Strain effect on the electronic transport properties of carbyne

Gofur Eshonqulov
National University of Uzbekistan, g.eshonqulov@nuu.uz

Golibjon Berdiyorov
Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, gberdiyorov@hbku.edu.qa

Hicham Hamoudi
Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University

Follow this and additional works at: https://uzjournals.edu.uz/mns_nuu

Part of the Physics Commons

Recommended Citation
Available at: https://uzjournals.edu.uz/mns_nuu/vol2/iss3/3

This Article is brought to you for free and open access by 2030 Uzbekistan Research Online. It has been accepted for inclusion in Bulletin of National University of Uzbekistan: Mathematics and Natural Sciences by an authorized editor of 2030 Uzbekistan Research Online. For more information, please contact brownman91@mail.ru.
STRAIN EFFECT ON THE ELECTRONIC TRANSPORT PROPERTIES OF CARBYNE

ESHONQULOV G.1, BERDIYOROV G.2, HAMOUDI H.2
1National University of Uzbekistan, Tashkent, Uzbekistan
2Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, Doha, Qatar

e-mail: g.eshonqulov@nuu.uz, gberdiyorov@hbku.edu.qa

Abstract

Quantum transport calculations are conducted using density functional theory in combination with Green’s functional formalism to study the effect of external strain on the electronic transport properties of carbyne, 1D carbon allotrope, which has recently received a revival of interest due to its extraordinary mechanical, thermal and electronic properties. The current in the system increases monotonically by increasing the compressive strain, whereas the tensile strain results in the reduction of the charge transport. The obtained results are explained by spatial variations of the electrostatic potential along the carbon chain and nanoscale localization of the charge carriers. These findings can be of practical importance for carbyne-based nanotechnology development.

Keywords: carbyne, electronic transport, charge localization.

Introduction

Recent advances in nanofabrication made it possible to synthesize low dimensional systems with advanced mechanical, chemical and electronic properties. One of such systems is carbyne, which consists of linear chain of sp-hybridized carbon atoms. This material has received a lot of interest in recent years due to its exceptional mechanical, thermal and optoelectronic electronic properties. For example, carbyne outperforms any known material (including diamond) in terms of mechanical properties (e.g., specific stiffness, strength, and elastic modulus) [1]. Thermal conductivity in carbyne much exceeds the one for graphene [2]. Optical, electronic and transport properties of this material is also found to be suitable for carbon-based nanotechnology development [3, 4].

Synthesis of long carbyne chain is very challenging using conventional growth techniques [5, 6] due to high chemical reactivity of carbon. However, defect-free long carbon chains can be grown inside carbon-nanotubes (CNTs), as was shown in many of recent experiments [7, 8, 9, 10, 11]. Record-long linear carbon chain consisting of over 6000 carbon atoms has been obtained inside double-wall CNTs [11]. However, such CNT encapsulation can have profound effect optoelectronic properties of this 1D material [12, 13]. Such an effect mostly originates from the structural changes imposed on carbyne from the environment (e.g., cross-linking between the atoms of carbyne and CNT [14]). On the other hand, extraction of carbyne from the host CNT is technologically very challenging [15].
Recent studies show that [16, 17, 18, 19] the pressure plays an important role in determining the electronic properties of carbyne encapsulated by CNT. For example, insulating-metallic transition can be obtained under the strain [16, 17]. However, such changes in the electronic and structural properties of carbyne are mostly related to the interaction with the environment. In this respect, it is of fundamental importance to study the effect of pressure on the properties of stand-alone carbyne, where computational tools became very useful. Therefore, in this work we study the effect of external strain on the electronic transport properties of carbyne using density functional theory (DFT) in combination with the Landauer-Büttiker formalism. We found profound effect of pressure on the conductivity of the material. For example, the current along the chain increases monotonically by applying compressive strain whereas tensile strain leads to considerable reduction of the electronic transport. The obtained results are explained by the strain-induced charge localization and electrostatic potential variations in the system. These results can be useful to nanotechnology development based on carbon chains.

