Ph.D. position in Data-Driven Molecular Material Design

The Multiscale Modeling of Fluid Materials group at the Technical University of Munich seeks talented and ambitious scientists interested in unique interdisciplinary research, integrating molecular simulations, machine learning, statistical physics, multiscale modeling, and uncertainty quantification. By integrating state-of-the-art machine learning models (graph neural networks, diffusion models) with quantum chemistry and molecular simulations, the project aims to accelerate bottom-up material discovery for applications 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 chemistry, physics, or informatics (candidates that will soon obtain the degree are also welcome to apply)
- strong background in machine learning
- proficiency in programming (especially Python)
- experience with ab initio/molecular simulations and knowledge of statistical physics is beneficial
- fluent in spoken and written English (knowledge of German is 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 three years. Salary is based on the Free State of Bavaria public service wage agreement (100%, TV-L E13). Additional funding is available for computational equipment and conference travel expenses.

How to apply?

Please send your application in English by e-mail 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 1 **May 2025**.

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

Contact

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