

BSc / MSc thesis or Hiwi

Dynamics of water molecules at nanoparticles– a quasi-elastic neutron scattering experiment

Water-nanoparticle interfaces play a crucial role in various applications ranging electrochemistry, fuel cells, industrial catalysis as well as biomedicine. In the three to five closest water layers at any interface, the physicochemical properties of the water are modified compared to the bulk. This affects both, the geometrical and the transport properties of the interface.

For nanostructured interfaces, our knowledge of the structure and dynamics of water molecules within the interfacial regime is still very limited. Yet, such insight is crucial to understand how organic ligand molecules diffuse and react at nanoparticle surfaces and how water diffusion can impact catalytic processes. Recently, we could for the first time measure the structure of hydration layers at such facets, see Fig. 1. Now, we want to additionally shed light onto the dynamics of water and possibly organic molecules at iron oxide nanoparticle surfaces as an important catalytic model system. In order to measure the **dynamics of water molecules at facets of magnetic iron oxide nanoparticles, we carry out quasi-elastic neutron scattering (QENS) experiments.**

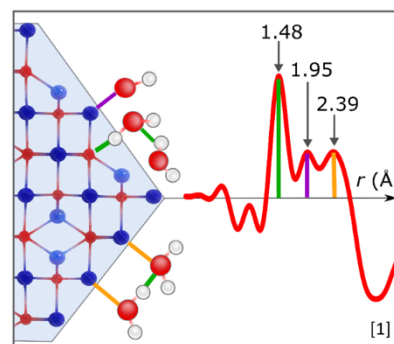


Fig. 1: Structure of water around an iron oxide nanoparticle (left) and density profile from the partially ordered liquid (from X-ray scattering (PDF) [1])

This project involves one or several of the following tasks:

- **QENS experiments** at a research neutron reactor or spallation source.
- **Data analysis** of neutron scattering data with software of your choice (Origin, Matlab, Igor, etc.).
- **Prepare samples** by adjusting relative humidities, perform water and nitrogen physisorption isotherm measurements or TGA-MS.
- Regular group meetings to discuss your results.

You will gain. / Our young research group can offer you:

- Training in **neutron scattering**.
- Participation in our **winter school** on structure and dynamics, 10-14th Feb 2020 in Austria.
- Understanding of structure and dynamics at interfaces.
- Participation in **beamtimes** for neutron scattering experiments.
- Become member of a small **international research team** (3 to 5 people).
- Presentation of your research work at a **conference** (QENS/WINS in Spain, June 2020).

The project can be split up into sub-topics to fit the scope of Hiwi projects, BSc or MSc thesis.

The topic is ample to continue for a PhD.

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October 2019

References: [1] S.L.J. Thomä, S.W. Krauss, M. Eckardt, P. Chater, M. Zobel, *Nature Communications* **10** (2019)
[2] H.-W. Wang, et al., *JACS* 2013, **135**, 6885 (2013)