

L-23

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Synchrotron radiation: an advanced tool for science under extreme conditions of pressure and temperature

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Science at extremes of pressure and temperature is a vibrant field of international research that addresses fundamental questions in domains as diverse as fundamental condensed-matter physics, Earth and planetary science, material synthesis and characterisation, and biology. Pressure strongly alters interatomic distances without changes in thermal energy or chemical environment, and is thus a better thermodynamic variable than temperature and chemical composition to explore free energy landscapes. Research at light-based large scale facilities has always been at the leading edge of extreme conditions science, and the recent advent of powerful laser sources (Omega, NIF, ELI, ...), X-ray free electron laser facilities (LCLS, European XFEL, ...), and the exciting perspective of a new generation of diffraction-limited synchrotrons will allow the exploration of material properties at conditions far in excess of those currently achievable. The current third-generation synchrotron facilities have pioneered many of the major breakthroughs in extreme conditions research over the last two decades. Indeed, compared to other large-scale facilities, synchrotron radiation offers a unique diversity of state-of-the-art techniques for characterisation of matter. At the ESRF, the scope of this research field has been constantly expanding and developing such that, remarkably, the structural, dynamical, electronic and magnetic properties of materials at pressure up to 100 GPa can now be determined with the same precision as at ambient conditions. This lecture will be focus on key instrumental and scientific achievements at the high pressure XRD beamline ID27.

L-24

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Time resolved X-ray scattering of molecules in liquids

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XFELs have dramatically improved our ability to measure and understand ultrafast structural changes with X-ray scattering. Here we attempt to draw a few lines from our work at synchrotron sources to a recent series of hard X-ray pump-probe experiments conducted at the XPP end-station at LCLS and at SACLA in Japan.

X-ray scattering of molecules in solutions is sensitive to all atoms in the illuminated volume of the sample. This gives both opportunities and challenges. The opportunities include being able to study structural changes following photo excitation of the solute molecule, how the excitation leads to changes in the solvation shell around the molecule, and how the excitation energy is eventually dissipated in the surrounding solvent. This great sensitivity is also a challenge, as it can lead to ambiguities in the interpretation of the measurements, since the scattering signal contains a combination of all the above contributions as well as instrument response functions.

However, some of these ambiguities may be resolved by combining scattering experiments with element specific spectroscopic techniques. In recent experiments, we utilized concurrent detection of complementary data, namely both X-ray Diffuse Scattering and X-ray Emission Spectroscopy. Doing so significantly aids in the interpretation of the results, as information from one set of measurements can inform the analysis of the complementary set. Further, it allowed us to address simultaneously both the electronic and the structural degrees of freedom, greatly enhancing the information obtained from a single experiment.

In these experiments, we investigated the ultrafast solvent response as well as structural and electronic dynamics in Fe(bpy)₃ as well as in a structurally related, linked Ru-Co complex. In a second set of experiments, we studied the ultrafast structural dynamics following excited-state bond formation in Ir₂(dimen)₄.

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