Destructive Quantum Interference in Graphene-like Single Molecule Junctions

Ozlem Sengul
Angelo Valli, Robert Stadler
Vienna University of Technology, Wiedner Hauptstrasse 8-10, Vienna Austria
oezlem.senguel@tuwien.ac.at

Destructive quantum interference (DQI) has been a source of interest as a new paradigm for molecular electronics with low power consumption advantage, and the electron conductance is widely dependent on the occurrence or absence of DQI effects. We perform non-equilibrium Green's function calculations within the framework of density funcitonal theory, and consider different configurations of pyrene moiety as single-molecule bridges between Au and graphene electrodes with different topological properties. Thiol and acetylene anchor groups with linkers at either meta- or para- positions are studied to asses the strucure-function relationship of molecular juncitons with different connectivities to probe electronic transport features and DQI effects. The analysis of charge transfer and frontier molecular orbitals allows to gain further insight into the nature of the transport mechanisms and the shape of the transmission function.

References

[1] O. Sengul, A. Valli, and R. Stadler, in preparation (2020).

Figures

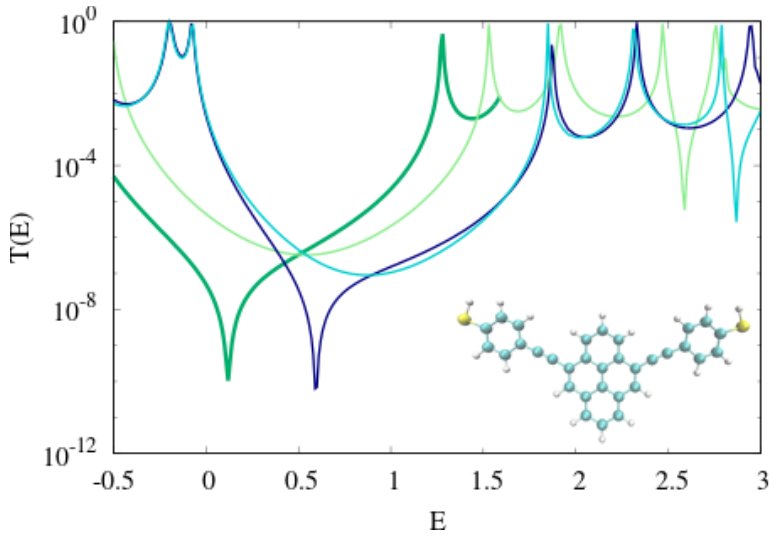

Figure 1: Transmission function with DQI for pyrene single-molecule junction.