Spin-dependent Transport in Metal-Organic Molecule-Metal Systems

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Due to their potential applications in the future electronics, there has been intense interest in the electron transport of organic molecular systems sandwiched between conducting molecules. Effects of molecular length, structure, chemical bonding, conjugation-length, strength of metal-molecule interaction, and rotation of molecule along single-bond have been investigated. The effect of electron spin on molecular electron transport has, however, received little attention. Electron spin is an important quantum mechanical parameter which has already played an important role in the development of solid-state magneto-resistance devices and may play an important role in molecular spintronics. In order to understand the effect of spin orientation, we have investigated electron transport in metal-organic molecule-metal (MOM) systems consisting of C60, benzenediothiole, and bicyclooctane sandwiched between Ni electrodes. The effects of molecular structure, molecule-electrode interaction, and chemical binding on the current-voltage (*I-V*) characteristics of the model structures are investigated by *ab initio* density functional theory (DFT), in the framework of non-equilibrium Green's function approach. In this paper, we shall present the results of our calculations of the effect of the relative spin orientations at the two electrodes on the *I-V* characteristics of of our model MOM architecture.