



Figure 1. Experimental setup of coupling XANES and SAXS using an acoustic levitator as sample holder. XANES spectra were collected using an XRF-detector.

Keywords: Iron oxide nanoparticles, XANES, SAXS, time-resolved

MS24. Short range order and diffuse scattering

Chairs: Alexei Bosak, Thomas Weber

MS24-P1 Modeling charge density variations in molecular crystals

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I will describe our efforts to accurately model charge density variations in molecular crystals. A key goal is to fill a gap in traditional crystallography by providing more detailed information about molecular motions. Our approach integrates molecular dynamics simulations, fast quantum mechanical computations, and information from diffuse X-ray scattering. It is timely as the necessary computations are becoming increasingly feasible, and as traditional structure determination methods are approaching the limits of their achievable accuracy. Elements of our approach have been applied to protein and small molecule systems, yielding new insights. Computational methods are being made available in publicly available software (<https://github.com/mewall/lunus>).

Keywords: diffuse X-ray scattering, molecular motions, charge density variations