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# Effect of number of carbon atoms on the electron transport properties of carbon chain-graphene junctions

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Abstract. Using nonequilibrium Green's functions in combination with densityfunctional theory, we investigate the electronic transport properties of carbon chains covalently connected with two bear armchair graphene electrodes. The results show that the transport properties are obviously dependent on the odd and even length chains located between graphene nanoribbons. For graphene nanoribbons connected to the chain with even chains, the negative differential resistance (NDR) is also observed in the *I-V* curves. The reason is that the even-odd effects are related to the connection structure between electrodes and carbon chains.

#### 1. Introduction

Recently, Jin et al have successfully achieved stable linear carbon atom chain structures from graphene [1-3]. The electronic transport properties of linear carbon have attracted much attention theoretically. For example, single carbon chain can be used as spin-filter by bridging two zigzag graphene nanoribbon (ZGNR) electrodes or bridging two modified armchair graphene nanoribbon (AGNR) electrodes [4, 5].

The NDR feature finds remarkable application in molecular switch, logic cell and memory [6]. Fullerenes, carbon nanotubes and graphene nanoribbons (GNRs) were proposed for NDR devices [7-9]. Carbon atomic chains have also been found the NDR behavior between Al electrodes [10] or between carbon nanotube electrodes [11].

In this present paper, we study the electron transport properties in carbon chain-graphene junctions with different numbers of carbon atoms. It is found that the transport properties are obviously dependent on the odd-numbered and even-numbered chains located between two chain-graphene nanoribbons. For two graphene nanoribbons connected to the chain with even chains, the negative differential resistance (NDR) is also observed in the I-V curves. Further analyses show that the evenodd effects are related to the number of carbon chains between electrodes.

#### 2. Computational method and model





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We use the model geometry consisting of a carbon chain including carbon chains with evennumbered and odd-numbered carbon atoms, bridging two bear AGNR electrodes. Figure 1 is the case of six carbon chains between bear AGNR electrodes.



Figure 2. The transmission spectrums of (a)-(c) the odd-numbered carbon chains ( $C_5$ ,  $C_{11}$  and  $C_{17}$ ) and (a)-(d) the even-numbered carbon chains (C6,  $C_{12}$  and  $C_{18}$ ).

In Figure 2 We show the transmission coefficients at zero bias voltage for odd-numbered carbon chains ( $C_5$ ,  $C_{11}$  and  $C_{17}$ ) and even-numbered carbon chains ( $C_6$ ,  $C_{12}$  and  $C_{18}$ ). The transmission at the zero bias voltage shows that the transmission peak increases with the increase of number of carbon atoms both odd-numbered carbon chains and even-numbered carbon chains.



Figure 3. Number-dependent conductance oscillation of the carbon chain-graphene junction.

Figure 3 shows that the conductance shows the characteristics of oscillation, and the conductance of the odd-numbered carbon chain is larger than that of the even-numbered, which due to their conductance at the Fermi level, as shown in Figure 2.

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Figure 4. (Color online) The *I*-V curves of the odd and even number of carbon chains ( $C_3$ - $C_8$ ).

To explain the conductance oscillation characteristic of the two probe systems, we present the *I-V* curves of the odd-numbered and even-numbered carbon atoms ( $C_3$ - $C_8$ ) at low voltage, as shown in Figure 4, calculated from

$$I(V) = \left(\frac{2e}{h}\right) \int_{\mu_L}^{\mu_R} T(E, V_b) dE$$
<sup>(1)</sup>

where  $\mu_{L,R}$  are the electrochemical potential of the left and right electrodes.  $T(E,V_b)$  is the transmission coefficient at energy *E* and bias voltage  $V_b$ .  $\mu_L(V_b) \ \mu_L(0) \ eV_b/2$  and  $\mu_R(V_b) \ \mu_R(0) \ eV_b/2$ .  $[\mu_L(V_b), \ \mu_R(V_b)]$  is the energy region, it contributes to the bias window.

In Figure 3, the current of odd-numbed carbon atom is larger than the even-numbed carbon atom at the same voltage. Interestingly, for even-numbed carbon atoms, the I-V curve exhibits NDR characteristic, the current decreases with the increase of voltage at the range of 0.1V to 0.3V. To understand the physical origin of the NDR feature in the number of carbon atoms, in Figure 5, we give the transmission coefficients at three biases.



Figure 5. (a) and (b) describe the transmission coefficient of the odd and even number of carbon atoms ( $C_3$ - $C_8$ ), respectively. The integral window have been denoted by the solid lines, and the shaded area denotes the integral area inside the integral window.

Figure 5 (a) displays the transmission coefficients T(E) for even number of carbon atoms under biases  $V_b=0$ , 0.3 and 0.6V, respectively. The integral area inside the integral window is related to the two factors, one is the range of the bias window and another is the transport coefficient. From the Figure 5(a), It is found that when the voltage is increased from  $V_b=0.3V$  to  $V_b=0.6V$ , the transport coefficient is increased and integral area becomes larger in the bias window, so the current increases.

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From the Figure 5(b), we can clearly see that when the bias voltage is increased from  $V_b=0.3$ V to 0.6V, the transmission coefficient is decreased in the bias window and the integral area gets smaller, so the current is decreased, and the NDR behavior can be founded.

#### 3. Conclusion

In conclusion, we investigate the transport properties of electrons in carbon chain-graphene junctions with odd and even number of carbon chains. The calculated show that the transport coefficient of the odd-numbered carbon chains is larger than the even-numbered carbon chains at zero bias voltage, and the conductance shows the characteristics of oscillation. In even-numbered carbon chains-graphene junction, the NDR behavior can be founded.

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