Study and comparison of the electronic and transport properties of pentacen and perfluropentacene

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Abstract

In this study, the electronic and transport properties of pentacene and perfluropentacene are investigated using first principle calculations based on density functional theory and non-equilibrium Green's function. The results show that the HOMO-LUMO gap of perfluropentace is about 0.2 eV smaller than that of pentacene which is comparable with the reported value of 0.2eV. For both molecules, the most contribution in DOS around Fermi energy is related to 2p orbitals of carbon. Electron transport calculations are investigated for both molecules of pentacene and perfluropentacene in Au(111)/molecule/Au(111) junction. Transmission coefficients and I-V curves up to 2V have been calculated and compared for both molecules. The transmission coefficients are composed from resonant peaks which are mostly originated from HOMO and LUMO peaks of the molecules. The calculated current in Au/pentacene/Au junction is more than the current in Au/perfluropentacene/Au junction except a small interval around 1V, in a way that the difference between the currents get the maximum value of $5\mu A$ at $2V$.

Keywords: Pentacene, Perfluropentacene, Electronic and transport properties, Transmission coefficient, I-V curve, Molecular Electronics, Non-equilibrium Green's Function