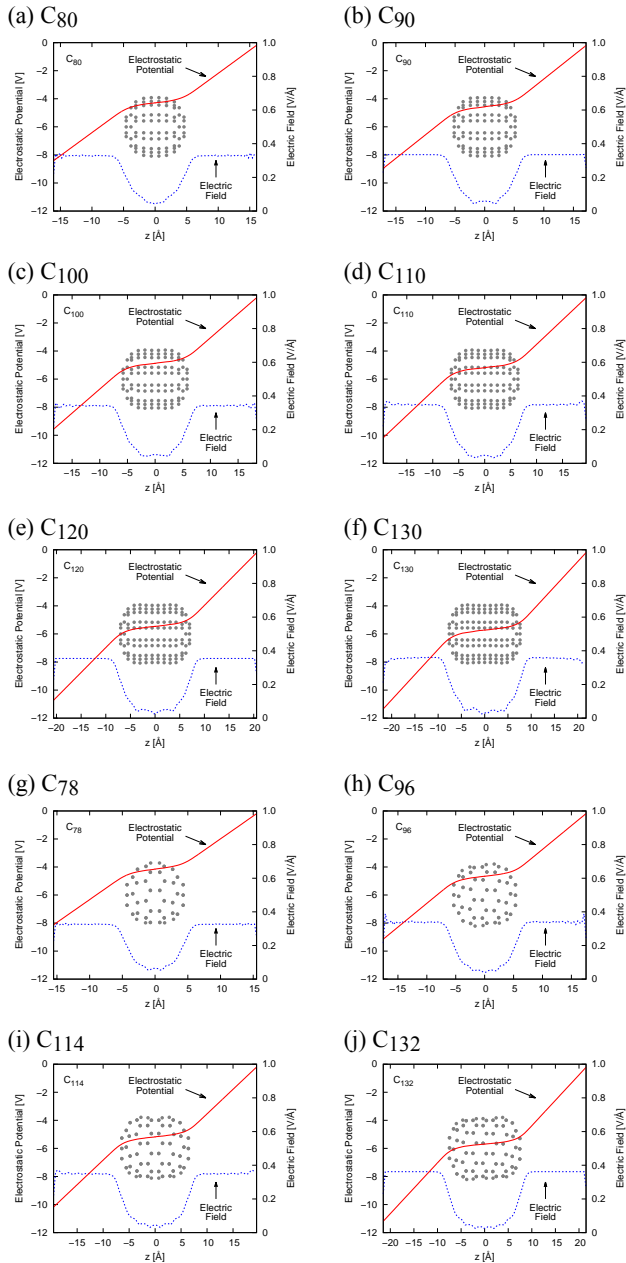


Fig. 2 Plane averaged electrostatic potential and electric field of capped armchair nanotubes, C₈₀-C₁₃₀ and zigzag nanotubes, C₇₈-C₁₃₂.

Since the potential modulation strongly depends on the atomic site, it is worth to investigate the electrostatic potential on each C atomic site of C₁₃₀ and C₁₃₂ nanotubes which are representative for the capped armchair and zigzag nanotubes, respectively. Figure 3 is the electrostatic potential on each C atomic site of the capped armchair nanotube C₁₃₀ and the capped zigzag nanotube C₁₃₂ under the electric field.

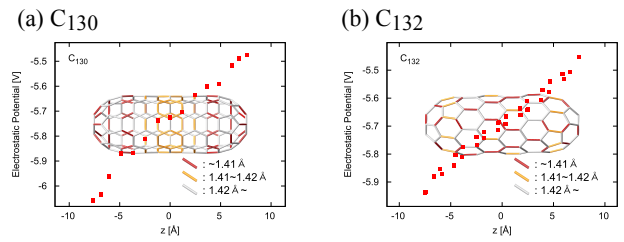


Fig. 3 Electrostatic potential on each atomic site of (a) the capped armchair nanotube C₁₃₀ and (b) the capped zigzag nanotube C₁₃₂.

In the case of armchair nanotubes, the potential exhibits stepwise nature indicating the fact that the screening strongly depends on the bond alternation of the carbon nanotube. We found that the potential keep almost constant values for the atomic sites those are connected via short C-C bond (less than 1.42 angstrom). Thus, these C-C bonds lead to strong screening on the external field. While, we found the substantial potential difference between the atoms connected via longer C-C bonds (longer than 1.42 angstrom). These facts are consistent with the chemical picture of the covalent bond of sp² materials. The short bonds possess double bond nature in which the electron density is higher than that of the single bonds which correspond with the long bonds. In sharp contrast to the armchair nanotube, it appears there is no clear correlation between screening strength and atomic site in the zigzag nanotubes. This unclear site dependence is ascribed to the nonuniform bond alternation for the atoms belonging to the cylindrical part of the zigzag nanotube. However, by focusing on the some armchair lines from one cap to the other cap, the screening strength also depends on the bond length. The fact indicates that the electric field inside the nanotube is nonuniformly screened by the valence electrons on the nanotubes.

References

- [1] M.S. Dresselhaus, G. Dresselhaus, P.C. Eklund: Science of Fullerenes and Carbon Nanotubes, Academic Press (San Diego, 1996).
- [2] S.J. Tans, A.R.M. Verschueren, and C. Dekker: Nature (London), 393 (1998) 49.
- [3] R. Martel, T. Schmidt, H.R. Shea, T. Hartel, and Ph. Avouris: Appl. Phys. Lett. 73 (1998) 2447.
- [4] P. Hohenberg and W. Kohn: Phys. Rev. 136 (1964) B864.
- [5] W. Kohn and L.J. Sham: Phys. Rev. 140 (1965) A1133.
- [6] Y. Morikawa, K. Iwata, and K. Terakura: Appl. Surf. Sci. 169-170 (2000) 11.
- [7] J.P. Perdew and A. Zunger: Phys. Rev. B 23 (1981) 5048.
- [8] D.M. Ceperley and B.J. Alder: Phys. Rev. Lett. 45 (1980) 566.
- [9] D. Vanderbilt: Phys. Rev. B 41 (1990) 7892.
- [10] M. Otani and O. Sugino: Phys. Rev. B 73 (2006) 115407.