Professorship of Multiscale Modeling of Fluid Materials
TUM School of Engineering and Design
Technical University of Munich

Modelling Self-Assembly Dynamics and Developing Machine Learning Potentials for Metal-Ligand Systems

Project Description

Self-assembly processes, where metal-ligand complexes organize into ordered structures (e.g., supramolecular assemblies or metal-organic frameworks), are central to materials science, catalysis, and nanotechnology. These dynamics depend on metal-ligand binding, solvent interactions, and steric effects, which are challenging to model with classical force fields due to their static nature or with *ab initio* methods due to steep computational costs.
This project focuses on developing machine learning potentials (MLPs) to study and simulate self-assembly dynamics in metal-ligand systems. Combining expertise in theoretical chemistry (Prof. Stein) and multiscale modeling (Prof. Zavadlav), the student will investigate how metal-ion coordination, ligand flexibility, and solvent effects govern hierarchical assembly. By bridging quantum accuracy with classical efficiency, this work aims to uncover design principles for functional materials while establishing MLPs as reliable tools for predicting and engineering self-assembled systems. This project is a collaboration between **Prof. Dr. Christopher J. Stein** (Associate Professorship for Theoretical Chemistry) and **Prof. Dr. Julija Zavadlav** (Professur für Multiscale Modeling of Fluid Materials).

Objectives

1. **Protocol Development:** Train MLPs with optimized hyperparameters and validate their performance
2. **Ligand Exchange Dynamics Analysis:** Employ trained models to simulate the effects of metal-ligand coordination, solvent interactions, and supramolecular organization during self-assembly

Application Process

If interested, email **m.sanocki@tum.de** with:

1. A brief introduction (background, interests, and motivation).
2. Your transcript of records.