Contribution ID: **147** Type: **Talk**

QENS Study of the Interface Dynamics of Humid Iron Oxide Nanoparticles

Iron oxide nanoparticles (IONPs) are extensively used in many different fields ranging from heterogeneous catalysis to biochemistry. Optimizing their performance especially under humid conditions where water interactions significantly influence the functional behavior depends on an understanding of the atomic-scale dynamics of surface-bound species. The interface dynamics can be probed by QENS in the form of energy-resolved spectra (ERS) and fixed window scans (FWS). Adequate data treatment is essential for elucidating these processes, particularly when dynamics from different molecules coexist.
We have synthesized citrate-capped IONPs and equilibrated them at relative humidities (RH) ranging from 8% to 98%. The water surface coverage varies from monolayer to multilayer. ERS and FWS of these samples were measured on IN16B in the temperature range of 2–380 K. A global fitting procedure with shared parameters between the ERS and FWS fits was used to analyze ligand and water dynamics, [1] as well as magnetic relaxations in 8% RH IONPs. [2] Extending this approach to the 85% RH sample, analysis of FWS also reveals distinct dynamical regimes in temperature space. While below 150 K there are signs of a weak magnetic process, water and ligand dynamics become observable above 200 K, evolving into a rapid decrease in elastic intensity. We interpret this feature as a pre-melting phase transition in hydration water. Before the phase transition, the dominant process can be described by Fick's law with a diffusion coefficient at 245 K of $1.57\times10^{-12}\ m^2\ s^{-1}$. This is much slower than would be expected from any residual supercooled water on the surface.
Our analysis demonstrates that the interfacial dynamics of citrate-capped IONPs can be probed under application-relevant, wet conditions by QENS.

[1] M. S. Plekhanov, et al., J. Phys. Chem. C, 2024, 128, 11661–11671.
[2] M. Zobel, et al., Phys. Rev. B, 2025, 111, L060406.

Author: PASCARIU, Matei (Forschungszentrum Jülich, JCNS-3)

Co-authors: Prof. MAGERL, Andreas (Friedrich-Alexander University, Erlangen); Dr PLEKHANOV, Maksim (RWTH Aachen University); Dr APPEL, Markus (Institut Laue-Langevin, Grenoble); Prof. ZOBEL, Mirijam (Forschungszentrum Jülich, JCNS-3)

Presenter: PASCARIU, Matei (Forschungszentrum Jülich, JCNS-3)

Session Classification: Parallel: Materials (RT2)

Track Classification: RT2