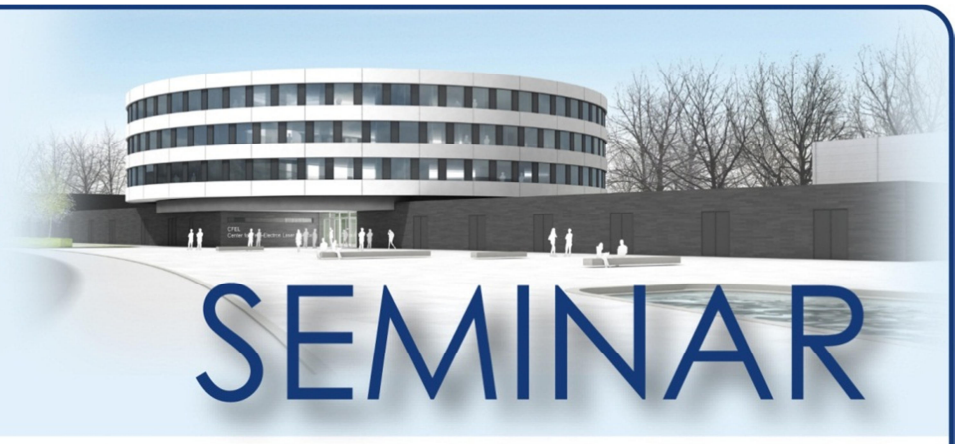
CFEL SCIENCE



SEMINAR

27th March 2012 - 14:15
Building 28c, seminar room

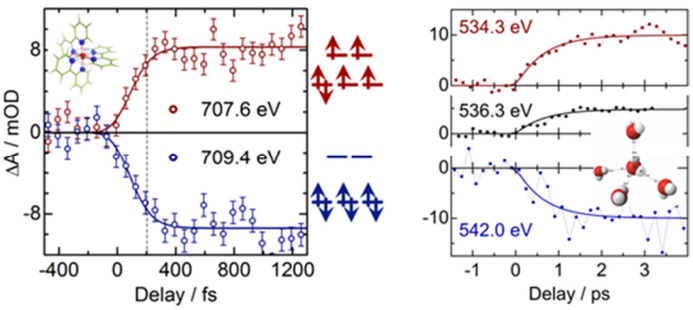
Nils Huse

Ultrafast Molecular Dynamics Group, Max Planck Department for Structural Dynamics at the University of Hamburg, Center for Free Electron Laser Science

From the infrared to X-rays: New insights into solution-phase chemistry via ultrafast spectroscopy

The liquid phase provides unique environments for chemical reactions but poses experimental and theoretical challenges in deciphering chemical dynamics. To study solution-phase systems experimentally, multidimensional infrared spectroscopy is a very sensitive tool, to probe structural dynamics with high chemical specificity while the visible analogue provides insight into the evolving valence charge density. More recent developments in the field of ultrafast hard X-ray spectroscopy have provided complementary probes to transient molecular structures and spin conversion. Ultrafast spectroscopy in the soft x-ray range is relatively new [1,2] due to the underlying experimental challenges but it is very powerful method to study first-row transition metal compounds and important lighter elements (C,N,O) in solution because of the information on valence charge distributions and spin-states not accessible via diffraction techniques. Combining information on nuclear, charge, and spin degrees of freedom gathered from these techniques is crucial for a microscopic understanding of reaction pathways and transient intermediates.

Ultrafast spectroscopy of water highlights the ultrafast nature of energy transfer, structural fluctuations and energy relaxation in this intriguing liquid which has been probed with ultrafast infrared and core-level spectroscopy. In another research area, solvated transition-metal spin cross-over compounds have been studied intensely for the past decades due to the complicated ultrafast spin interconversion on 100 fs time-scales. The underlying evolution of atomic structure and valence charge density has been elucidated by visible and core-level spectroscopies. These liquid-phase studies will set the stage for introducing some future directions in the ultrafast molecular dynamics group to investigate charge-transfer reactions, molecular magnetism, and hydrogen-bond dynamics of solvated systems.



1. Wen et al., *JCP* **131**, 234505 (2009)
2. Huse et al. *JPCL* **2**, 880 (2011)

Host:Valentyn Prokhorenko