Electronic transport through benzene molecule and DNA base pairs

A. A. Farajian, T. M. Briere, R. V. Belosludov, H. Mizuseki, and Y. Kawazoe

Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

One of the possible applications of electronic transfer through organic materials is in the area of molecular devices. Current trend of the miniaturization of electronic devices has resulted in intensive interest in molecular devices, which basically consist of a group of a few atoms, in contrast to the previous 'bulk' materials. The reason is that molecular devices possess two main characters that are important for probable applications: They are self-assembled and rather abundant.

As the molecules that are to be used as the main functional part of the device are typically a few angstroms in size, a natural question arises here, namely when these small building blocks are attached to the electrodes, how would their main characters of interest depend on the actual arrangement of the atoms in the electrode. This is an issue of concern for both experimentalists and theoreticians: In experiments, it should be known that which surface in general, and which part of the surface in particular, are more suited for to be used as the electrode. As for the theoretical calculations, it should be known that what model should be used in the description of the electrodes.

In the present study we first investigate the above-mentioned issues for a typical case of a simple organic molecule, i.e., benzene, attached to two gold electrodes via sulfur clips. Two models are used for the gold electrodes: a simple chain and the Au(111) surface. We use ab initio modeling, from which the Hamiltonian of the system is deduced. Moreover, as we use a non-orthogonal basis, the overlap matrix is also needed for our study. The conductance of the system is then calculated via the Green's function approach, by finding the surface Green's functions of the two electrodes, and attaching them to the Green's function of the organic molecule. It is shown that the atomistic model used for the electrodes indeed affects the calculated conductance, at least for the case of strong coupling between the organic molecule and the metallic electrodes. The same Green's function procedure is then used to calculate the electronic transport properties of DNA base pairs. The results will be useful in both describing the scanning tunneling microscope (STM) images of DNA, and exploring the possibility of using DNA base pairs as part of electronic molecular devices.

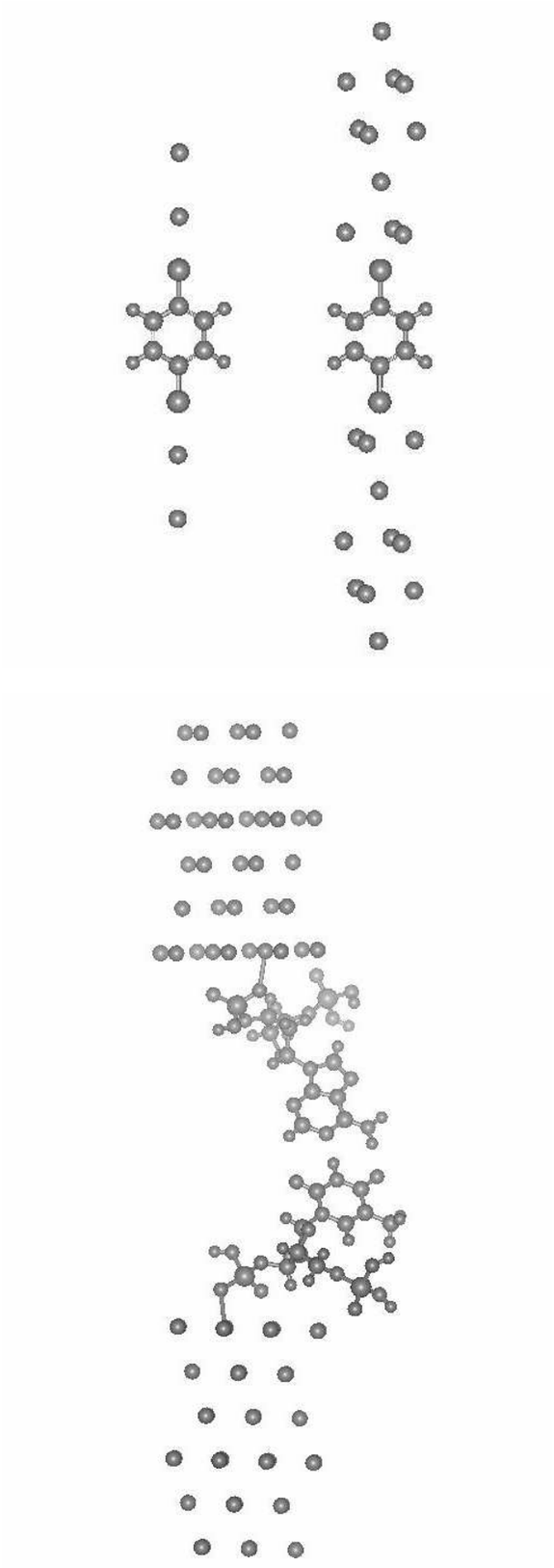

Fig. 1: Two models for gold contacts in calculating electronic transfer through a benzene-1,4-dithiolate molecule: simple gold chain (top left) and Au(111) surface (top right). The same procedure is used to calculate transport through DNA A-T base pairs attached to Au(111) electrodes (bottom).