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Quasielastic neutron scattering to study the diffusion of water molecules on the surface of iron oxide nanoparticles at different relative humidities

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Iron oxide nanoparticles (IONPs) are vital in many applications ranging from biomedicine to heterogeneous catalysis. While their structure is well-studied, the interfacial dynamics of surface molecules have been barely addressed up to now. Quasielastic neutron scattering (QENS), though, is highly suited to access the dynamics of water and ligand molecules on surfaces of metal oxide nanoparticles. For instance, rotational and translational diffusion dynamics of interfacial water molecules on the surface of TiO2 nanoparticles were shown to be different from bulk water [1,2]. Recently, we disentangled magnetic signatures from water and ligand diffusive modes on the surface of iron oxide nanoparticles from QENS data –yet for comparably dry powders equilibrated at 8 % RH (relative humidity). [3]
Here, we report on QENS experiments on 7 nm IONPs performed at IN16B at ILL using fixed window scans (FWS) and a wavelength of 6.271 Å. The IONPs were synthesized according to ref 4, are stabilized with the ligand citrate and equilibrated at four distinct RH, reflecting different numbers of water layers on the IONP surface: from nominally dry powders at 8 %RH, via 75 and 85 % RH to multilayer water coverage at 98 %RH. FWS were carried out at the elastic line and at an energy offset of 3 μeV. A temperature range of 2 –373 K and a Q-range of 0.19 –1.83 Å-1 were used.
The elastic and inelastic FWS allow us to quickly identify distinct differences in the diffusion dynamics of samples equilibrated at different RH. While at very low RH of 8 %, we are also highly sensitive to the dynamics of magnetism and the citrate ligand, with increasing RH these contributions to the quasielastic signal decrease. Compared to the 8% RH sample, the FWS of the IONPs equilibrated at 75 % RH already show on first sight the dominating contribution of diffusion dynamics of water molecules. Activation energies and relaxation times are derived from refinements of the FWS.

References:
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Sitzung Einordnung: Mounting Posters, Beer and light Dinner

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