Technische Universität Berlin

Technische Universität Berlin offers an open position:

Research assistant - salary grade E 13 TV-L Berliner Hochschulen - for qualification

part-time employment may be possible

The Berlin Institute for the Foundations of Learning and Data (BIFOLD) at TU Berlin (Prof. Klaus Robert Müller) is seeking a Research Associate in Machine Learning for an Agility subproject. The agility project will be carried out in the research groups "Machine Learning for Molecular Simulation in Quantum Chemistry" (https://www.bifold.berlin/people/dr-stefan-chmiela.html) led by Dr. Stefan Chmiela and "Probabilistic modeling and inference" (https://web.ml.tu-berlin.de/author/dr.-shinichi-nakajima/) led by Dr. Shinichi Nakajima.

Dr. Chmiela's team is engaged in the modeling of multi-body systems with applications in quantum chemistry, particularly for predicting solutions to the Schrödinger equation. The overarching goal of the team is the development of models to accelerate accurate molecular dynamics simulations for the calculation of dynamic and thermodynamic observables of physical systems.

Faculty IV - The Berlin Institute for the Foundations of Learning and Data (BIFOLD) / Machine Learning (ML)
Reference number: IV-354/24 (starting at the earliest possible / for 3 years / closing date for applications 07/11/24)

Working field:

Independent and responsible research in the field of machine learning. The goal of the advertised project is the development of new explanation methods (Explainable Artificial Intelligence, XAI) for atomistic modeling in quantum chemistry. The focus is on acquiring physically grounded insights to guide hypotheses in quantum chemistry. The associated tasks are:

- Development and implementation of XAI methods for ML models in quantum chemistry
- Incorporation of physical knowledge about the target systems into the models, e.g., distinguishing different kinds of short- and long-range interactions between atoms
- Evaluation of the developed methods using benchmark problems and contextualizing observations within physical theory
- Communication of results through presentations

Requirements:

- Successfully completed university degree (Master, Diplom or equivalent) in Physics, Mathematics, or Computer Science
- Proven experience in machine learning with a strong understanding of algorithms, linear algebra, functional analysis, and related mathematical concepts
- Solid knowledge in physics, including methods for solving the Schrödinger equation
- Excellent programming skills in Python and solid knowledge of common machine learning frameworks such as PyTorch or TensorFlow
- Strong communication skills in English and the ability to explain complex topics to a broad audience with diverse backgrounds (i.e., both computer scientists and physicists)
- Familiarity with state-of-the-art machine learning models and approaches for modeling molecular force fields with ML
- The ability to teach in German and/or in English is required; willingness to acquire the respective missing language skills

Desirable:

- The ability to interact with a team of ML experts and physicists

Please send your written application, quoting the reference number, with the usual application documents (i.e. at least cover letter, CV, graduation certificates, grade overviews, etc.) to Technische Universität Berlin - Die Präsidentin - Fakultät IV, Institut für Softwaretechnik und Theoretische Informatik, FG Maschinelles Lernen, Prof. Dr. Müller, MAR 4-1, Marchstr. 23, 10587 Berlin or by e-mail (one PDF file, max. 5 MB) to: **jobs@bifold.berlin**.

For cost reasons, application documents sent by mail will not be returned. Please submit copies only.

By submitting your application via email you consent to having your data electronically processed and saved. Please note that we do not provide a guarantee for the protection of your personal data when submitted as unprotected file. Please find our data protection notice acc. DSGVO (General Data Protection Regulation) at the TU staff department homepage: https://www.abt2-t.tu-berlin.de/menue/themen_a_z/datenschutzerklaerung/ or quick access 214041.

To ensure equal opportunities between women and men, applications by women with the required qualifications are explicitly desired. Qualified individuals with disabilities will be favored. The TU Berlin values the diversity of its members and is committed to the goals of equal opportunities. Applications from people of all nationalities and with a migration background are very welcome.

The vacancy is also available on the internet at
https://www.personalabteilung.tu-berlin.de/menue/jobs/