Graduate School Seminar

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AG Molecular Quantum Dynamics

Simulation of non-equilibrium electronic and spin-state dynamics in transition metal complexes

The ultrafast electron dynamics of the charge-transfer processes in organometallic compounds has been attracting almost attention both from experimental and theoretical viewpoints. The reason for this interest stems from the fact that transition metal complexes represent prospective highly efficient light-harvesting and light-emitting materials for photovoltaics and photoelectronics. The recent progress in this field is connected to the rapid development of time-resolved experimental techniques in different energy ranges and development of theoretical approaches.
In the present work we focus on the investigation of ligand to metal electron transfer and spin-state dynamics in the organoleptic $[Fe(H_2O)_6]^{2+}$ complex. The coupling between the different energy levels is calculated using the restricted active space configuration interaction approach. The spin-orbit coupling between electronic states of different multiplicity is considered within the atomic mean-field integral (AMFI) approximation. The non-equilibrium electron dynamics is studied through the real-time propagation of the reduced density matrix. We also consider the intramolecular vibrational states as a thermal bath within Redfield theory.

Talk: English
Slides: English

Location: Institute of Physics, Albert-Einstein-Str. 24, HS1

Talks in WS 2015/16

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