MOLECULAR CONDUCTANCE IN TERMS OF ORBITAL DENSITIES AND POLARIZABILITIES

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In molecular electronics, molecules are connected to macroscopic contacts. In our work we focus on modeling the transmission of electrons through a molecular electronic device (MED). We use conventional perturbation theory (where the contacts are represented by a perturbing potential[1]) to calculate the transmission probability T(E) for an electron to pass through the molecule. This allows us to express T(E) in terms of properties of the bare molecule. We show that, in general, it is the electron density (first-order contribution) on the atoms that connect to the contacts that contributes the most to the transmission probability of the MED. The second-order correction, determined by the orbital polarizability, adds little improvement on the first-order results for the system studied. Using this approach, we obtain a simple qualitative answer to the question why the molecule studied by M. Mayor[2] shows orders of magnitude difference in the conductance by changing the contact attachment points in the molecule. We outline an extension of our method that accounts for correlation effects.

References:

[1] F. Goyer, M. Ernzerhof and M. Zhuang, J. Chem. Phys., **126**, (2007) 144104
[2] M. Mayor *et al.*, Angewandte Chemie Int. Ed., **42**, (2003) 5834