University of Stuttgart
Institute for Theoretical Chemistry
Computational Chemistry Group

Open Ph.D. Student Position in Molecular Machine Learning

Want to join the Computational Chemistry Group as a fully-funded doctoral researcher?

We search for highly motivated people with an MSc. degree in physics, chemistry, materials science, astrochemistry, computer science (machine learning), or related fields and an interest in chemistry and computing. The project is embedded in the priority program SPP 2363 on "Utilization and Development of Machine Learning for Molecular Applications – Molecular Machine Learning." It builds on our Gaussian-Moment Neural Network code (gitlab.com/zaverkin_v/gmnn) and includes method and code development in areas like active learning, learning on-the-fly, explainable machine learning in cooperation with the institute for computational physics on the simulation of ionic liquids.

To fit into the team, you should be willing to collaborate with experimentalists and theoreticians. Our team communicates in English. We offer the successful candidates an intellectually challenging position in the inspiring atmosphere of an interdisciplinary, diverse team connected to the SimTech cluster of excellence at the University of Stuttgart. We offer a structured doctoral training program within the SimTech graduate school, a research stay abroad in a cooperating group for three months, and participation at international conferences. Ample computer time is available.

We highly encourage applications from underrepresented groups, explicitly (but not exclusively) first-generation students, women, immigrants, parents, POC, LGBT*IQ.

If you are interested, please send your application (CV, list of publications if applicable, contact details for references) via email to kaestner@theochem.uni-stuttgart.de, Johannes Kästner, Institute for Theoretical Chemistry, University of Stuttgart, or informally contact him.