Design and Modelling of Single Molecular Switch with Graphene Electrodes

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Abstract:

The electronic transport properties of molecular device based on molecular switches with graphene electrode are investigated by density functional theory and non-equilibrium Green's function. The devices with open and closed configurations show a switching effect. It is found that doping of different amounts of nitrogen atoms and boron atoms on left and right graphene electrodes results in different electronic transport properties. In addition, the observed oscillation of current in the devices induced by doping using transmission eigenstates and transmission spectra of the device. The local density of states of the device is calculated to analyze the observed rectifying behavior. The results suggest that doping of nitrogen atoms on the left electrode can be considered as a factor to modulate the electronic transport properties of molecular device.

The single-molecule junction, which is the basic unit of molecular device, has been extensively studied since the first discovery in 1974. Since then several numerous experiments and theoretical studies have been performed through molecules placed between two nano electrodes within a nano gap. Since the pioneering work of Reed et al. who first measured by mechanically controllable break junctions (MCBJ), the conductance of a single benzene-1,4- dithiol (BDT) molecule attached to a gold surfaces, BDT has been considered the benchmark molecule for both theoretical and experimental studies. Performed a systematic investigation of the evolution of the conductance of a benzene molecule with different electrodes and different anchoring groups combination. When junctions are formed using gold metal electrodes, thiol links are frequently used. However, the conductance of the single-molecule junction varies significantly from junction to junction, making it difficult to map the relation between molecular structure and junction conductance. Measurements of single molecule junctions in a molecular switch with different metal electrodes results in a broad distribution of conductance, attributed to different binding geometries for ON and OFF. In particular, the conductance of aromatic molecules is strongly influenced by the orientation of the π system relative to the electrode-anchoring bond.

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