Freie Universität Berlin - Department of Biology, Chemistry, Pharmacy – Institute of Chemistry and Biochemistry - Keller group “Theoretical Chemistry” – VW Momentum “Molecules move!”

The Keller research group focuses on the modeling and simulation of molecular dynamics, with an emphasis on multiscale systems and processes whose dynamics are driven by rare events. These questions require an interdisciplinary approach, applying methods from mathematics and physics to solve chemical problems. A central research topic is the modeling of the influence of the environment on the mechanism and speed of chemical reactions. Particularly challenging is the simulation of such reactions in complex solvents or on surfaces, where machine-learned force fields theoretically allow for the simulation of chemical reactions. However, the timescales of chemical reactions are far beyond those that can be achieved with current simulations. In the project 'Molecules move!', the Keller research group leverages its expertise in the simulation of rare events and dynamic reweighting methods to address this research question. Specifically, we plan to combine the path reweighting technique (Girsanov reweighting) with machine-learned force fields to develop a simulation method for chemical reactions. https://www.bcp.fu-berlin.de/en/chemie/chemie/forschung/PhysTheoChem/agkeller/index.html https://www.fu-berlin.de/en/presse/informationen/fup/2024/fup_24_126-volkswagenstiftung-bettina-keller-momentum/index.html https://portal.volkswagenstiftung.de/search/projectDetails.do?ref=9D387

Research assistant (postdoc) (m/f/d)

Full-time job limited to 4 years salary grade (Entgeltgruppe) 13 TV-L FU reference code: BC-AGKeller_VWMomentum_2025_E

City: Berlin; Starting Date: At the earliest possible; Renumeration: Entgeltgruppe 13 TV-L FU; Reference number: BC-AGKeller_VWMomentum_2025_E; Closing date: 25/11/24

Working field

You will be working on the project 'Molecules move!'. Your tasks include training neural network potentials based on DFT data, implementing Girsanov reweighting in molecular dynamics packages, simulating chemical reactions in solvents and on surfaces, as well as publishing the results.

Requirements

Completed university degree (M.Sc. or Diploma) and PhD (completed or close to completion) in Computational or Theoretical Chemistry, Computational Physics or a related subject.

Desirable:
- excellent PhD and a strong publication record
- Experience in one or more of the following areas:
- parametrization of machine-learned force fields
- machine learning, in particular neural networks
- simulation of molecular systems, in particular enhanced-sampling and reweighting

techniques.
- quantum mechanical calculations, in particular DFT
- programming, preferably Python- LaTeX
- very good English language skills, both spoken and written.

Application documents:
- Motivation letter with information about previous research projects and future goals
- Curriculum vitae (CV)
- Publication list
- Contact details of two referees/former supervisors

For further information, please contact Prof. Dr. Bettina Keller (bettina.keller@fu-berlin.de / 838 50614).

Application
Applications should be sent by e-mail, together with significant documents, indicating the **reference code, no later than November 25th, 2024** in PDF format (preferably as one document) to Prof. Dr. Bettina Keller: **bettina.keller@fu-berlin.de** or postal to

Freie Universität Berlin
Fachbereich Biologie, Chemie, Pharmazie
Institut für Chemie und Biochemie
AG Keller - VW Momentum “Molecules move!”
Prof. Dr. Bettina Keller
Arnimallee 22
14195 Berlin (Dahlem)

With an electronic application, you acknowledge that FU Berlin saves and processes your data.
FU Berlin cannot guarantee the security of your personal data if you send your application over
an unencrypted connection.

Freie Universität Berlin is an equal opportunity employer.

More information at https://stellenticket.de/188380/
Offer visible until 13/11/24