

## MO 32: Poster: Experimental Techniques

Time: Thursday 16:00–18:00

Location: P1

MO 32.1 Thu 16:00 P1

**Multiplex-CARS microspectroscopy and multivariate statistics for characterisation of biological samples** — ●CHRISTOPH POHLING, TIAGO BUCKUP, and MARCUS MOTZKUS — Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, D-69120 Heidelberg, Germany

Multiplex Coherent Anti-Stokes Raman Scattering (MCARS) provides labelling free and fast characterisation of samples in nonlinear microscopy. In case of unknown biological tissue, CARS has been, however, often limited to the visualisation of lipid rich structures. Combined with additional steps of data processing such as imaginary part extraction followed by multivariate statistics, this limitation was compensated [1]. In this context, techniques like (functional-) Principal Component Analysis (PCA) and Maximum Entropy Method (MEM) have been successfully employed in the analysis of complex samples. Here we compare these methods based on the characterization of several biological samples such as different types of cellulose-rich samples as well as mammalian brain tissue. Particularly, chemical contrast obtained from PCA analysed MCARS data shows equivalent information as the well known HE-stained samples. [1] Pohling, C., Buckup, T., Motzkus, M., Hyperspectral data processing for chemoselective Multiplex CARS microscopy of unknown samples, *J. Biomed. Opt.*, 2010, accepted.

MO 32.2 Thu 16:00 P1

**X-ray diffraction from single molecules at the worlds first X-ray Free-Electron Laser source** — ●STEPHAN STERN, JOCHEN KÜPPER, HENRY CHAPMAN, and DANIEL ROLLES — Center for Free-Electron Laser Science (CFEL), DESY, Hamburg, Germany

The advent of the first X-ray Free-Electron Laser, the Linac Coherent Light Source (LCLS), opens up a new approach for diffractive imaging of even single molecules that cannot be crystallized into macromolecular crystals of sufficient size necessary for conventional X-ray crystallography.

Here, we present the concept, the experimental parametric space that has to be addressed together with first experimental results of x-ray diffractive imaging of single molecules in the gas phase at LCLS. We use a supersonically cooled molecular beam to provide an ensemble of test-molecules, laser-align them, and subsequently probe them with the LCLS in order to get diffraction patterns of single molecules.

This work was carried within a collaboration, for which J. Küpper, H. Chapman and D. Rolles are spokespersons. The collaboration consists of CFEL (DESY, MPG, University Hamburg), Fritz-Haber-Institute Berlin, MPI Nuclear Physics Heidelberg, MPG Semiconductor Lab, Aarhus University, FOM AMOLF Amsterdam, Lund University, MPI Medical Research Heidelberg, TU Berlin, Max Born Institute Berlin, and SLAC Menlo Park USA. The experiments were carried out using CAMP (designed and built by the MPG-ASG at CFEL) at the LCLS (operated by Stanford University on behalf of the US DOE.)

MO 32.3 Thu 16:00 P1

**Electron detachment spectroscopy on a fast ion beam using a magnetic bottle spectrometer** — ●MARKO FÖRSTEL<sup>1</sup>, CHRISTIAN DOMESLE<sup>2</sup>, BRANDON J. JORDON-THADEN<sup>2</sup>, LUTZ LAMMICH<sup>3</sup>, TIBERIU ARION<sup>1</sup>, MELANIE MUCKE<sup>1</sup>, ANDREAS WOLF<sup>2</sup>, UWE HERGENHAHN<sup>1</sup>, and HENRIK B. PEDERSEN<sup>3</sup> — <sup>1</sup>Max-Planck-Institut für Plasmaphysik, EURATOM Association, 85748 Garching, Germany — <sup>2</sup>Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany — <sup>3</sup>Department of Physics and Astronomy, Aarhus University, DK-8000 Aarhus C, Denmark

Electron spectra after photodetachment of O<sup>-</sup> and OH<sup>-</sup> in a 4.2 keV fast ion beam were measured by using a magnetic bottle spectrome-

ter and the third harmonic of a Nd:YAG laser. Fast ion beams imply their own approach to the investigation of their physical properties. The broadening of photoelectron lines due to momentum transfer with the emitting ion is an example. In angle-integrating electron spectrometers this effect leads to a substantial line broadening. We introduce a method to overcome this limitation and gain additional information on the angular distribution of the emitted electrons. We simulated the combined effect of the angular distribution function, described by the  $\beta$ -parameter and the velocity shift by momentum exchange. A mapping between  $\beta$  and the lineshape observed in the spectra recorded with a magnetic bottle spectrometer was found. Results determined from an analytical expression and from numerical ray-tracing will be compared to measurements. Spectroscopy of ions at higher photon energies by use of the FLASH Free Electron Laser will be discussed.

MO 32.4 Thu 16:00 P1

**IR - Transition Moment Orientation Analysis and its application to thin polymer films** — ●WILHELM KOSSACK<sup>1</sup>, PERIKLIS PAPADOPOULOS<sup>2</sup>, and FRIEDRICH KREMER<sup>1</sup> — <sup>1</sup>Universität Leipzig, Institut für experimentelle Physik 1, Abteilung Molekülphysik, Leipzig, Germany — <sup>2</sup>Max-Planck-Institut für Polymerforschung, Mainz, Germany

Infrared Transition Moment Orientation Analysis (IR-TMOA) is a spectroscopic technique, that reveals a complete characterization of the quadratic averaged orientation of transition dipole moments in any IR-translucent material. Since it is based on the polarization and inclination dependence of the recorded transmission spectra, it enables one to measure the absorption coefficient matrix independently for different molecular moieties and, thus, their orientation distribution [1]. To study surface interactions and confinement effects IR-TMOA is applied to thin, spin coated polymer films on various substrates. Results for different polymer films will be discussed and compared to the ones of other methods.

[1] Wilhelm Kossack, Periklis Papadopoulos, Patrick Heinze, Heino Finkelmann, Friedrich Kremer, DOI: 10.1021/ma101121f, *Macromolecules* 2010

MO 32.5 Thu 16:00 P1

**Soft x-ray absorption spectroscopy of ultrathin liquid films** — ●SIMON SCHRECK, CHRISTIAN WENIGER, GIANINA GAVRILLA, and PHILIPPE WERNET — Institute for Methods and Instrumentation for Synchrotron Radiation Research, Helmholtz-Zentrum Berlin

Applying soft x-rays to liquid samples is a challenging task due to the incompatibility of the vacuum environment required for soft x-rays and the high vapor pressure of liquids. When recording soft x-ray absorption spectra in transmission mode, which is the most direct and efficient way, the strong attenuation of soft x-rays in nearly all elements calls for ultrathin samples. For water and aqueous solutions, sample thicknesses clearly below one micrometer are necessary.

Here we present an experimental setup for preparing ultrathin liquid films separated from vacuum or He atmosphere with controllable thickness from nm to  $\mu\text{m}$ . These ultrathin liquid films allow for transmission measurements with soft x-rays to record high quality soft x-ray absorption spectra of different kinds of samples such as bulk liquid water (H<sub>2</sub>O) and heavy water (D<sub>2</sub>O), aqueous salt solutions and solvates molecules. The high quality and reproducibility of the spectra is shown by comparing measured data with reference data and the high sensitivity for small structural differences is demonstrated by resolving the spectral differences in the x-ray absorption spectra of H<sub>2</sub>O and D<sub>2</sub>O. Furthermore the data prove the ability to measure solvated systems and solutions at very low concentrations of down to the millimol/l range. The measurements were performed at the synchrotron radiation source BESSYII at the Helmholtz-Zentrum Berlin.