Doping-Enhanced Current Rectification in Carbon Nanotube–Metal Junctions for Rectenna Applications

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ABSTRACT: Using density functional theory in combination with Green’s functional formalism, we study the effect of chemical doping on the electronic transport properties of carbon nanotube (CNT)–metal junctions. Both surface doping (i.e., surface fluorination) and substitutional doping with different dopant atoms (e.g., B, N, and P) are considered. Profound current rectification is obtained for the fluorinated samples, whereas substitutional doping results in only small asymmetry in the current–voltage characteristics of the system despite the smallest differential resistance. The current rectification originates from voltage-dependent charge localization in the system as revealed in our transmission spectrum analysis. We also study the effect of CNT morphology (i.e., tip opening, radius, length, chirality, and multiple walls) on the electronic transport properties of the CNT–metal junction. CNT–insulator–metal junctions are also investigated as a reference to our doped systems. The results show the possibility of creating fluorinated CNT-based diodes for practical nanoelectronic applications, such as rectenna solar cells.

I. INTRODUCTION

It is well known that chemical doping dramatically changes both structural and electronic properties of carbon nanotubes (CNTs).1 Consequently, charge transport properties (such as, mean-free path and conducting mechanisms) are also strongly affected by doping.2,3 Current rectification can also be achieved by doping CNTs with appropriate chemicals.4 In this work, we study the effect of chemical doping of the outer surface of CNT on the charge carrier transport through the CNT–metal interface, which has received lots of interest in recent years as a potential system for optical rectenna applications.5,6 Contrary to conventional photovoltaic technologies where the solar conversion efficiency is limited by the properties of the absorbing semiconducting material (e.g., the band gap), the rectenna device does not have such a restriction for solar energy harvesting.5–11 However, there are two main challenges, which prevent the progress in rectenna device development.12 First, the antenna part of the device should be small and electromagnetic/ergonomic (optoergonomic) enough to collect waves at optical frequencies and to convert the signal into an alternating current, which will be passed through a diode for direct current conversion. Second, the response of the rectifying diode must be fast enough to accommodate the changes in the polarity of the electron oscillations in the antennas, which is experimentally very challenging to achieve using conventional semiconductor-based technologies. These key limitations can be circumvented in the CNT-based rectenna design5–7 where each CNT acts as a receiving antenna and forms a tunnel diode in contact with the transparent top electrode. Because of the small contact area between CNT and the metal electrode, the capacitance of this diode is very small. However, this may increase the diode resistance resulting in a large impedance mismatch between the diode and antenna. Therefore, further research is needed to improve the diodes for better conversion efficiencies.7

Here, we study the possibility of enhancing current rectification in CNT–metal junctions by altering the electronic properties of CNTs through chemical doping. The latter has already been used to create CNT-based p–n junction diodes operating at different frequencies.13 A particular focus will be given to surface fluorination14,15 since fluorinated carbon structures are known by their chemical inertness and high thermal stability.16,17 The analyses are based on the computer simulations using density functional theory (DFT) in combination with nonequilibrium Green’s functional formalism. We show that, depending on the level of fluorination, more than an order of magnitude larger rectification can be obtained. Transmission spectrum analysis show that such large current rectification originates from bias-dependent nanoscale charge localization in the system. We also study the effect of substitutional doping using different dopants such as N, B, and P. The effect of CNT morphology, such as radius, length, tip opening, and chirality on the transport properties of the CNT–metal systems is also studied. CNT–insulator–metal (CNT–I–M) junctions are also studied as a reference to our doped systems. We show that chemical doping (i.e., fluorination) has advantages over the direct insulating layer deposition in terms of current rectification.

