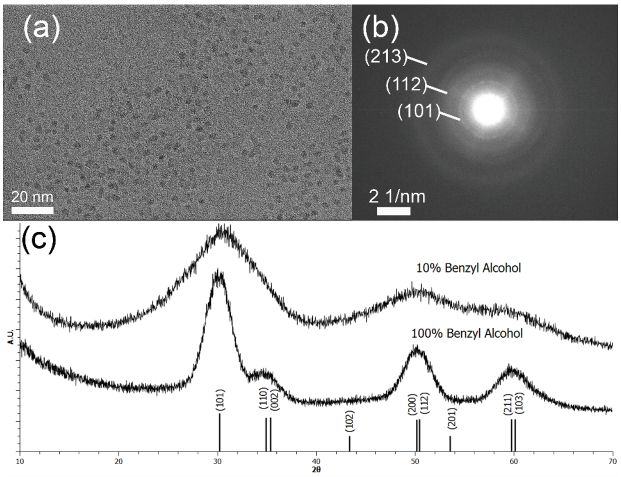

Figure 1. TEM image (a), selected area electron diffraction image (b) and XRD images of tetragonal phase zirconia (c) prepared via nonhydrolytic route

Keywords: ultrasmall, nanoparticles, nonhydrolytic sol-gel, zirconia, pair distribution function

MS23-P18 Combining fast-XANES and SAXS for time-resolved studies on the formation mechanism of iron oxide nanoparticles

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Iron oxide nanoparticles find application in different areas like sensing [1], catalysis [2], magnetic storage media [3], and biomedicine [4,5], due to their magnetic properties and environment-friendliness. Different synthesis routes are intensively studied, one of which is the co-precipitation. The synthesis is performed by precipitating the iron precursor in an alkaline, aqueous solution. Despite many studies based on *ex situ* investigations, information on the particles formation mechanism in the aqueous solution is still scarce [6,7]. Time-resolved *in situ* investigations allow to clarify the pathways and intermediates occuring during the formation. In the present contribution, we report on the *in situ* investigation of an iron oxide nanoparticle synthesis by coupled X-ray absorption near-edge structure (XANES) and small-angle X-ray scattering (SAXS) (Fig. 1). The combination provides simultaneously information about the size and shape of particles (SAXS) and on the oxidation state and the local structure of the iron atoms (XANES). The co-precipitation synthesis was exemplary studied, using a stabilization agent to decelerate the fast precipitation of the iron oxides. This allows to detect intermediates *in situ*. The measurements were performed using a custom-made acoustic levitator as sample holder. From the data, a mechanism was derived indicating different phases of particle formation and oxidation state changes. The information obtained provided the basis for an improved control of the product of the synthesis.

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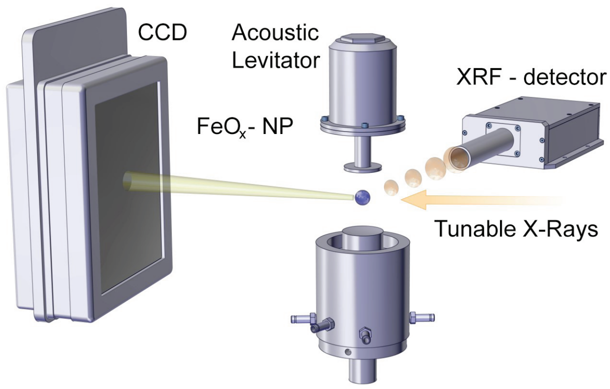

Figure 1. Experimental setup of coupling XANES and SAXS using an acoustic levitator as sample holder. XANES spectra were collected using an XRF-detector.

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 notions, charge density variations