The electronics proprieties of conjugated molecular shelf-assembled monolayer -The intermolecular interactions

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Abstract:

The purpose of this paper is to study the electronic transport of molecular wire. The calculations were performed using an approach based on Landauer formula. The investigated self-assembled monolayer (SAM) system is composed of 1,4-dithiol benzene (HSC_6H_4SH) molecules isolated or connected between two gold electrodes. We present the density functional theory (DFT) to describe the molecular electronic structure with the first principle DFT-KS (Khon-Sham) method. The electron transport within a single molecule unit or more than two molecules connected in parallel will be investigated. We will focus on the description and influence of the structural and energy characteristics of the assembly, as well as the π-coupling on the electron transport process. This allows us to obtain molecule-molecule or molecule-metal coupling description. The research work involves also the studied of the influence of π-orbital coupling on the electronic proprieties and on molecular assembly. We will also investigate the influence of π-coupling on electronic and structural properties as function of the intermolecular distance.

The conduction of molecules benzene 1,4-dithiol connected in parallel is obtained and compared as the intermolecular distances are reduced to below 10 Å. The effect of the number of molecules connected in parallel and the molecular orientation of one molecule to another molecule on the conduction will be discussed. A specific arrangement of packing molecules as function of the intermolecular distance and orientation of molecular assembly should be investigated to predict a larger conduction.

It was found that the intermolecular distance between single molecular unit as well as the number of molecules connected in parallel play an important role for controlling the electronic proprieties. The HOMO-LUMO gap (HLG) of one single SAM unit is reduced when decreasing the intermolecular distance and increasing the number of molecules.