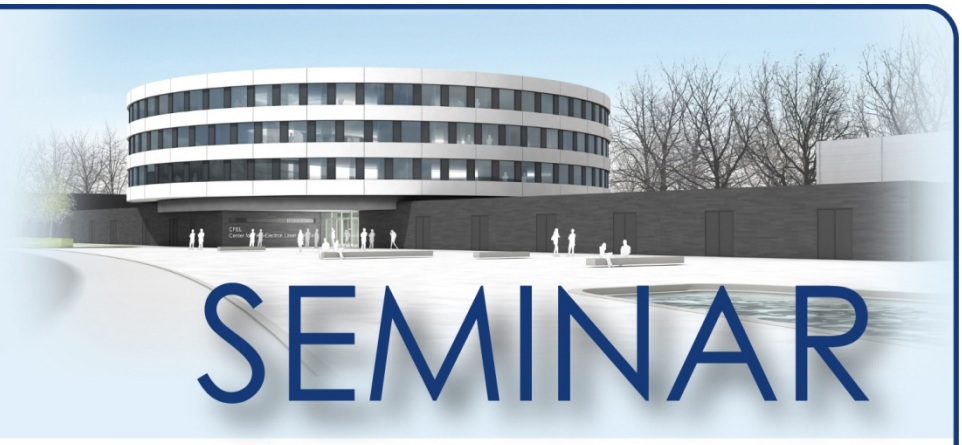
CFEL SCIENCE



SEMINAR

29th March 2011 - 14:15

Building 28c (FLASH hall), Seminar Room

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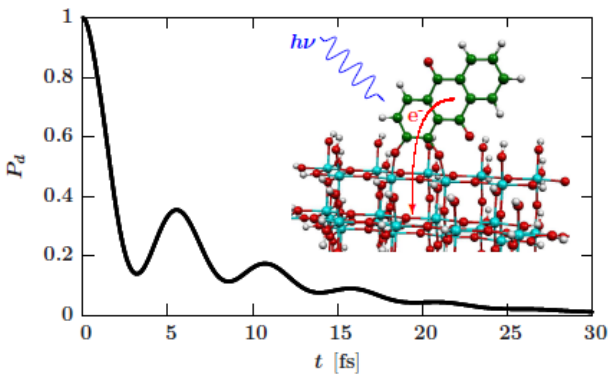
Dynamics of electron transfer processes in molecular systems at surfaces

Dynamical processes involving the transfer or transport of electrons are ubiquitous in many areas of physics, chemistry and biology. Among the variety of different types of reactions, electron transfer processes of molecular systems at semiconductor or metal surfaces have been of great interest recently. Important applications of such reactions include photonic energy conversion in organic solar cells and single-molecule conduction in nanoscale molecular electronics.

In this talk, two types of surface electron transfer reactions are considered. The first part addresses electron transfer processes at dye-semiconductor interfaces as an example for an ultrafast photoinduced reaction. Employing quantum dynamical simulations, various aspects of these reactions are investigated including electronic population dynamics, vibrational wave-packet motion associated with the ultrafast electron transfer process as well as the mutual influence of electronic and nuclear dynamics. Moreover, the influence of the anchor group that mediates the electron transfer from the dye molecule to the semiconductor substrate is discussed.

In the second part, electron transport through single molecules that are bound to metal electrodes is considered. Based on a first-principles modeling and transport calculations, the influence of the nuclear degrees of freedom of the molecular bridge on the conductance properties of the junctions as well as the nonequilibrium character of the process are studied. Furthermore, possibilities for switching of molecular junctions via photoinduced hydrogen transfer are discussed.



Host: Oriol Vendrell – CFEL Theory Group