WIDTH EFFECTS IN OPG-Z NANORIBBON SYSTEMS

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Molecular electronics has become an alternative to overcome the problems related to materials commonly used in electronics (such as silicon), which are reaching the limit of their miniaturization capacity. This area of research involves the use of atomic and molecular systems to produce an electronic device, the so-called electronic molecular devices with performance equal to or superior to existing devices[1]. The aim of this work was to propose and investigate the width effect in a new system based on a 2D carbon allotrope called OPG-Z[2] and verify the potential of its application in nanoelectronics. The systems were investigated by means of ab-initio calculations based on Density Functional Theory (DFT), using the PBE/GGA/DZP approximation implemented in the SIESTA computational package[3]. We obtained the energetic and electronic properties considering of five nanoribbons (NR, with width (W) from 1 to 5) (zzOPGZNR-PO). The results indicated that the systems are energetically stable, with cohesive energy from -7.48 to -8.39 eV/Atom. The molecular devices were designed from the unit cell structure, considering the NR with widths from 1 to 3. We observe that the device with (W=1) the smallest width presents an I-V curve behavior that resembles a Field-Effect Transistor (FET) in the voltage range from -0.3 V to +0.3 V and linear behavior between -0.3 (+0.4) V and -1.0 (+1.0) V. For W = 1 and W = 2, the I-V curve tends to linear behavior throughout the analyzed voltage range (-1.0 V to +1.0 V). From the results obtained in the calculations via DFT/NEGF, we note that the systems present behavior similar to some electronic devices in the analyzed voltage range, for example: the field effect transistor (FET) and the ohmic resistor. These results indicate possibilities in the development of new molecular electronic devices based on OPG-Z nanoribbons, and suggest applications for these materials in nanoelectronics using the width of the systems as a control parameter.

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