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Pushing PDF experiments for weakly scattering samples –tackling solvation shells

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The pair distribution function (PDF) technique exploits the total, i.e. the Bragg and diffuse, scattering of crystallographically challenging materials to derive their structure - with nanoparticles (NPs) being the biggest showcase in recent years. [1] The strong increase in flux at high X-ray energies combined with novel detector technologies at synchrotron radiation facilities allowed to push both the time resolution of in-situ studies and the concentrations to new, low borderlines. [2,3] Recently, we proved the existence of nanoscopic solvation shells around colloidal NPs < 10 nm in various solvents (alcohols, hexane). [3] The solvent molecules reorient over 3 to 5 molecular layers away from the NP surface before bulk properties are regained. Such insight requires caution in data treatment as slight flatfield imperfections or insufficient polarization corrections have the same contribution to the overall scattering signal as the restructured solvent. Our approach to analyse double-difference PDFs of restructured solvent layers is now readily applied to colloidal iron oxide NP dispersions in organic solvents, nanodiamonds in water and palladium NPs in tetrahydrofuran. Novel focus is on the interfacial solvent structures in liquid-phase catalysis as well as extending the measurable temperature and NP size range.
[1] S. J. L. Billinge, et al., Chem. Commun. 7 (2004), 749
[2] M. Zobel, et al., CrystEngComm 18 (2016) 2163
[3] M. Zobel, et al., Science 347 (2015), 6219, 292

Primary author: ZOBEL, Mirijam (University Bayreuth)

Co-authors: ECKARDT, Mirco (Universität Bayreuth); THOMÄ, Sabrina (Universität Bayreuth)

Presenter: THOMÄ, Sabrina (Universität Bayreuth)

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