Ph.D. position in Machine Learning for Molecular Simulations

The Multiscale Modeling of Fluid Materials group at the Technical University of Munich is looking for talented and ambitious scientists interested in unique interdisciplinary research, integrating molecular simulations, machine learning, statistical physics, multiscale modeling, and uncertainty quantification. The successful applicant will work on molecular dynamics simulations, where molecular interactions are predicted by neural network potentials. These state-of-the-art neural network models promise simulations at unprecedented accuracy, giving quantitative insight into physical processes at the nanoscale. The candidate will develop the next generation of neural network potentials and apply them to problems from different scientific fields, ranging from life sciences to engineering. For more information, visit our webpage www.epc.ed.tum.de/en/mfm.

Your profile
- M.Sc. degree in informatics, physics, chemistry, or engineering (candidates who will soon obtain the degree are also welcome to apply)
- strong background in machine learning
- proficiency in Python programming
- experience with molecular simulations and knowledge of statistical physics is beneficial
- fluent in spoken and written English (knowledge of German is beneficial but not required)

Our offer
You will join a young research group working on state-of-the-art research in molecular modeling and become part of TUM, a top European university. The position is available immediately and for a duration of three years (possible extension). Salary is based on the Free State of Bavaria public service wage agreement (100%, TV-L E13). Additional funding is available for scientific equipment and conference travel expenses.

How to apply?
Please send your application in English by email to **info.mmfm@mw.tum.de** with the subject "**PhD Application**". The application should include (one PDF document) a cover letter (motivation to join our group, how your previous work/knowledge/interest relates to our research topics and publications), a CV, a grades transcript, two references' contact information, and a desired starting date. Provide evidence of your programming skills (e.g., GitHub repository) if possible. Applications will be reviewed on a rolling basis until the position is filled. Preference will be given to applications received before the **15th of July 2025**.

For any questions, please do not hesitate to contact Prof. Dr. Julija Zavadlav (info.mmfm@mw.tum.de).

Contact
Technical University of Munich
Multiscale Modeling of Fluid Materials (Prof. Julija Zavadlav)
Boltzmannstr. 15, 85748 Garching b. München
www.epc.ed.tum.de/en/mfm.