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II. COMPUTATIONAL METHOD

Structural optimizations and electronic structure calculations are conducted using DFT within the generalized gradient approximation of Perdew–Burke–Ernzerhof (PBE) for the exchange-correlation functional.\(^\text{18}\) The Brillouin zone is integrated using the Monkhorst–Pack sampling method.\(^\text{19}\) van der Waals interactions are taken into account using the Grimme’s empirical dispersion correction to PBE.\(^\text{20}\) The electronic structure is obtained self-consistently within DFT/PBE, and the electrostatic potentials are defined on a real-space grid with a mesh cutoff energy of 150 Ry. Double-zeta-polarized basis sets of local numerical orbitals are used in the calculations. The convergence criterion for Hellman–Feynman forces was 0.05 eV/Å. Electronic transport calculations are performed using the nonequilibrium Green’s function formalism. The current–voltage (I–V) characteristics are calculated using the Landauer–Büttiker formula:\(^\text{21}\)

\[
I(V) = \frac{2e}{h} \int_{\mu_L}^{\mu_R} T(E, V) [f(E - \mu_L) - f(E - \mu_R)] dE,
\]

where \(T(E, V)\) is the transmission spectrum for the given value of voltage biasing \((V)\), \(f(E, E_F)\) is the Fermi–Dirac distribution function, and \(\mu_L/\mu_R\) is the chemical potential of the left/right electrode. All the calculations are conducted using the computational package Atomistix toolkit.\(^\text{22}\)

From the calculated I–V curves, we have extracted diode figures of merits (resistance, nonlinearity, responsivity, and asymmetry) as:

\[
R = \left( \frac{dI}{dV} \right)^{-1} \text{(differential resistance)},
\]

\[
N = \frac{d^2I}{dV^2} \text{(nonlinearity)},
\]

\[
\beta = \frac{1}{2} \frac{dI}{dV^2} \frac{dI}{dV} \text{(responsivity)},
\]

\[
A = \frac{I(+V)}{I(-V)} \text{(asymmetry)},
\]

where the asymmetry is defined as the forward-to-reverse current ratio.

III. RESULTS AND DISCUSSIONS

A. Effect of CNT Tip Opening. One of the key factors limiting the solar conversion efficiency of CNT-based rectennas is the large impedance mismatch between the antenna and diode due to large electrical resistance of the CNT–I–M diodes.\(^\text{5,6}\) As was shown in recent experiments, the resistance of CNT–I–M diode arrays can be reduced significantly by opening the tips of the multiwalled CNTs by, for example, plasma etching.\(^\text{6}\) This is because of opening of extra channels for electronic transport as the inner walls of multiwalled CNTs also form contacts with the electrodes. In this section, we study how the tip opening in single-walled CNT will affect the transport properties of CNT–metal junctions.

As a representative example, we consider single-walled armchair CNT (5,5) capped by a C\(_{16}\) hemispher. Both closed-ended and open-ended CNTs are in contact with 100 surfaces of silver. We first optimized these structures with respect to the distance between the CNT and metal surface. For the capped CNT, the minimum energy distance was found to be \(d = 2.2\) Å. This distance becomes smaller \((d = 1.8\) Å\) when the tip of CNT is open. Using these optimized interface structures, we have constructed device geometries, each of which consists of left and right regions (i.e., electrodes), which are connected to a central region (i.e., two-probe configuration). As shown in Figure 1a,b, the left electrode consists of the extension of CNT, and the right electrode consists of silver atoms. The sizes of the electrodes are 4.92 and 4.09 Å for left and right electrodes, respectively. Figure 2a shows the I–V curves of both samples calculated using 1×1×100 k-point sampling. In both cases, we have obtained a small asymmetry with reverse current being larger than the forward one for the given value of the applied voltage. However, the current in the system becomes more than 3 times larger when the tip of CNT is open (open-red circles in Figure 2a). Figure 2b shows the calculated differential resistance of both samples. For the considered range of the applied bias, the differential resistance of the system decreases at least 2 times due
to the tip opening. These results are in good qualitative agreement with the recent experiments.6

