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Disconnect armchair carbon nanotube as rectifier predicted by first-principles study

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ABSTRACT

For electronics devices based on carbon nanotube, we propose that the localization of the density of the states can enhance the rectification effect. The proposal is confirmed according to the first-principles study of the transport characteristics of several disconnected armchair nanotubes where only one side of armchair edge is hydrogenated. We find that the rectification effect increases as the diameter of armchair carbon nanotube and has no trend of decrease, which originates from the localization of the density of states of the pristine armchair edge. Our investigations indicate that the quantum size effect is helpful for molecular or nano-scale electronics devices.

1. Introduction

The Si-based semiconductor transistor based on CMOS technology is approaching the geometrical and physical limits because of the continued miniaturization. In the future generation of electronics, the nano-scale or molecular devices are considered as the most potential substitutions of the Si-based semiconductor transistor. In the field of the nano-scale or molecular electronics, carbon nanotubes (CNTs) and graphene nanoribbons (GNRs) are considered as the potential materials to construct the nano-scale or molecular devices [1–3]. The CNTs are carbon cylinders whose diameter is a few nanometers and the length is up to several millimeters. As the quasi one-dimensional materials, they belong to the fullerene structural family and were discovered by Iijima [4]. Much researches show that the field effect transistors (FETs) [5–8], diodes [9–22] and negative differential resistors [23–27] based on CNTs have superior performance over the traditional Si-based devices because they exhibit the exceptional electronics properties such as high current carrying capability and low scattering rates [28,29].

As mentioned above, the Si-based semiconductor transistor is approaching the physical limits because of the quantum size effect (QSE). With the continued miniaturization of Si-based transistor, the impact of the QSE is more and more obvious and eventually inhibits the further miniaturization. In this work, we propose that the QSE is harmful for the traditional Si-based semiconductor devices which using "top-down" technical route but may be helpful for the molecular or nano-scale electronics devices which using "bottom-up" technical route. The QSE some extent not only enhances the performance but also reduces the power depletion for the molecular or nano-scale electronics devices. According to the first-principles calculations of the transport properties of the disconnect armchair CNTs where only one armchair edge is hydrogenated, our proposal is confirmed. We find that one of the QSEs, the localization of the density of energy states (DOS), increases when the diameter of armchair CNTs increases. That results in the enhancing of the rectification effect and the decreasing of the forward and reverse current. The increased rectification effect and the decreased current mean the enhanced performance of rectifier and low power depletion, respectively.

2. Computational details

Our investigation is based on a self-consistent first-principles technique which combines the Keldysh non-equilibrium Green's-function formalism with a self-consistent density-functional theory. The package we use is the Atomistix Toolkit [30]. The k-points sampling is 1, 1, and 30 in the *x*, *y*, and *z* direction respectively. The cutoff energy and basis set is 150 Ry and SingleZeta, respectively. The exchange–correlation interaction is treated within generalized gradient approximation using the Perdew–Burke–Ernzerhof functional [31]. The convergence criterion for the total energy is 10^{-5} via the mixture of the Hamiltonian. The hydrogenated and pristine armchair edges are relaxed until the force tolerance 0.05 eV/Å is achieved. The current [32] is calculated as

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$$I = \frac{2e}{h}\int_{-\infty}^{+\infty} T(E,V_b)[f_l(E-\mu_L) - f_r(E-\mu_r)]dE \quad (1)$$

where f is the Fermi–Dirac distribution, $\mu_{L,R}$ are the chemical potentials of left lead (L) and right lead (R), h is Planck constant, V_b is bias and $T(E, V_b)$ is transmission spectrum. The $T(E, V_b)$ is the transmission coefficient at the energy E and bias V_b and is calculated by the standard equation

$$T(E,V_b) = Tr[\Gamma_L(E,V_b)G(E,V_b)\Gamma_R(E,V_b)G(E,V_b)] \quad (2)$$

where the $G(E, V_b)$ is Green's function of the scattering region and $\Gamma_{L,R}$ is the coupling matrix.

Fig. 1 shows the schematics of the transport systems of the disconnected armchair CNTs. According to the $2n + m = 3q$ rule (the n and m is integer, they are two unit vectors along two directions in the honeycomb crystal lattice of graphene [33], q is also integer), the armchair CNTs are metallic and can be used as good lead. In the scattering regions, only the left armchair edges are pristine. The length of vacuum between pristine and hydrogenated edge is 3.70 Å. To eliminate the contribution of leads to the rectification effect, the left and right leads including carbon atoms in scattering region are mirror symmetry in all transport systems.

