USING COMPLEX POTENTIALS TO DESCRIBE ELECTRON TRANSMISSION THROUGH MOLECULES

Francois Goyer, Matthias Ernzerhof
Department of Chemistry, University of Montréal, Montréal, Canada
francois.goyer@umontreal.com

The understanding of electron transport through molecular electronic devices (MEDs) is essential for the conception of new types of circuits, such as quantum transistors. We present our newly developed Source-Sink Potential (SSP)[1] method for the calculation of the transmission probability.
Using SSP we explore simple relationships between molecular structure and conductance to analyze and predict experiments. The systems studied range from small aromatic compounds to nanotubes. In these systems, phenomena, such as destructive interference, are studied to provide insight on their impact on the conductance of MEDs.
We also present an approach to include correlation effects in the description of MEDs. A generalization of density functional theory (DFT) has been proposed[2] to allow for the use of complex (SSP) potentials. We apply the SSP method in the framework of this complex DFT. The implementation of this new DFT[2] is explained, as well as preliminary results of the conductance of model MEDs.

References:

[1] Goyer, Ernzerhof, and Zhuang, *The Journal of Chemical Physics* ***126***, (2007) p. 144104.
[2] Ernzerhof, *The Journal of Chemical Physics* ***125***, (2006) p. 124104.