To understand the origin for the difference in the electronic transport in the considered systems, we have calculated transmission pathways at different energy levels. As an example, we presented in Figure 1 the pathways for electron transmission from the left to the right electrode for both samples at the Fermi level. In these plots, the volume of each arrow shows the magnitude of the local transmission between each pair of atoms, whereas the arrow and the color indicate the direction of the current (blue corresponds to the electron flow from left to right, and red corresponds to the flow from right to left, i.e., scattered electrons). In the case of the capped CNT, large scatterings of the electrons are obtained from the tip of CNT (see Figure 1a). Consequently, the current in the system reduces due to such electron back-scattering. On the contrary, we did not observe such scattering in the open tip CNT (Figure 1b). This explains the enhanced current in the open-tipped CNT geometries. We expect that this effect will be even more pronounced in the case of multiwalled CNTs due to the formation of extra channels for the charge carrier transport in the system.

B. Effect of an Insulating Layer. We start with studying the electronic transport properties of the CNT−I−M junction as a reference to our further calculations. Figure 3a shows our reference device, which consists of metallic (i.e., armchair) CNT (3,3) connected to the 100 surface of the silver electrode. No strain is applied to the metal electrode during the interface formation because of the vacuum region near CNT. As insulating layers, we have chosen HfO2(100) (Figure 3b) and ZnO(100) (Figure 3c) layers. This is because HfO2 gives better rectification, and ZnO results in better electronic transport among the other insulating layers.6 Only insulating layers were strained during the interface formation with the mean absolute strain values 0.69 and 1.44% for HfO2 and ZnO layers, respectively. In both cases, the interface area was 133.5 Å2. During the structural optimization, all the atoms of CNT are fully relaxed and insulating, and metallic layers are optimized as rigid bodies.

Figure 3. Device geometries: CNT(3,3)−Ag(100) junctions (a) without and (b) with HfO2 and (c) ZnO layers.

Figure 4a shows the I−V curves of the considered systems for the voltage range from −2 to 2 V. Calculations are conducted using 5×5×100 k-point sampling. Introduction of the insulating layer decreases the current in the system considerably for all considered voltage biases. To see how the resistance changes in the presence of the insulating layer, we plotted in Figure 4b the calculated differential resistance $R$ as a function of applied voltage. The insulating layers increase the resistance of the system for all voltage values, except small bias range around 1.5 V. The HfO2 layer results in higher resistance as compared to the ZnO layer, which is in good agreement with the recent experiments.6 To estimate the current rectification, we plotted in Figure 4e the asymmetry in the I−V curves as a function of bias voltage. For the reference sample (solid-black circles), the maximum rectification is obtained at 1.2 V voltage biasing and the asymmetry is just 1.26. Current rectification increases up to 50% when the ZnO layer is introduced (filled-green triangles). The current rectification becomes more pronounced for the CNT−HfO2−Ag system (open-red circles): the asymmetry level increases monotonically by increasing the applied voltage and becomes more than 3 at $\Delta V = 2$ V. Figure 4c,d shows nonlinearity in the I−V curves and responsivity of the considered systems. It is seen from these figures that these diode parameters are also pronounced for the system with the
is substitutionally doped with di replaced by N atoms (see Figure 5d). In this case, the ratio of the reverse current to the forward one is less than 1.7. We also considered the case when more carbon atoms are substituted by B, Be, N, Nb, and P atoms (see Figure 5 for the substituted system (open-blue squares in Figure 6b), whereas, for all other dopants, the reverse current is larger than the forward current. However, the current rectification (defined now as a ratio of the reverse current to the forward one) is less than 1.7. We also considered the case when more carbon atoms are replaced by N atoms (see Figure 5d). In this case, the rectification level increases only at larger bias voltages (>1 V). The reverse current becomes larger at small voltages. Thus, the substitutional doping does not provide better current rectification as compared to CNT−I−M junctions (see Figure 4e). However, substitutionally doped systems give a larger current as compared to CNT−I−M samples. For example, the Nb-doped system (Figure 5e) shows a larger current even as compared to the undoped (Figure 3a) system (compare solid-black circles and solid-magenta triangles in Figure 6a).

