Simulation of quantum transport in molecular junctions using multiconfiguration wavefunction and reduced density matrix methods

Michael Thoss

University of Erlangen-Nuremberg, Staudtstrasse 7 / B2, 91058 Erlangen, Germany

Nonequilibrium electron transport in molecular junctions often involves correlation effects due to electron-electron or electron-vibrational interaction. In this talk, methods are discussed, which allow an accurate description of correlated electron transport, including the hierarchical master equation approach [1] and the multilayer multiconfiguration time-dependent Hartree (ML-MCTDH) method [2]. Moreover, the combination of the ML-MCTDH method with reduced density matrix theory is outlined [3]. The performance of the methods is discussed based on models for vibrationally coupled electron transport in molecular junctions, including both time-dependent and steady-state transport.

[1] C. Schinabeck, A. Erpenbeck, R. Härtle, M. Thoss, Phys. Rev. B 94, 201407(R) (2016).

[2] H. Wang and M. Thoss, J. Chem. Phys. 131, 024114 (2009); 138, 134704 (2013); 145, 164105 (2016).

[3] E. Wilner, H. Wang, G. Cohen, M. Thoss, E. Rabani, Phys. Rev. B 88, 045137 (2013); 92, 195143 (2015).