ARL/Master Thesis

in the group of *Theory of Magnetic Materials* (FB11)

TECHNISCHE UNIVERSITÄT DARMSTADT

EXAFS: Simulation and Machine Learning

Understanding the local coordination environment around atomic species is crucial for unraveling the mechanisms of operation in various functional materials. Extended X-ray Absorption Fine Structure (EXAFS) has emerged as a powerful tool in this domain, providing exceptional elemental specificity and spatiotemporal resolution. By focusing on the interference patterns generated by photoelectron waves, EXAFS enables researchers to delve deep into the atomic and electronic structure of materials.

Recent advancements in machine learning have opened up new possibilities for mapping between EXAFS spectra and pair distribution functions (PDF)[1], offering more precise insights into atomic structures. The combination of machine learning and EXAFS is especially promising for complex systems with multimodal bond distributions, such as catalysts, ionic liquids, and nanomaterials[2]. The use of DFT-based FEFF codes, a widely used software for calculating EXAFS spectra, provides a robust framework for these studies.

In this context, we are looking for a motivated master student to join our research team as part of their Advanced Research Lab (ARL) or Master thesis project. The student will primarily focus on testing and benchmarking the EXAFS calculation workflow using FEFF, while also exploring the forward mapping and the inverse design of local structures based on EXAFS data.

Please write to Prof. Hongbin Zhang (Email: hongbin.zhang@tu-darmstadt.de) if you are interested.

References

[1] N. Marcella, S. Lam, V. S. Bryantsev, S. Roy, and A. I. Frenkel, "Neural network based analysis of multimodal bond distributions using extended x-ray absorption fine structure spectra," *Physical Review B*, vol. 109, no. 10, p. 104201, 2024.

[2] K. Zheng, N. Marcella, A. L. Smith, and A. I. Frenkel, "Decoding the pair distribution function of uranium in molten fluoride salts from x-ray absorption spectroscopy data by machine learning," *The Journal of Physical Chemistry C*, vol. 128, no. 18, pp. 7635–7642, 2024.