CFEL SCIENCE

Colloquium

7th November 2014 - 14:00

CFEL Seminar rooms I-III (DESY Bldg. 99)

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Ab initio simulation of photon-matter interactions: non equilibrium dynamical processes within QED-TDDFT

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 modelling 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 characterisation 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. The goal of the group activities in the long-run 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.

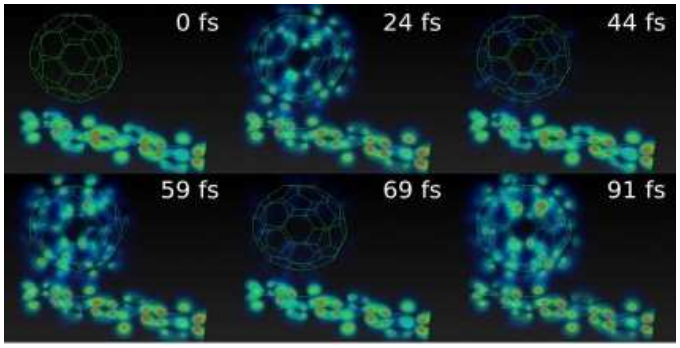

Figure: Photos of the simulation of the evolution in the transfer of charge from the polymer to the fullerene in femtoseconds. (From: Coherent ultrafast charge transfer in an organic photovoltaic blend.

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Host: Andrea Cavalleri, MPSD-CFEL