

# Seminář odd. 26

## Tenkých vrstev a nanostruktur

*Fyzikální ústav AVČR, Cukrovarnická 10, Praha 6*

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### TÉMA

## Devices in single molecule electronics based on quantum interference and redox switches

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The talk will be divided into two parts. Part one is related to quantum interference [1],[2],[3]: 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 (QI) effects are likely to provide an useful starting point. In order to be able to use QI 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 and the derivation of this method and the range of its applicability will form the center piece of this presentation.

Part two is related to redox switches [4],[5],[6]: In a joint experimental and theoretical investigation of the transport properties of organometallic molecules containing either Fe, Ru or Mo centers, hysteretic transport properties with continuous transitions were found for all compounds, and additionally an abrupt switching for Mo [4]. The latter could be modelled by taking into account bias-driven charging and explained by an oxidation/reduction mechanism mediated by a localized MO with weak coupling to the electrodes that is unique to the Mo compound because of the latter's spin-polarized ground state. Di-nuclear Fe compounds with various different anchor groups were also investigated, where excellent agreement of the trends in conductance between theory and experiment were obtained [5].

#### References:

- [1] R. Stadler, S. Ami, M. Forshaw, and C. Joachim, *Nanotechnology* 15, S115-S121 (2004).
- [2] T. Markussen, R. Stadler, K. S. Thygesen, *Nano Lett.* 10, 4260-4265 (2010).
- [3] R. Stadler, *Nano Lett.*, 15, 7175–7176 (2015).
- [4] F. Schwarz, G. Kastlunger, F. Lissel, C. Egler-Lucas, S. N. Semenov, K. Venkatesan, H. Berke, R. Stadler and E. Lörtscher, *Nature Nanotechnology*, in print (2015); DOI:10.1038/nnano.2015.255
- [5] F. Schwarz, G. Kastlunger, F. Lissel, H. Riel, K. Venkatesan, H. Berke, R. Stadler and E. Lörtscher, *Nano Lett.* 14, 5932-5940 (2014).
- [6] G. Kastlunger and R. Stadler, *Phys. Rev. B* 91, 125410 (2015).