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

HiWi position

Mapping Liquid Structure: Experimental Data for Machine-Learning Potentials

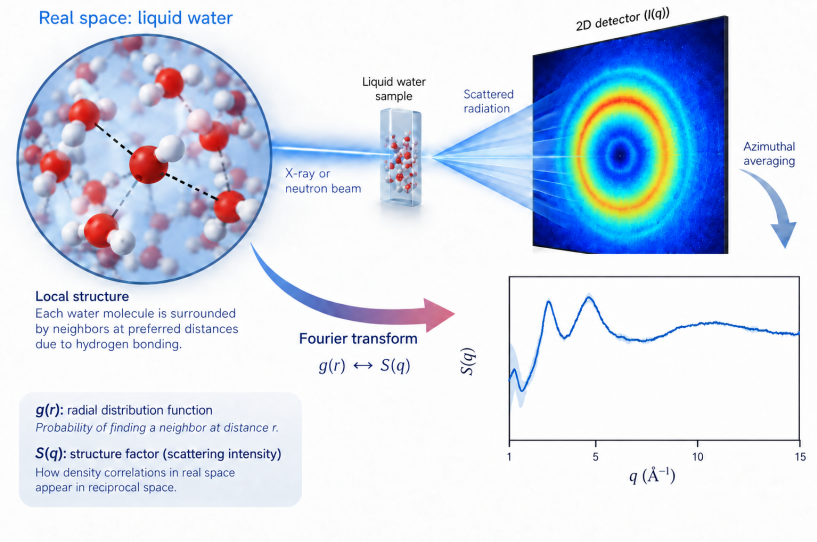
Project Description

In recent years, machine-learning interatomic potentials (MLIPs) have become powerful tools for simulating molecular liquids. Their reliability, however, depends on high-quality experimental data for systematic validation and benchmarking. Scattering experiments provide detailed structural information: neutron and X-ray diffraction probe collective correlations, radial distribution functions (RDFs) describe local atomic organization, and bulk densities provide a complementary benchmark. Yet these data are scattered across publications and repositories and vary in units, normalization, experimental conditions, and reported uncertainties. A reusable, well-documented collection is therefore still missing.

Objectives

The project will establish a curated, provenance-aware dataset of experimental scattering and density data for multiple liquid solvents, enabling consistent validation of accurate and transferable MLIPs. The student will:

- learn how scattering and molecular interactions reveal liquid structure and relate to RDFs and density;
- collect, standardize, and document experimental diffraction, RDF, and density data;
- create basic tools to check data quality, consistency, and provenance.



Prerequisites / Candidate Profile

We are looking for a motivated Bachelor's or Master's student interested in computational molecular science and scientific data analysis. A suitable candidate will ideally have:

- experience with Python programming and numerical data analysis;
- basic knowledge of molecular simulation, statistical mechanics, or materials characterization;
- an interest in machine learning, MLIPs, molecular simulation, or scattering experiments;
- careful and systematic working habits.

Experience with molecular dynamics, RDF analysis, diffraction data, or Git is helpful but not required.

Project Information

Project type: HiWi position
Starting date: Flexible
Duration: To be agreed
Supervisor: Claudio Colturi
Location: Chair of Multiscale Modeling of Fluid Materials, Technical University of Munich

Application Process

This project is offered by the Chair of Multiscale Modeling of Fluid Materials under the academic supervision of Prof. Julija Zavadlav. Interested candidates should contact Claudio Colturi at claudio.colturi@tum.de and include:

1. a brief introduction describing their background and motivation;
2. their transcript of records;
3. a short description of relevant programming, data-analysis, or simulation experience;
4. optionally, a GitHub repository or other examples of previous work.