C. Effect of Substitutional Doping. We start by considering the effect of substitutional doping on the charge carrier transport through CNT−metal junctions. We use our CNT(3,3)−Ag(100) system (see Figure 3a) as a reference to our further calculations. We start with considering the systems where edge carbon atoms near the Ag(100) surface are substituted by B, Be, N, Nb, and P atoms (see Figure 5 for the different elements.

Figure 5. (a)−(f) CNT(3,3)−Ag(100) device geometries where CNT is substitutionally doped with different elements.

In this section, we study the effect of fluorination of the tip area of CNT on the quantum transport through the CNT−metal junction. We have chosen fluorine atoms for the doping, knowing the fact that fluorine atoms form strong covalent bonding with carbon atoms, which is necessary for the operational stability of the proposed devices. Only the outer surface of CNT is fluorinated, which still makes the charge transport more complex across the CNT−metal junction due to the interplay of surface and bulk properties. The optimized device geometries are shown in Figure 7 where the edge carbon atoms (i.e., first carbon ring, Figure 7a), two (Figure 7b), and four (Figure 7c) carbon rings are fluorinated. For the sake of simplicity, we named these systems as samples F1, F2, and F4 in the rest of the text.

Figure 7. CNT(3,3)−Ag(100) device geometries with different levels of fluorination: (a) first carbon ring, (b) two carbon rings, and (c) four carbon rings.

Figure 6 shows the $I−V$ curves (a) and asymmetry (b) of the doped samples together with the results for the undoped sample (solid-black circles). The largest forward-to-reverse current ratios are obtained only for the N-doped system (open-blue squares in Figure 6b), whereas, for all other dopants, the reverse current is larger than the forward current. However, the current rectification (defined now as a ratio of the reverse current to the forward one) is less than 1.7. We also considered the case when more carbon atoms are replaced by N atoms (see Figure 5d). In this case, the differential resistance of the fluorinated samples reduces considerably starting from the voltage bias $ΔV > 0.5$ V, which is not obtained for the reference system. Despite such an increase in the resistance, the fluorination results in dramatic enhancement of the rectification effect in the system. For example, only the edge fluorination gives the asymmetry level of more than 2 (see open-red circles in Figure 8a), whereas the maximum forward-to-reverse current ratio does not exceed 26% in the case of the undoped system (filled-black circles in Figure 8a). The rectification effect enhances further with increasing the level of doping; the asymmetry becomes more than an order of magnitude depending on the value of the applied bias (triangles in Figure 8a).
strongly suppressed at electron energies below the Fermi level. This reduced transmission is due to the nanoscale charge localization (see panel 3 in Figure 9), which is not obtained in the other two systems (panels 1 and 2). The presence of the insulating layer also reduces the electron transmission, despite larger DDOS (see red curves in Figure 9a,b). For electron energies above the Fermi level, the electronic states extend to the doped region, leading to enhanced electron transmission. With an increase in the positive voltage biasing, these nonzero transmission regions shift to the energy range that covers the bias window (see the shaded and highlighted areas in Figure 9c). Such energy- and voltage-dependent transmission of the electrons is responsible for the large current rectification in fluorinated systems.

**E. Effect of CNT Morphology.** In this section, we study the effects of length, radius, and chirality of CNT on the obtained rectification behavior of fluorinated CNT–metal junctions. We start with studying the effect of the CNT length on the electronic transport properties of fluorinated-CNT–metal junctions. As a typical example, we consider the F2–CNT system with the length of the active layer of 21.05 Å (short sample, see the lower inset in Figure 10a) and 51.58 Å (long sample, see the upper inset in Figure 10a). The reference system will be the one shown in Figure 7b with a layer length of 31.68 Å, the results for which are shown in Figure 8. Figure 10 shows the $I$–$V$ curves (a) and asymmetry (b) of both samples. It is seen from this figure that both samples give the same current values for the reverse voltage biasing. Slightly larger current values are obtained for the short sample only for the voltage values (>0.6 V). The rectification ratio is also slightly larger for the shorter sample. However, no qualitative changes are obtained in the current voltage characteristics of the system by increasing the length of CNT.

