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Energy transfer dynamics in molecular junctions under ultra-short excitation pulses from non-equilibrium Green's function formalism

The problem of energy transfer is emerging as one of the most crucial issues of our occidental societies. At a fundamental level, how energy flows at the nanometre scale is gaining specific interests due to its implications in both alternative energy production and basics of quantum thermodynamics. The nature of our work is hence two-fold. In the first part, we provide a definition of energy current operator in the Heisenberg representation, while discussing certain conditions which an operator shall fulfill. The obtained expression is applicable to non-stationary as steady-state situations. We implement this definition to derive time-dependent energy current using non-equilibrium Green's function formalism, which represents a suitable approach for calculating measurable quantities in opened nanosystems. The second part applies these developments to molecular junctions sandwiched in between two thermal reservoirs. Molecular electronic devices are indeed a promising alternative to standard electronic switches due to their fast response on the picosecond time scale. Here, the approach is used for the study of molecular junctions subjected to ultra-short excitation pulses. We thus analyze the electronic energy fluxes across the molecular junction engendered by femtosecond laser pulses. Our numerical implementation enables us to correlate the time-dependent energy current to the underlying intra-molecular dynamics, with special attention paid to the impacts of intra-molecular coupling and incoherence on the energy transfer time-resolved measurables.

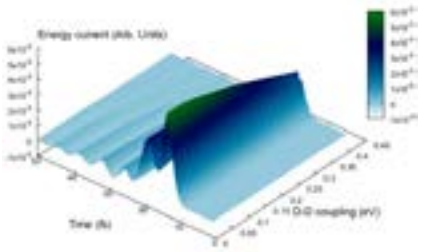

Figure1: We consider a junction made of two donors (D) that interact with light and an acceptor (A), the whole is in contact with tow thermal reservoirs. Effects of the intra-molecular D-D coupling on the time-resolved energy current flowing from D to A during a 30 fs laser pulse

Biography

Fabienne Michelini has worked on the theoretical/numerical building of empirical models within the k•p method to understand the electronic properties of realistic condensed-matter systems. In parallel, she has gained a great expertise in high performance computing for large-scale numerical problems. For the last years, she has investigated the transport properties of opened quantum structures for novel nanodevices using effective methods within the Green function formalism. She is now focusing on time-dependent and non-linear regimes of nanosystems interacting with light for optoelectronic and thermoelectric applications at the nanoscale.

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