Spin polarization induced by electric fields in carbon-atom-chain molecular devices

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The response of large molecular systems to an external electric field (EF) plays an underlying role in the development of efficient nanoelectronic devices. In this sense, molecular rectifiers have long been the holy grail of molecular electronics. We employing EF, with sufficiently high strength, to generate and control spin polarization in molecular systems containing small carbon atomic chains interconnected by graphene-like flakes. This is performed within density functional theory. Our theoretical study indicates that the application of an external EF along the direction of the carbon chains allows to control both energy gap and spin-polarization, within the limit of the structural restoring of the systems. In this sense, by applying electric fields with magnitudes in the 1-5 V/nm range, we obtain semiconductor-to-metallic transitions for odd-numbered carbon-chain systems. Moreover, high-spin-to-low-spin transitions are determined for these systems as a function of the EF magnitude. In the case of the even-numbered carbon-chain systems, the overall effect is pushing electron density near the Fermi level, leading to a gapless or metallic regime at 3.0 V/nm. However, an electric-field control of the spin-polarization of these latter systems is only achieved by doping the extremities of the graphene-like terminations with sulfur atoms. This finding is beneficial for applications of these systems in spin-controlled carbon-based devices connected by gold electrodes. Financial Suport: CNPq and CAPES.