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

Investigating the Generalizability of Machine Learning Potentials Across Chemical Space

Project Description
Machine learning potentials (MLPs) have shown great promise in accurately describing interatomic interactions while being computationally efficient. However, a critical challenge in their application is ensuring generalizability—i.e., the ability to perform well across diverse chemical systems and reproduce physically meaningful behaviour. Understanding how MLPs generalize across chemical space is essential for their reliable use in molecular dynamics (MD) simulations and materials discovery.
This thesis focuses on developing methods to investigate the generalizability of MLPs. The student will analyze how model performance varies with chemical features (e.g., functional groups, bond types, or atomic environments) and identify regions of chemical space where the model may fail. Additionally, the student will design and test systems to evaluate whether the MLP can reproduce known physical behaviour, or structures.

Objectives

1. **Chemical Space Analysis:** Develop a method to investigate the relationship between chemical features (e.g., atomic environments, functional groups) and model errors.
2. **Generalizability Insights:** Provide insights into the limitations of MLPs and propose strategies to improve their transferability across chemical space.

Outcomes

- A systematic method for analyzing the generalizability of MLPs across chemical space.
- Demonstration of the MLP's ability (or inability) to reproduce physical behaviour in selected test systems.

Requirements

- **Machine Learning Practice:** Experience with training and evaluating machine learning models, particularly neural networks.
- **Programming Experience:** Strong proficiency in Python. Familiarity with machine learning frameworks (e.g., PyTorch, JAX)
- **Chemistry Knowledge:** Basic understanding of chemical features, and molecular structures is advantageous.

What We Offer

- Access to high-performance computing resources for running simulations and analyzing data.
- An opportunity to work on a cutting-edge project with potential applications in materials science, chemistry, and beyond.

Application Process
If you are interested in this project or have further questions, please send a short email to m.sanocki@tum.de with the following:

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