

3rd Workshop on the Simultaneous Combination of Spectroscopies with X-ray Absorption, Scattering and Diffraction Techniques



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En-Light-ening Photo-crystallography with X-ray Absorption

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Photo-excited state crystal structures are now possible via photo-crystallography - a technique that pumps optical light upon a crystal which is, in turn, probed by X-ray diffraction. While this technique is still very much in a developmental phase, results have already demonstrated important findings in the area of optoelectronics.

Such photo-crystallography experiments are now being technically extended to incorporate X-ray absorption spectroscopy and anomalous X-ray scattering. Two case studies are shown. In the first case, XANES has been used to identify solid-state photoisomerism in these materials where suitable crystals could not be grown for photo-crystallography. The XANES data analysis also clarified the redox property changes owing to light-excitation. In the second case, anomalous X-ray scattering has been embraced within photo-crystallography experiments in order to gain superior scattering contrast in the areas of the molecule that pose special interest with respect to light-induced effects. The associated X-ray absorption cross-sections are determined using EXAFS spectra that are obtained in tandem with the X-ray diffraction experiment.

The paper concludes by forecasting the likely combinations of techniques that will create a result whose sum is far greater than its parts.

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