Next, we study the effect of the CNT size on the rectification properties of the F2–CNT–metal junction. We use the 100 surface of silver as the right electrode material. Figure 11 shows the $I$–$V$ curves (a) and asymmetry (b) for armchair CNTs with size (2,2) (solid-black curves, panel 1), (4,4) (open-red circles, panel 2), (5,5) (solid-green squares, pane 3), and (6,6) (open-blue circles). It is seen from the $I$–$V$ results that both voltage onsets for the finite current in the system and value of the current for the given bias voltage depends on the size of CNT. For example, the largest current for small positive values of the voltage is obtained for the (2,2) CNT system. With further increasing the positive voltage, the largest current is generated in CNT with larger size. For negative biasing, the CNT(5,5) system gives the largest current. However, regardless of the size of the CNT, significant current rectification is obtained in all considered systems (see Figure 11b). The smallest current rectification is obtained for CNT(5,5) (filled-green squares), and the largest asymmetry is obtained for the CNT(6,6) system (open-blue squares).

So far, we have considered armchair CNTs, which have a metallic nature. To see how the chirality of CNT affects the rectification properties of CNT–metal junctions, we have conducted quantum transport calculations for single-walled zig-zag CNTs with chiral indices $(n,n)$, which present a semi-conducting nature. Figure 12a shows the $I$–$V$ curves of fluorinated zig-zag CNT–metal systems for different sizes of CNT and for the voltage range from $-2$ to $2$ V. There are two main differences in the $I$–$V$ characteristics of these samples as compared to the systems with armchair CNTs (compare Figures 11a and 12a). First, the value of the current for a given voltage biasing is larger in the case of zig-zag CNTs because of the

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**Figure 8.** (a) $I$–$V$ curves, (b) differential resistance, (c) nonlinearity, (d) responsivity, and (e) asymmetry of CNT-Ag(100) system without (solid-black circles) with different levels of fluorination. The current values in (a) are multiplied by 10, 100, and 100 for F1, F2, and F4 samples, respectively.
smaller doping level. Second, the reverse current is larger than
the forward one. Therefore, the rectification level (i.e., asymmetry) is in these systems defined as the ration of the reverse current to the forward one. Figure 12b shows the asymmetry for different sizes of the zig-zag CNTs. Significant current rectification is also obtained for this type of CNTs with the largest asymmetry for the CNT (8,8) system.

Finally, we study quantum transport through the double-walled CNT–metal interface. As a typical example, we consider double-walled CNT consisting of inner (3,3) CNT and outer (6,6) CNT (i.e., both CNTs have metallic character) (see inset of Figure 13b). Figure 13a shows the I–V curve of the system for the voltage range of −2 to 2 V. Current rectification is clearly seen from this figure with forward current being larger than the reverse current at larger voltage biasing. For the given level of fluorination (see the inset of Figure 13b), the asymmetry of more than 3 is obtained as shown in Figure 13b. Thus, current rectification can also be obtained due to fluorination for the systems containing multiwalled CNTs.

IV. CONCLUSIONS

Using first-principle density functional theory in combination with Landauer–Büttiker formalism, we study the quantum transport through CNT–metal interfaces. We start by considering the case when an insulating layer is inserted between the CNT and metal electrode. We obtained a clear current rectification where the rectification level depends on the
type of insulating layer. Enhanced current rectification is obtained by fluorinating the outer surface of CNTs, which originate from the bias-dependent charge localization in the system. We also study the effect of CNT morphology (i.e., tip opening, length, radius, and chirality) on the obtained results. These results show the potential of chemical doping (i.e., fluorination) as compared to direct evaporation of insulating layers in creating higher rectifying diodes. The obtained nonlinear and asymmetric diode behavior as well as low turn-on voltage can be beneficial for developing CNT-based devices for high-frequency optoelectronic applications, such as rectenna-based solar energy harvesting.

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Notes
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