

Seminar on Condensed Matter Theory

Group of Theoretical Physics at the Department of Condensed Matter Physics
of Charles University has a pleasure to invite you to attend the seminar

on 25 April 2019 at 13:00

at Faculty of Mathematics and Physics of Charles University, Ke Karlovu 5, 121 16 Praha 2

Seminar room F052



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Institute of Physics, FMP CU

Modeling of atomic force microscopy control of single molecule electron transfer

We model non-equilibrium electron transfer within a single molecule (two ferrocene units linked by a naphthalene linker) under the driving by an oscillating probe of an atomic force microscope. The model enables us to discuss the interplay of the environmental reorganization with the electron transfer process, especially the role of the relative time-scale of this process with respect to the time-scale of the electron transfer. Experimentally measured electron transfer rates show only a mild dependence on temperature, at odds with a straightforward application of the canonical detailed balance condition. We explain the breakdown of the canonical detailed balance by the non-equilibrium nature of the steady state into which the system is driven by the probe. Comparison between the theory and the experiments hints at the non-equilibrium state of both the electron and at least some of the environmental degrees of freedom. However, a very good agreement can be obtained already with the model of an equilibrium environment. The non-equilibrium character of the electronic state remains crucial for the explanation of the experimental observations.

