Scientific report on a short visit grant within the ESF program: Electron Induced Processes at the Molecular Level

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Title of the project: Nonequilibrium theory of vibrationally inelastic electron transport through molecular junctions

The purpose of the my visit in the group of Prof. J. Horaček and Dr. M. Čížek at the Institute of Theoretical Physics, Charles University, Prague, was to extent the previously proposed theory of vibrationally inelastic electron transport through molecular junctions to take the nonequilibrium character of the process into account.

To this end, the following work was carried out in close collaboration with Dr. M. Čížek:

- A rate theory of electron conduction through a molecular junction was formulated which describes the consecutive transmission of electrons through a molecular bridge. Extending the previous theory, this approach includes the stationary state of the vibrational degrees of freedom of the molecular bridge. This rate theory will allow us to study the process of current induced heating and dissociation of the molecular bridge which is one possible source of instability of molecular junctions.
- We have started to develop a nonequilibrium Green's function theory of charge transport through molecular bridges beyond the commonly used harmonic approximation. This theory appears promising to study vibrationally inelastic effects in molecular junctions with large-amplitude motion, such as, e.g., the torsional motion of two phenyl rings between gold electrodes.

Furthermore, I gave a talk in the Theoretical Physics seminar of the group of Prof. J. Horaček on 'Quantum dynamics of ultrafast photoinduced electron transfer reactions'.

It is planned to continue the collaboration in the future including a visit Dr. M. Čížek in the group of Dr. Michael Thoss at the Department of Chemistry, Technical University of Munich, in July 2005.

It is also planed to publish the above mentioned methodological developments as well as their applications to charge transport in experimentally relevant systems.