Electron transport properties of the fluorocarbon chain bridging two graphene leads

Małgorzata Wawrzyniak-Adamczewska, Tomasz Kostyrko

Faculty of Physics, A. Mickiewicz University, ul. Umultowska 85, 61-614 Poznań, Poland

Inspired by the experiment showing realization of the stable free-standing carbon atomic chains connected to graphene flakes [1], as well as by the theoretical electron transport studies in such systems [2, 3, 4], the numerical analysis of the electronic properties of the fluorocarbon chain bridging two graphene leads is presented and discussed. Such a system may be possibly realized during the fluorine-passivation process of the graphene-chain-graphene junction. The role of the type of the graphene edges, the length and parity of the formed chain, as well as the range of the fluorine passivation is examined. The electronic properties such as partial and local density of states, the transmission function and the current-voltage characteristics is studied within density functional approach using SIESTA package [5]. The *ab initio* results are then compared to tight-binding model ones.

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