3. Results and discussions

Fig. 2 shows the current–voltage (I–V) curves of the disconnected armchair CNT transport systems. We calculate the I-V curves within the voltage region [−1.50 V,+1.50 V], which is enough for obtaining all the I–V characteristics. The current at forward bias ($+V_b/2$ is applied to the left lead, $-V_b/2$ is applied to the right lead) are always larger than that at reverse bias ($-V_b/2$ is applied to the left lead, $+V_b/2$ is applied to the right lead). Thus, the rectification effect is present. From Fig. 2, one can see that both forward and reverse current decrease when the diameter of armchair CNT increases. This phenomenon originates from the localization of the DOS of pristine armchair edge in the scattering regions. Fig. 3 shows the curves of the bias voltage dependent rectification effect for the armchair CNT transport systems. The rectification effect is defined as $|I(+V_b)/I(-V_b)|$. From Fig. 3, one can see that the rectification effect increases with bias voltage and then decreases for every armchair CNT transport system. One can also see that the rectification effect increases with the diameter of the armchair CNT from (4, 4) to (10, 10) CNT transport system. These phenomena also originate from the localization of the DOS of pristine armchair edge in the scattering regions. From (4, 4) to (10, 10) CNT transport system, the maximum value of rectification effect increases from 2.02 to 10.24 and have no trend of decrease. One can predicts that the maximum value of the rectification effect can be large enough when the diameter of nano-scale diode constructed by armchair CNT increases, which promise the potential applications in the field of molecular or nano-scale electronics. As mentioned above, the decrease of the current and the increase of the rectification effect all originate from the QSE of the localization of DOS. That's to say the QSEs may not only decrease the

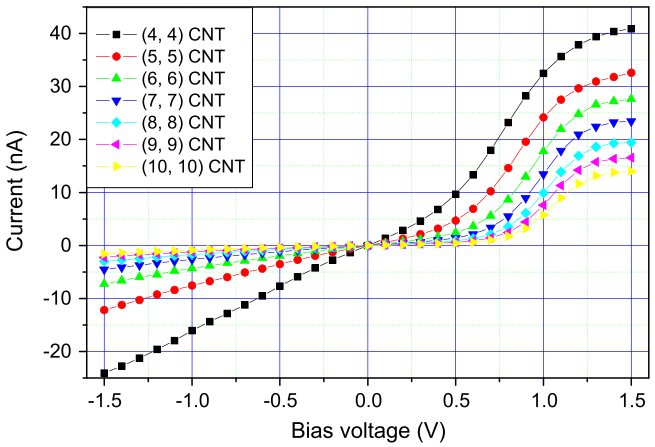

Fig. 2. The curves of the bias-dependent current for the armchair CNT transport systems.

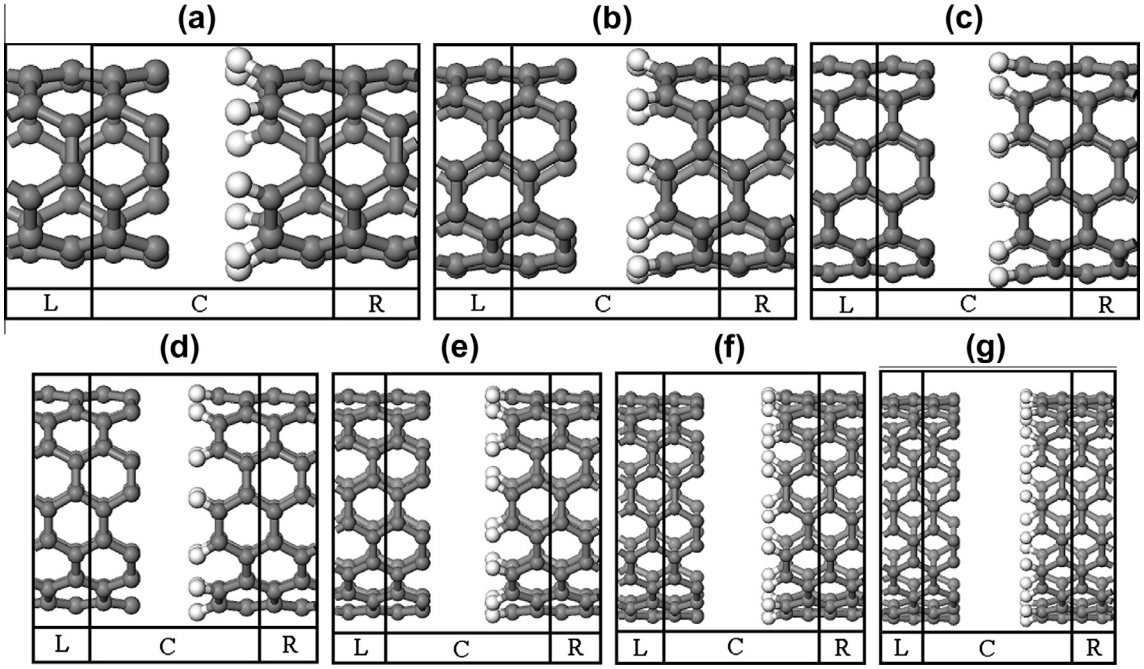

Fig. 1. Schematics of transport systems of the disconnected armchair CNTs where right armchair edges are hydrogenated. (a–g) are (4, 4), (5, 5), (6, 6), (7, 7), (8, 8), (9, 9) and (10, 10) carbon nanotube transport systems, respectively. Color code: C atom (black) and H atom (grey). The L, C and R are left lead, scattering region and right lead, respectively. The z direction is from left lead to right lead.