The Polarizability and Electric Field-Induced Energy Gaps In Carbon Nanotubes

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A simple method to calculate the static electric polarization of single-walled carbon nanotube (SWNTs) are significant application as nanoscale devices \[1\] due to their extraordinarily small diameter and versatile electronic properties \[2\]. It is suggested that individual SWNT may act as devices such as field-effect transistors (FETs) \[3\], single-electron-tunneling transistors (SETs), rectifiers \[4\], or p-n junctions \[5\]. The most exciting expectancy lies in the devices fabricated on a single tube \[6\]. In recent years, the interplay between mechanical deformation and electrical properties of SWNTs have been extensively studied \[7,8\]. Tombler et al. \[9,10\] used an atomic force microscope tip to manipulate a metallic SWNT, leading to a reversible two-order magnitude change of conductance, and Lammert et al. \[11\] applied a uniaxial stress to squash SWNTs and detect a similar reversible metal-insulator (M-I) transition. It is also well known that a magnetic field can also change the conductance of carbon nanotubes \[12,13\]. A possible electric field-controlled M-I transition are considered to be more exciting because of its easy implementation in the actual applications. Yet, a question remains: Can electric field change the electronic properties of a tube?

In previous studies on electronic transports \[14,15\], the potential of a weak longitudinal electric field (bias voltage) in conductors was treated approximately to a slowly change variable in the range of the primitive unit cell. The electric field makes all the electronic energy and the Fermi level have a gradient along the field direction, but the energy-band structure is not change. The controlled potential, such as the gate voltage without a drop of component in the direction perpendicular to the tube axis in the case of FET, is only used to shift the Fermi level or changed the carrier concentration \[16\]. In the literature, according to our knowledge, there is no report on using a transverse electric field to control the longitudinal electronic transport of conductors. In \((n, n)\) metallic SWNT, the electrons nearby Fermi energy are nonlocal in the circumference of the tube since their circumference-Fermi wavevector is zero \[17\], the classic wave-package approximation in slow-change voltage may be not suitable in the presence of the strong transverse electric field. The V/\(\mu\)m order electric field is enough to obviously break the rotational symmetry about the tube axis, and create new interband and intraband coupling, which may change the low energy electronic properties of SWNTs, and hence affect the electronic transport. In the other hand, the field is still less than the V/\(\mu\)m order of the atomic interior electric field, can be treated as perturbation.

In this Letter, we first report the result by using a tight-binding (TB) model to calculate the polarizability of SWNTs in the application of an external electric field perpendicular to the tube axis. The calculated polarizability of SWNTs is in agreement with the previous results within the random-phase approximation (RPA) \[18\]. Then we calculate the low energy electronic structure of SWNTs in the electric field. The results show obviously valuable effects: (1) The electric field can always induce an energy gap in \((n, n)\) metallic SWNTs; (2) There is a maximum gap strongly depended on the radius of the tubes; (3) Universal scaling is found for the gap as a function of the field and the size of the tubes, and the numerical results are testified by the second order perturbation calculations. Our results indicate that the magnitude of the electric field required to induce a sizable energy gap in metallic SWNTs falls into the range of currently available experimental conditions.

In density function theory, single electronic Kohn-Sham Hamiltonian is

\[ \mathcal{H} = T + V_{KS}[\rho(r)] + V_{xc}(r), \]

where \(V_{KS}[\rho(r)]\) is the effective potential, self-consistently depended on the electronic density \(\rho(r)\),
uniform polarization approximation. From small \[21\]. Here we will only report the results within the
electrostatic potential. If we suppose the polarization in (3) in small tubes with the calculated TB-electron-energy
correlation approximation, we have numerically solved
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gap decreases as $E$ increases further. When $V_0 = 3.0$ V, the zero gap is found, but the Fermi point dramatically moves from $K_0$.

To probe the above effect in general, we performed the computation for a series of $(n, n)$ tubes. Fig. 4 shows the gap as a function of the applied field $V_0$ in $(n, n)$ tubes, where $n$ is from 5 to 15. From the figure, we find the determined effect: The electric field can always induce a gap in $(n, n)$ tubes, and the size of the gap strongly depends on the amplitude of the transverse field and the tube parameter $n$. For any $(n, n)$ tubes, the gap first increases with increasing field, and reaches a maximum value $E_{gm}$ at the $V_{0m}$, then drops again. Both the maximum gap $E_{gm}$ and the corresponding $V_{0m}$ are approximately proportional to $1/n$, and hence inversely proportional to the radius of tubes, i.e.,

$$E_{gm} \approx 6.89 \text{ eV}/n, \quad c_n \approx 12.09 \text{ eV}/n.$$  \hspace{1cm} (13)

The finding shown in (13) that electric field effects fastly decrease as the size of conductor increases might be the reason why people have not yet recognized the effect in previous studies. The field dependence of the gap is quite similar for tubes with various cross-sectional radii, which invites us to scale both $E_g$ and $V_0$ up $n$ times their original values. The obtained results are shown in Fig. 5.

