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

Active Learning-Driven Development of Machine Learning Potentials for Molecular Self-Assembly Dynamics

Project Description

Multiscale modelling is essential for understanding complex phenomena in fields ranging from life biochemistry to materials engineering. A promising research area in this area is the development of machine learning potentials (MLPs), particularly those based on Graph Neural Networks (GNNs), which have emerged as a powerful tool for bridging the gap between quantum-mechanical accuracy and classical molecular dynamics efficiency. This project focuses on the implementation of new **active learning** strategies for the development of machine learning potentials (MLPs) that can efficiently and accurately model molecular interactions.
By combining **active learning** with **multiscale modeling**, this project offers a unique opportunity to push the boundaries of computational chemistry while developing transferable ML tools for materials design. This project, 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. **Active Learning for MLP Development:** Implement active learning workflows to train MLPs, focusing on high-impact regions of chemical space (e.g., transition states, rare coordination geometries).
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.