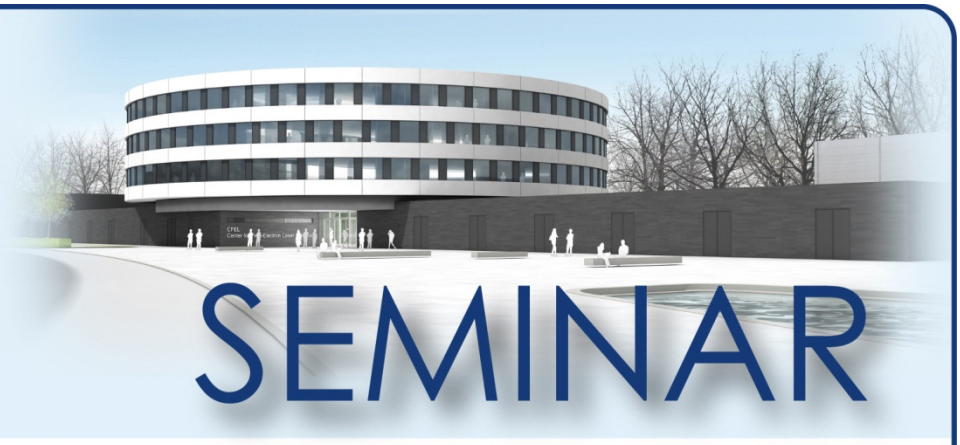
CFEL SCIENCE



SEMINAR

10th June 2011 - 10:15
Building 49 - Seminar Room 108

Yunjie Xu

Department of Chemistry, University of Alberta, Edmonton, Canada

Exploring chirality and chirality recognition using experimental spectroscopic and ab initio methods

Chirality and chirality recognition are essential for living systems and are of great importance in the life sciences. To quantitatively characterize the related phenomena on the molecular level, we use experimental spectroscopic techniques and ab initio calculations. I will present a series of high resolution rotational and vibrational spectroscopic studies of propylene oxide, a basic chiral building block, and of its homo- and heterochiral complexes with ethanol, 2-fluoroethanol, and itself. Using the experimentally established structures and stability ordering, complemented with the ab initio calculations, we examine the chiral discriminating forces at play in these molecular systems. In the second part of the talk, I will discuss our two-pronged approach to study the effects of solvent-solute hydrogen-bonding on chiroptical measurements using both high resolution spectroscopy and vibrational circular dichroism (VCD) spectroscopy. We observed that some vibrational bands of an achiral molecule, such as water can show significant VCD strength through hydrogen-bonding to a chiral molecule. This effect, termed chirality transfer, will be discussed.

Host: Jochen Küpper, Coherent Imaging Division - Controlled Molecule Imaging Group