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Solvent restructuring at colloidal nanoparticle surfaces

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Interfaces are the key to understand manifold chemical and physical processes, for instance catalytic reactions as well as nanoparticle nucleation and growth. Nanoparticle surfaces have a strong tendency to restructure to strained atomic arrangements in order to stabilize themselves at their finite size [1,2]. But also restructuring of the solvent molecules takes place. The presence of colloidal nanoparticles in bulk solvents induces a reorientation of the solvent molecules and a change of the hydrogen bond network in the vicinity of the particle surface.

We could for the first time experimentally prove the universality of solvent restructuring around nanoparticles for a matrix of redispersed nanoparticles (ZnO, TiO2, ZrO2, Ag) in the primary alcohols methanol to 1-propanol as well as in nonpolar hexane and water. We carried out high-energy x-ray scattering experiments on colloidal dispersions with a metal ion concentration of ca. 0.4 wt% / 30 mM. We observe primarily the reorientation of solvent molecules along the surface normal, yielding a sinusoidal oscillation of the solvent electron density profile in the corresponding pair distribution functions (PDF). The rearrangement of molecules reaches out as far as 2 nm into the bulk liquid and the decays exponentially [3].

Molecular dynamics modelling predict that the solvent restructuring is influenced by the particle size, shape, crystallinity or the facetting [4]. Nucleation and growth depend on the attachment of new primary building blocks like ions or precursor clusters to existing particle surfaces. This process is determined by the interaction of the building blocks with the surface. The interaction and the electric field of the nanoparticle is however modulated by the solvent layering at the surface. We carried out in-situ PDF experiments on the nucleation of 3 nm large ZnO nanoparticles from precursor clusters in ethanol and revealed that the layering of the solvent molecules at the nanoparticle surface changes during nucleation. Understanding these changes will help us in the future to better model nanoparticle nucleation and growth.

[1] Zhang, H., et al. Nature 424 (2003), 1025
[2] Gilbert, B., et al. Science 305 (2004), 651
[3] Zobel, M., et al. Science 347 (2015), 292
[4] Spagnoli, D., et al. Geochimica et Cosmochimica Acta 73 (2009) 4023
[5] Silvera Batista, C. A., et al. Science 350 (2015), 6257

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