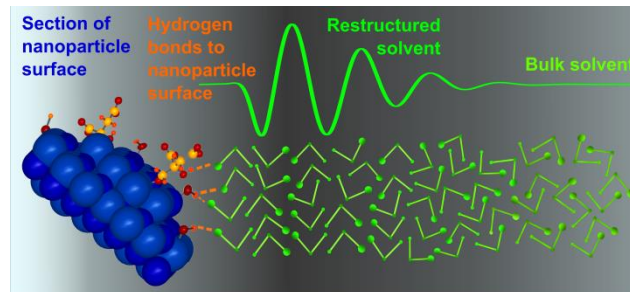


Interfacial solvent layering around nanoparticles via high energy X-ray scattering

Jun.-Prof. Mirijam Zobel, Department of Chemistry, University Bayreuth

Pair distribution function (PDF) measurements have originally been used to study the structure of bulk liquids and glasses about 100 years ago. During the last two decades, the big revival of the method was in the structural refinement of nanoparticles and in-situ studies of chemical reactions.

Thanks to the increase in flux and improved signal-noise ratio with novel detector technology, even the molecular arrangement of solvent molecules in solvation shells around nanoparticles can be accessed nowadays. We showed that primary alcohols reorient perpendicular to the particle surface and hereby create a sinusoidal oscillation of the solvent electron density profile in the corresponding PDF. The rearrangement of molecules reaches out as far as 2 nm into the bulk liquid and decays exponentially.



In this talk, an introduction to PDF analysis of nanoparticles and solvents is given. It is shown how we extract information about interatomic distances from layers of adsorbed molecules and restructured solvent layers around iron oxide nanoparticle dispersions in organic solvents and water. A novel focus is on the interfacial solvent structures in liquid-phase catalysis, showcased by in-situ PDF experiments on palladium nanoparticles in hydrogenation reactions.