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Report on the PhD thesis by Mgr. I. Pshenichnyuk

Since the first experimental realization of single molecule junctions, where molecules are chemically bound to metal or semiconductor electrodes, about a decade ago, the field of molecular electronics has seen a rapid development. Employing a variety of experimental techniques, including break junctions methods and scanning tunneling microcopy, the transport properties of single molecule junctions have been investigated in detail. The experimental investigations have revealed a multitude of interesting transport phenomena, including Coulomb blockade, Kondo effects, hysteresis, switching, current-induced vibrational excitation, and have stimulated theoretical studies to elucidate the underlying transport mechanisms.

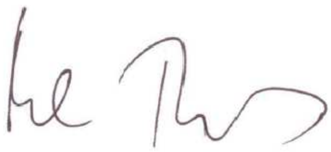
Within this context, the major focus of the research presented in the thesis of Ivan Pshenichniyuk is the theoretical study of the influence of electronic-vibrational coupling on the transport properties of molecular junctions. The often strong coupling of the electrons to local vibrational modes of the molecular bridge is one mechanism that distinguishes transport in molecular junctions from that in semiconductor devices or quantum dots. The adequate theoretical description of such effects is a challenging project at the forefront of theoretical nanophysics.

To study vibrationally-coupled electron transport in molecular junctions, two different transport methods are employed in this thesis: inelastic scattering theory and master equations. The scattering theory approach allows the treatment of strong molecule-lead coupling. However, in its original formulation, it neglects vibrational nonequilibrium effects, which are necessary to describe current-induced vibrational excitation and the resulting heating of molecular junctions. In the present thesis, the scattering theory approach is extended to include vibrational nonequilibrium effects. To this end, a kinetic equation for the nonequilibrium vibrational distribution at finite bias voltage is formulated. The comparison with results of the master equation approach, which includes vibrational nonequilibrium effects but cannot be applied for larger molecule-lead coupling, shows good agreement and thus validates the novel extended scattering theory approach.

The influence of electronic-vibrational coupling on transport in single-molecule junctions is analyzed in the present thesis for a series of models with increasing complexity. Most studies of electron-vibrational effects in molecular junctions in recent years employ the harmonic approximation for the vibrational degrees of freedom, which is valid for small amplitude motion. The study of models with large-amplitude torsional motion, presented in the second part of this thesis, goes well beyond these simpler models, both with respect to the required theoretical methodology and the underlying physical transport mechanisms. To describe transport in these systems, the master equation method had to be extended to allow the treatment of anharmonic degrees of freedom. The analysis of the results reveals a multitude of interesting transport phenomena, in particular current-induced vibrational cooling, negative differential resistance, and, most interestingly, current-induced rotational motion. These results will be of great interest to both experimental and theoretical researchers in the field of molecular electronics.

The thesis is clearly written, the results are carefully analyzed and discussed. The English language is not always perfect, but this minor issue never deteriorates the presentation and understandability of the results.

To summarize, this thesis presents interesting research at the forefront of current work in the field of molecular electronic, including both the development of novel theoretical methods, the implementation of the methods in efficient numerical algorithms as well as the analysis of interesting transport phenomena. Ivan Pshenichnyuk has thus demonstrated his ability for independent scientific work. I recommend to accept his work as a PhD thesis.



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