1 Computational details

We use DFT within the generalized gradient approximation of Perdew-Burke-Ernzerhof (PBE) [20] to study the structural and electronic properties of carbyne. Carbon atoms are described using double-zeta-polarized basis sets of local numerical orbitals and Monkhorst-Pack method is used for Brillouin zone integration [21]. Geometry optimization is conducted using the convergence criterion for Hellman-Feynman forces as 0.01 eV/Å. For the reference (i.e., unstrained) sample, the lattice parameters are optimized for a stress less than 0.02 GPa. van der Waals interactions are taken into account using Grimme’s PBE empirical dispersion correction [22].

Figure 1: Carbyne device geometry. The electronic transport is calculated along the z-direction.
The nonequilibrium Green’s function formalism is used for electronic transport calculations, where the current-voltage ($I$-$V$) characteristics are obtained using the Landauer-Büttiker formula [23]:

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

(1)

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. The calculations are performed using the computational package Atomistix toolkit [24].

2 Results and discussions

Geometry optimization is conducted for a carbyne supercell consisting of 4 carbon atoms using 21 k-points along the chain. Vacuum spacing of 20 Å is applied in the other two directions. The optimized geometry has alternating interatomic distances 1.321 Å and 1.273 Å. Using this geometry, we have constructed a two-probe device geometry which consists an active (scattering) region and left/right electrodes (see Fig. 1). The length of the scattering region is 7 times larger than the electrode size in order to avoid the interference of the electrodes. The electrodes are modeled as a semi-infinite extension of the unit cell (5.188 Å) to avoid the effect of contacting leads on the conductivity [25].

![Figure 2: Current voltage characteristics of carbyne under compressive (open symbols) and tensile (filled symbols) strain.](image-url)
Figure 2 shows the $I-V$ curves of carbyne for different values of the external strain, which will be the main result for our further discussions. The transport calculations are conducted using $1\times1\times120$ $k$-points. For the pristine (i.e., unstrained) sample (solid-black curves), the finite current in the system is obtained starting from applied voltage 0.5 V due to the semiconducting nature of carbyne. The energy band gap is estimated to be 0.42 eV from our devise density of states (DDOS) calculations (see Fig. 3 (a)). The current in the system increases monotonically with further increasing the applied voltage. The external strain affects both the current onset and the current value for the given voltage biasing. Namely, the compressive strain reduces the threshold voltage for the finite current in the system (see open symbols in Fig. 2), whereas the current onset shifts to larger voltage values in the case of tensile strain (filled symbols in Fig. 2). For a given value of the applied voltage, the electronic transport reduces for tensile strain. For the largest strain we have considered ($\varepsilon = 0.03$), the current in the system becomes more than twice smaller due to the tensile strain (filled-blue stars). On the contrary, compressive strain increases the current in the system considerably; twice larger current can be obtained for $\varepsilon = -0.03$ (open-blue stars). We expect further increase/decrease of the current with further increasing the compressive/tensile strain.

To explain the changes on the current-voltage characteristics of carbyne due to the external strain, we have analyzed the transmission spectra, device density of states (DDOS) and the transmission eigenstates of the considered samples for different values of the applied voltage. Zero-bias DDOS and transmission spectra are shown in Fig. 3 as a function of electron energy for different values of the external strain. Regardless of the strain, DDOS of the system is characterized by zero DDOS region due to the band gap and by sharp increase of DDOS near the band edges. The estimated band gap for the pristine carbyne is 0.42 eV, which is reduced to 0.24 eV for the compressive strain $\varepsilon = -0.03$ (thick-dotted-blue curve in Fig. 3(a)). On the contrary, the tensile strain increases the band gap and the maximum gap of 0.6 eV is obtained for $\varepsilon = 0.03$ (thin-dotted-blue curve in Fig. 3(a)). Such modulation of the energy band gap is reflected in the transmission spectra of carbyne as zero-transmission areas the size of which depends on the applied strain. Sharp increase of the transmission value from zero to 2 is obtained for all considered systems. Thus, the variations of the energy band gap with applied strain is responsible for the change in the threshold voltage for the current onset (see Fig. 2).

