MS40-05 | Atomic Insight into Hydration Shells around Facetted Iron Oxide Nanoparticles

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Whilst the strength of hydrogen bond networks within solvation shells around colloidal nanoparticles can be accessed with various spectroscopic techniques, the structure of those shells had hitherto remained inaccessible. Thanks to the increase of detection efficiencies and flux at high X-ray energies > 60 keV, we could recently access the solvent layering of alcohols with a robust data processing routine over 3 to 5 molecular layers for the first time via pair distribution function (PDF) analysis [1]. Detection of water remained challenging due to the small molecule size and the weak scattering contribution of hydrogen.

Now we have pushed the boundaries and even gained atomic insight into hydration shells around facetted iron oxide nanoparticles (IONPs). For this, we synthesized variably functionalized IONPs of two diameters – 7 and 15 nm – via coprecipiation in basic solution. TEM proved the faceting, TGA the partial ligand coverage and PDF analysis the hydration shell structure. Via double difference PDFs of the dispersions, nanopowders and bulk water, we identified three distinct interatomic distances within 2.5 Å from the IONP surface, irrespective of the capping agent. These distances correspond to molecularly and dissociatively adsorbed water molecules in accordance with theoretical predictions [2]. Despite the small IONP diameters, the interfacial fingerprint of the water structure is just like for large 2D interfaces.

[1] Zobel, M. *et al.*, Science 2015, 347 (6219), 292
[2] Thomä, S. L. J. *et al.*, Nat. Commun. 2019, 10 (1), 995