



Contribution ID: 2

Type: **not specified**

# Theoretical calculations on ultrafast anisotropic X-ray scattering in the condensed phase

*Monday, 21 November 2011 10:40 (5 minutes)*

The advent of X-ray free electron lasers offers new opportunities for X-ray scattering studies of the ultrafast molecular dynamics in liquids, which was so far limited to the 100 ps resolution of synchrotrons. Photoexcitation induces anisotropy in the sample, which enhances the contrast of the signal from excited molecules against the diffuse background, while allowing probing of their vibrational and rotational dynamics. In this poster, we present a computational approach for calculating the transient scattering intensities of iodine in n-hexane, based on molecular dynamics simulations. We also derive, using realistic parameters the anticipated signal-to-noise ratio for a large class of diatomic elements in solution.

**Primary author:** Dr PENFOLD, Thomas (EPFL/PSI)

**Co-authors:** Dr TAVERNELLI, Ivano (EPFL); Prof. CHERGUI, Majed (EPFL); Dr ABELA, Rafael (PSI)

**Presenter:** Dr PENFOLD, Thomas (EPFL/PSI)

**Session Classification:** Poster Presentation