Quantum interference effects in electron transport: How to select suitable molecules for logic gates and thermoelectric devices

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Since the concepts for the implementation of data storage and logic gates used in conventional electronics cannot be simply downscaled to the level of single molecule devices, new architectural paradigms are needed, where quantum interference effects (QIE) are likely to provide an useful starting point [1],[2]. In order to be able to use QIE for design purposes in single molecule electronics, the relation between their occurrence and molecular structure has to be understood at such a level that simple guidelines for electrical engineering can be established. We made a big step towards this aim by developing a graphical scheme that allows for the prediction of the occurrence or absence of QI induced minima in the transmission function (Fig. 1) [2]-[4] and the derivation of this method as well as a discussion of its range of applicability and limitations will form the center piece of my presentation. In addition I will address the possible usefulness of QIE for thermoelectric devices, where the peak shape around a transmission minimum is of crucial importance and different selection rules for suitable molecules have to be found (Fig. 2) [5].

References

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[3] T. Markussen, R. Stadler and K. S. Thygesen, Nano Lett. **10** (2010) 4260.
[4] T. Markussen, R. Stadler and K. S. Thygesen, Phys. Chem. Chem. Phys. **13** (2011) 14311.
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Figures

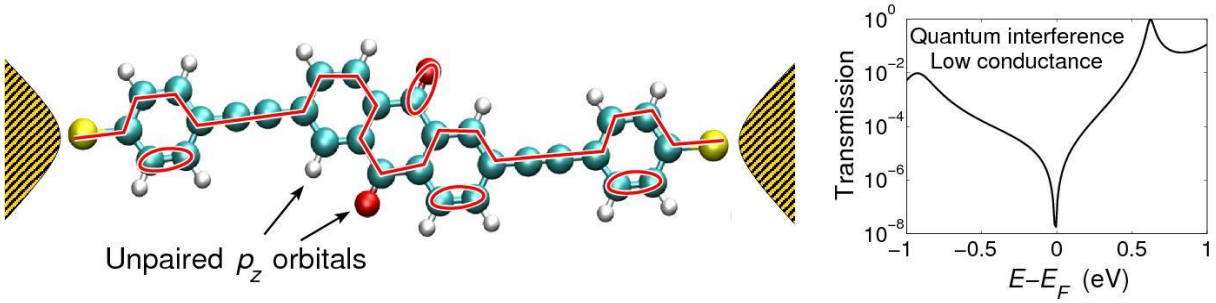

Fig. 1: Illustration of the graphical scheme (left) for predicting a QI induced minimum in the electron transmission function (right). For details see Ref. [3].

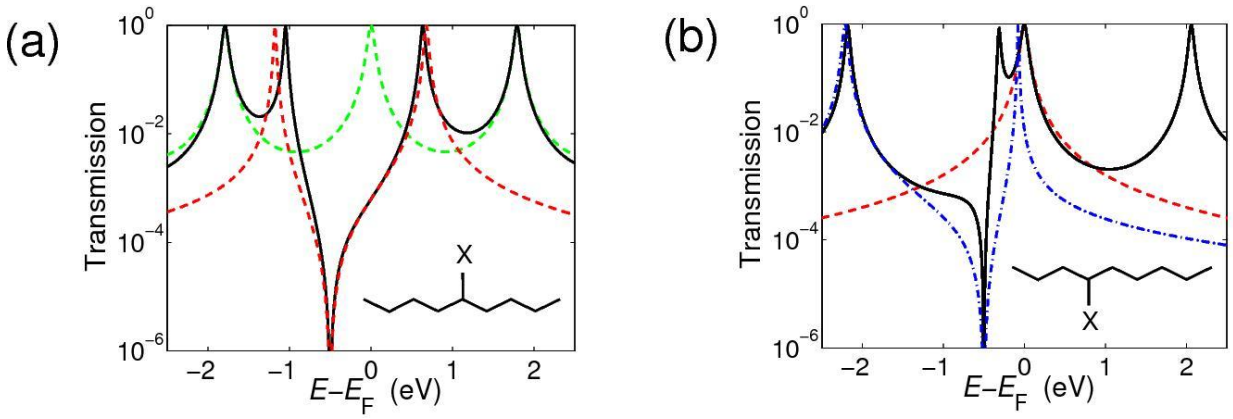

Fig. 2: Depending on the position and chemical nature of a sidegroup on a molecule, the transmission minimum can exhibit different peak shapes. For details see Ref. [5].