Electrical and optical properties of beta-graphyne nanoribbons.

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Abstract

The beta-graphyne is a class of graphyne that presents an interesting difference from other graphynes shapes. The Dirac cone is not located in a point of high-symmetry in reciprocal space [1-2]. In this work we perform a theoretical study of the electronic and optic properties of bi-nanoribbons of this material, for different stacking configurations. The electronic properties of the systems are obtained using the density functional theory (DFT) code OpenMX [3], which is based on localized pseudoatomic orbitals (PAOs) [4] and norm-conserving pseudopotentials [5]. The PAO of carbon atoms consists of two s-orbitals and two p-orbitals. The Perdew–Burke–Ernzerhof (PBE) exchange-correlation functional [6], which is derived within the generalized gradient approximation (GGA) is used, taking into account an energy cutoff equal to 150 Ry and a convergence criteria of 10^{-8} Hartree. All structures are relaxed using the Direct Inversion Iterative Subspace method [7] with a residual force criteria less than 10^{-4} Hartree/Bohr. Our results show that these systems have interesting optical and electrical conduction properties, depending on the stack and edges of nanoribbons. As an example, shown in Figure 1, the results of electrical conduction, of nanoribbon formed with a single layer.

References

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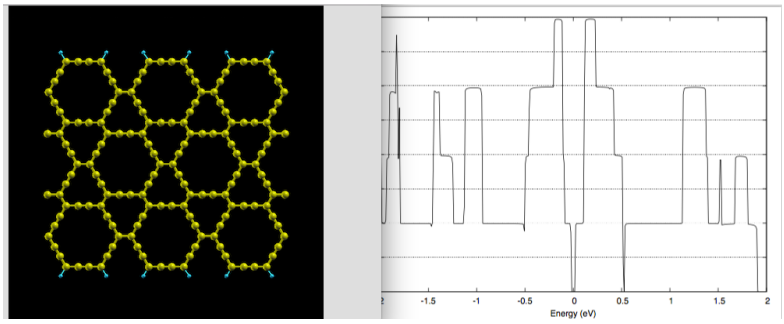

Figure 1. Schematic of beta-graphyne nanoribbon and electrical transmission.