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

Differentiable Molecular Physics

Differentiable physics facilitates the fusion of machine learning and molecular modeling for drug discovery, materials design, computational biology, and many other fields. At our chair, we leverage differentiable molecular dynamics to train next-generation models that scale to systems of millions of atoms with high accuracy.

Your thesis aims to develop neural network potentials through novel approaches that efficiently access new data sources. Prior knowledge of molecular modeling is not a prerequisite.

Your thesis will consist of the following tasks:

- Familiarize yourself with Molecular Dynamics
- Research state-of-the-art approaches to machine learning in Molecular Modelling
- Implement these approaches in our software
- Train new models on the chair's GPU cluster

If you are interested in the thesis, please reach out to paul.fuchs@tum.de with a short introduction and your transcript of records.