Julius-Maximilians-
UNIVERSITÄT
WÜRZBURG

Kolloquium der Physikalischen und Theoretischen Chemie

Dienstag, 11.02.2014 **Hörsaal D, Chemiezentralgebäude, 17:15 Uhr**

Sprecher: Angel Rubio

(San Sebastián, Spain)

Titel: Non equilibrium dynamical processes in low dimensional systems from a time-dependent density functional theory

Abstract:

In this talk we will review the recent advances within density-functional and many-body based schemes to describe spectroscopic properties of complex systems with special emphasis to modeling time and spatially resolved electron spectroscopies (including transient pump-probe techniques). Pros and cons of present functionals will be highlighted and provide insight in how to overcome those limitations by merging concepts from many-body perturbation theory and time-dependent density functional theory. We will discuss some of the theoretical approaches developed in the group (and under development) for the characterization of matter out of equilibrium, the control material processes at the electronic level and tailor material properties, and master energy and information on the nanoscale to propose new devices with capabilities. We will focus on examples linked to the efficient conversion of light into electricity or chemical fuels ("artificial photosynthesis") and the design on new nanostructured based optoelectronic devices based on inorganic nanotubes, among others.

We will discuss some of the new challenges we are facing linked to what is coined as "new states of matter" that rely on two fundamental developments: i) the ability to describe open-quantum-systems out-of-equilibrium and ii) the availability of a viable “quantum optimal control theory” of their processes. The description of non-equilibrium phenomena requires answers to a number of complex questions. What are the general rules that apply to microscopic relaxation on extremely long time scales? How can non-equilibrium processes be directed at the nanoscale? How do systems search free-energy landscapes? Can artificial systems be designed to mimic biological processes? Can matter be stabilized in non-equilibrium states, such as metamaterials, glass, or graded structures? Is it possible to understand and control phase transitions, diffusion, and chemical reactions? Mastering non-equilibrium phenomena should pave the way for dealing effectively with a host of issues related to energy, climate, materials, or biology. A time-dependent description of decoherence and dissipation in many-body quantum systems will answer the above questions and open the possibility for an ab-inito simulation of a wealth of experiments that are now accessible. Some examples include: Molecular relaxation after charge transfer in donor-acceptor complexes; relaxation of excited vibrational wavepackets in the context of photo-chemistry; real-time dynamics of formation, propagation, and decay of excitons in semiconductors, polymers and light-harvesting antenna complexes; relaxation after energy transfer between chromophores in Förster resonance-energy transfer; thermal transport and relaxation effects in molecular electronics. The goal for the newer future is to provide a detailed, efficient, and at the same time accurate microscopic approach for the ab-initio description and control of the dynamics of decoherence and dissipation in quantum many-body systems. With the help of quantum optimal control (QOC) theory and the mastery over spectroscopy we could direct the movement of electrons, selectively trigger chemical reactions and processes, and create new materials.

Organisation: T. Hertel

Kontakt: *Prof. Dr. Tobias Hertel, Institut für Physikalische u. Theoretische Chemie*
tobias.hertel@uni-wuerzburg.de

Weitere Informationen unter:
http://www.phys-chemie.uni-wuerzburg.de/startseite/veranstaltungen/