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

ML for Modeling of Metal–Organic Frameworks (MOFs)

Project Description

Metal–Organic Frameworks (MOFs) are a versatile class of porous crystalline materials with tunable structures and properties, making them highly promising for applications such as gas storage, separations, catalysis, sensing, and energy technologies. However, the space of possible MOF structures is extremely large, and experimentally measuring or computationally calculating their properties can be slow and resource-intensive. Machine learning (ML) offers a powerful way to accelerate MOF research by enabling fast, accurate prediction of important material properties across vast chemical and structural spaces.
This project focuses on developing, evaluating, and applying machine learning models to predict key MOF properties relevant to performance and stability. By building ML models that can generalize across diverse MOF families, the student will contribute to strategies for rapid materials screening and data-driven discovery.

Objectives

1. Benchmark ML Models for MOF Property Prediction

Train and evaluate different machine learning approaches—such as gradient-boosted trees, neural networks, and graph-based models—on selected MOF property tasks. Compare prediction accuracy, computational cost, and generalization.

2. Analyze Structure–Property Relationships

Use the trained models to identify which structural or chemical features most strongly influence the target properties. Produce interpretable analyses to better understand what drives MOF performance.

3. Build a Predictive Workflow for Screening New MOFs

Develop a practical ML-based pipeline that can rapidly estimate MOF properties and support high-throughput discovery efforts. Demonstrate its usefulness by screening candidate structures and identifying promising MOFs for further study.

Application Process

If interested, email m.sanocki@tum.de / linying.zhang@tum.de with:

3. A brief introduction (background, interests, and motivation).
4. Your transcript of records.