From it we do find the scaled gap to be a universal function of the scaled electric field for all $(n, n)$ tubes. In the low field range, for all calculated eleven $(n, n)$ tubes there exists a simple relation: $nE_g = \lambda (nV_0)^2$, where $\lambda$ is a constant, about 0.07 (eV)$^{-1}$. In the higher field range, except for a few small-radius tubes such as (5, 5) and (6, 6) tubes, the universal scaling law still holds.

To understand the above scaling relation, we use perturbation theory to calculate the field-induced gap in low field limit. The first-order perturbation approximation only causes shift in the Fermi level, showing no contribution to the gap change. Calculating up to the second order perturbation at $K_0$ point, we obtained the following analytic result

$$E_g \approx \frac{\sqrt{3}}{2 \pi h} n E^2 R^2,$$  \hspace{1cm} (14)

where $h (=3.033 \text{ eV})$ is the hopping parameter in the absence of the electric field [22, 23]. The contribution of the overlap integral $s$, which is very small, is neglected. Obviously, the second-order perturbation calculation gives almost the same scaling relation as the numerical results in the low field, though the obtained $\lambda \approx 0.09$ (eV)$^{-1}$ is slightly larger than the numerical result 0.07 (eV)$^{-1}$. In the high field range, since the Fermi wavevector is moved from $K_0$, the perturbation theory becomes not suitable. However, the low field range may be more compatible with the practical application. In order to open a 0.1 eV gap in the energy bands of $(n, n)$ tubes, $n$ must be smaller than $n_0 = 6.89/E_g \sim 68$, and the required electric field is,

$$|\mathbf{E}| = \frac{2\pi}{3\sqrt{3} \rho_0} \sqrt{E_g n^{-\frac{3}{2}}}.$$  \hspace{1cm} (15)

where $\rho_0$ is the bond length of carbon atoms in the SWNT. Therefore, for example for a (10, 10) tube, the required field is about $5 \times 10^8$ V/m, and for a (60, 60) tube, it is about $3 \times 10^7$ V/m. Considering the polarizing, the needed external field is about 0.5 V/Å and 0.06 V/Å, respectively. Our results are encouraged by an important fact that the perturbation approximation is suitable only required the small total field $\mathbf{E}$, need not the small external field $\mathbf{E} = e\mathbf{E}$. Even though $e$ is larger, our conclusion is still correct, but needing stronger external field. The magnitude of the required external field for inducing a sizable gap in tubes with larger radius can be reached by the currently available experimental conditions, we wish the above prediction can be checked in near future.

In summary, we have proposed an electric field-induced M-I transition in $(n, n)$ SWNTs for the first time. The results support the argument that SWNTs can be applied as nanoscale electric signal-controlled switching devices.

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Fig. 1 X. Zhou et al
FIG. 1. A uniform external electric field perpendicular to the axis of SWNT.

Fig. 2 X. Zhou et al
FIG. 2. The polarization of \((n,n)\) tubes: (a) \(\alpha_0 \sim n^\gamma\), where \(\gamma \approx 2.4\) (see text); (b) the dielectric function of tubes, circles and squares are the calculated results using \(R\) and \(R_{\text{eff}}\), respectively (see text).

Fig. 3 X. Zhou et al
FIG. 3. The energy bands of \((10,10)\) tube in the vicinity of the Fermi level under the application of a transverse electric field of certain magnitude. \(V_0 = 0 \text{V}\) is the result in the absence of the electric field.

Fig. 4 X. Zhou et al
FIG. 4. Field-induced gap of \((n,n)\) tubes versus the field \(V_0 = ER\). From the top to the bottom, the tube parameter \(n\) increases from 5 to 15. The clubs denote the position of the maximum gap point. In the inset, both the maximum gap \(E_{gm}\) and its corresponding electric field \(V_{gm}\) are found to be proportional to \(1/n\) The lines are fitting results.
FIG. 5. Universal scaling are found in the gap as a function of $V_0$ in different $(n, n)$ tubes. In the low field, the data of all tubes are very much consistent with the scaling relation $nE_g = \lambda(nER)^2$, as expected by the second perturbation theory. The line is the fitting result. Except for (5,5) and (6,6) tubes, the universal scaling is satisfied well up to high field region.

Fig. 5 X. Zhou et al