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Switching and negative differential resistance in a gated single-molecule transistor: Effects of fixed and shifting states AMIR FARAJIAN, RODION BELOSLUDOV, HIROSHI MIZUSEKI, YOSHIYUKI KAWAZOE, TOMIHIRO HASHIZUME, BORIS YAKOBSON — The quantum transport in a gated nanodevice based on polythiophene is studied. The functional polythiophene molecule is attached to two gold electrodes which are used as drain and source contacts. A third electrode, assumed to act as gate, is considered to shift the energy levels of the functional molecule. We use density functional theory to obtain the self-consistent electronic structure of the system under bias. The electronic structure is then used within the nonequilibrium Green's function approach to calculate conductance and current- voltage characteristics. We show that this molecular field effect transistor possesses two the of the main features of electronic components, namely abrupt switching and negative differential resistance. Ab- initio based explanations of these features are provided by distinguishing fixed and shifting conducting states, which are shown to arise from the interface and functional molecule, respectively. Optimization of the device characteristics by choosing proper bias range and doping is also discussed.

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