Electronic Transport in unidimensional carbon wire: Carbyne dopped Boron and Nitrogen atoms

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ABSTRACT

Carbon is a versatile material that is of interest in molecular electronics due to the variety of allotropes [1,2]. In the field of molecular electronics and miniaturization, nanowires constitute the lowest composition limits for a device [3], thus highlighting carbon allotropes with hybridization type -*sp* which are formed by thin wires of minimum sizes (atomic diameter) [1,2], constituting an allotropic group called carbyne [1] represented by two groups, whereas the continuous bond between the carbons is continuously classified as cumulene, whereas an alternation between single and triple bonds along carbon atoms is polyyne [1,2]. Using first-principle methods based on Density Functional Theory (DFT) [4,5], the solution for the generalized gradient approximation (GGA) based on the PBE with the solution for the exchange-correlation potential [4,5], with a base set DZP, as cutoff of 300 Ry implemented in the SIESTA package [6] and to investigate the molecular electronic transport, was used the non-equilibrium green function (NEGF) [7] method, based on the TRANSIESTA package [6,8] was used as a basis. Doping in the central region between carbon atoms with boron (B) and nitrogen (N) atoms has been proposed, see Fig. (1). The results for the structure of doped carbon with B and N revealed that there was no alternation in bond length, being 0 Å difference between r_i–r_{i+1} wherein i is an i-th atom, which characterizes the wire as cumulene [1, 2], thereby providing the system with a greater delocation of electrons π . The current and voltage curve (I – V_b) over a voltage range of -0.5V to 0.5V, the appearance of symmetry in the current is due to the influence of the electrodes, with range currents in the order of 40μA, see Fig. (2), indenting the doping guarantees the current asymmetry seen in Fig. (3), however the relationship between the current values and the direct and reverse voltage values provides the rectification rate [R(V_b)] [8] revealing the driving tendency feeling reverse tension, direction N to B, seen in Fig. (4).

[1] CASARI, C. S.; MILANI, A. Carbyne: from the elusive allotrope to stable carbon atom wires. **MRS Communications**, v. 8, n. 2, p. 207-219, 2018.
[2] HEIMANN, Robert B.; EVSYUKOV, Sergey E.; KAVAN, Ladislav (Ed.). **Carbyne and carbynoid structures**. Springer Science & Business Media, 1999.
[3] ZHANG, Anqi; ZHENG, Gengfeng; LIEBER, Charles M. **Nanowires: Building blocks for nanoscience and nanotechnology**. Springer, 2016.
[4] PAYNE, Mike C. et al. Iterative minimization techniques for ab initio total-energy calculations: molecular dynamics and conjugate gradients. **Reviews of modern physics**, v. 64, n. 4, p. 1045, 1992.
[5] KOHN, Walter; SHAM, Lu Jeu. Self-consistent equations including exchange and correlation effects. **Physical review**, v. 140, n. 4A, p. A1133, 1965.
[6] SOLER, J. M. et al. The SIESTA method for ab initio order-N materials simulation. **Journal of Physics: Condensed Matter**, v. 14, n. 11, p. 2745, 2002.
[7] BÜTTIKER, M. Four-terminal phase-coherent conductance. **Physical review letters**, v. 57, n. 14, p. 1761, 1986.
[8] AADHITYAN, A. et al. Electron transport analysis in positional isomers-A DFT-NEGF approach. **Materials Science in Semiconductor Processing**, v. 104, p. 104654, 2019.

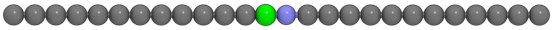

Fig. 1. Unidimensional device model Carbyne dopped with Boron and Nitrogen atoms. In gray to carbon atom, green to boron atom and blue to nitrogen atom.

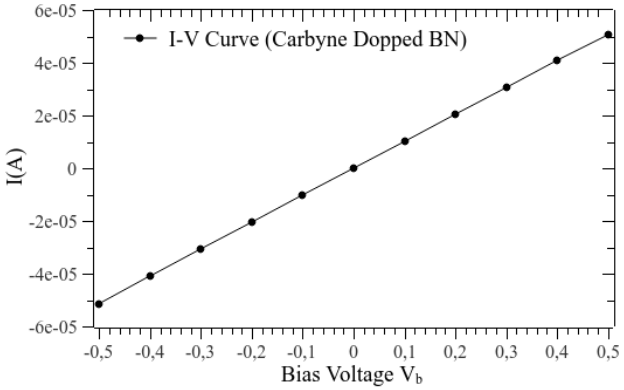

Fig. 2. Voltage versus current curve for carbyne dopped with B and N.

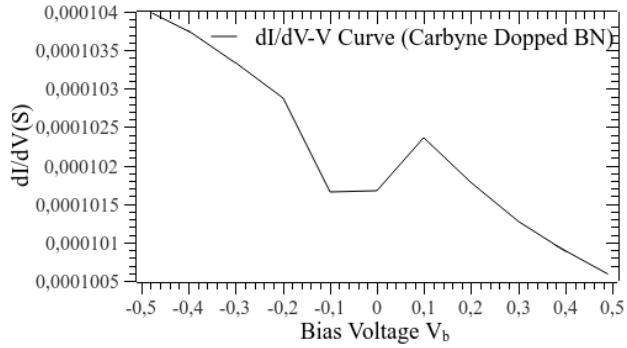

Fig. 3. Differential conductance versus voltage curve for Carbyne dopped with B and N.

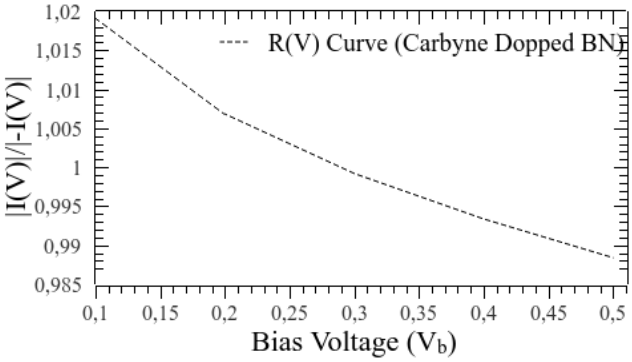

Fig. 4. Rectification ratio curve for carbyne dopped by B and N.