Electron Transport into Organized Low-Dimensional Molecular Systems

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One promising approach to assemble molecules into an active electronic component involves self-assembling monolayer (SAM) techniques. This would ideally lead to the formation of highly packed and organized molecular structures on a metallic template. Once a dense structure is formed, molecular interactions should become significant. We have studied the influence of π-orbital coupling in arenes-based assembly on its resulting electronic and electrical properties. The conduction and the field-switching properties of the assembly are compared as the intermolecular distances are reduced to below 5 Å. We have investigated the electron transport within a single molecule, and more importantly, between the molecules which form a 1D molecular wire. We have also explored different electrode geometries, such as the one shown in Figure 1. For this specific arrangement, we predict a large conductance modulation upon application of a transverse gate field, for which the switching mechanism involves a delocalized π-resonance - i.e. resonant tunneling in the intermolecular π- and π^*-bands of the molecular assembly.

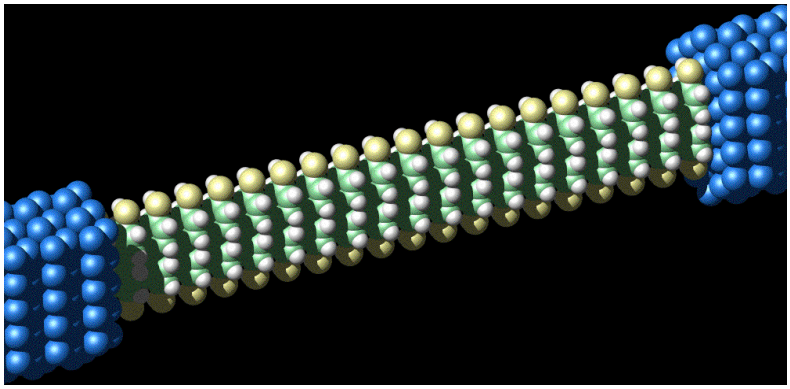

Figure 1. Model of a molecular wire made of 20 arenes molecules (4,4'-biphenyldithiol, BDT) perfectly stacked into a 1D structure, and connected at both ends to metallic electrodes (in blue).