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Neutron PDF for insight into hydration shells around iron oxide nanoparticles

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Interfaces between iron oxide nanoparticles (IONP) and water are of great importance in various fields spanning biomedicine, waste water treatment and catalysis. Recently, we could distinguish adsorbed water species and extended hydration layers around IONPs via a double-difference X-ray pair distribution function (dd-PDF) analysis.¹ Details of the interfacial hydrogen bond network shall now be addressed with neutrons.

Here we present neutron total scattering data on IONP powders and their aqueous dispersions (H₂O/D₂O), to which we apply our dd-PDF strategy.¹ 7 nm sized IONPs are synthesized in basic diethylene glycole and capped with citrate or phosphocholine. We developed a transferable, robust combination of TGA, AAS and elemental analysis to determine the exact composition of the powders, especially amount of the organic capping agents, important for absolute normalization of the neutron data.² Additionally, contributions of surface-OH (-OD) groups of wet powders with varying amount of surface water layers are investigated according to 3. Finally, we aim at elucidating interfacial structures like surface hydroxyls, ligand coordination and possibly contributions from in-plane co-adsorbed water molecules, via a contrast match study to bridge the gap between insight into wet powders and colloidal dispersions.

1. Thomä, S. L. J. et al., Nat. Commun. 2019, 10(1), 995.
2. Eckardt, M. et al., in preparation
3. Wang, H. et al., J. Am. Chem. Soc. 2013, 135, 6885-6895

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