To understand the changes in the value of the current at finite voltages, we have performed DDOS and transmission spectrum calculations for finite voltage biasing. Figure 4 shows the obtained results at 1 V for two values of the external strain. At the Fermi level, both DDOS and transmission spectrum becomes larger when compressive strain is applied ($\varepsilon = -0.03$, dashed-red curves). The calculated transmission eigenstates show that the electronic states are well delocalized along the carbon chain (see panel 1 in Fig. 4) which responsible for the obtained larger transmission. The integration of such enhanced transmission gives the larger current as shown in Fig. 2 (open-blue stars). Dotted-blue curve in Fig. 4 (b) show the transmission spectrum of carbyne for tensile strain $\varepsilon = 0.03$. In this case, the electron transmission becomes
Figure 3: Zero bias device density of states (a) and transmission spectra (b) as a function of electron energy (zero corresponds to Fermi energy) for different values of the external strain.

smaller as compared to the one for the pristine carbyne for all electron energies. Such reduced transmission is due to the localization of electronic states as was revealed in our transmission eigenstate calculations (see panel 3 in Fig. 4) which is not obtained for the pristine carbyne (panel 2 in Fig. 4). Consequently, the current in the system decreases (filled-blue stars in Fig. 2). Another interesting phenomenon is obtained for larger electron energies where the transmission values of the considered systems starts to saturate. Namely, finite transmission is obtained for compressively strained sample (see panel 4 in Fig. 4 for the isosurface plots of the transmission eigenstates.
at 0.7 eV), whereas zero transmission is found for the unstrained and tensile strained systems. This is despite the fact that the latter systems have larger DDOS.

Finally, we study the effect of applied strain on the electrostatic potential profile in the system, which is also one of the important factors determining the electronic transport properties of the system. Figure 5 shows the electrostatic difference potential at zero voltage biasing along the carbyne without (solid black curve), with compressive (dashed-red curve) and tensile (dotted-blue curve) strain. In all three cases, we obtained periodic oscillations with double minima in each period. Amplitude of the oscillations increases for the tensile strain, which increases the back-scattering of the electrons and reduce their transmission probability. Compressive strain decreases the amplitude of the potential oscillations, thus, reducing the potential barrier for the electrons to transit along the carbyne. Thus, the characteristic changes on the I-V curves of carbyne under external strain can also be explained by electrostatic potential profile along the carbon chain.

3 Conclusions

Quantum transport calculations are conducted to study the effect of external strain on the electronic transport properties of carbyne. The results show that compressive strain increases the current in the system considerably due to delocalization of electronic states and reduced electrostatic potential variations along the sample. On the contrary, tensile strain results in the reduced current in the system, which can also be explained by nanoscale charge localization and by the electrostatic potential profile. These findings can be useful for practical applications of carbyne in nanotechnology development.

4 Acknowledgements

Computational resources were provided by the research computing center at Texas A&M University in Qatar.

References


Figure 4: Device density of states (a) and transmission spectra (b) as a function of electron energy for bias voltage 1 V for different values of external strain. Panels 1-4 show the isosurface plots (isovalue 0.1) of the transmission eigenstates for unstrained (panel 2), compressive strain (panels 1 and 4) and tensile strain (panel 3) at electron energies indicated on the transmission curves.
Figure 5: Variations of the electrostatic difference potential along the carbyne chain without (solid-black curve), with compressive ($\varepsilon = -0.03$, dashed-red curve) and tensile ($\varepsilon = 0.03$, dotted-blue curve) strain.