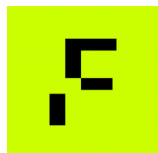


**Freie Universität Berlin - Fachbereich Biologie, Chemie, Pharmazie,  
Institut für Chemie und Biochemie, PTC / Theoretische Chemie / AG  
Keller**



**Research assistant (praedoc) (f/m/d)**

with 65%-part-time job limited to 4 years salary grade (Entgeltgruppe) E13 TV-L FU  
reference code: DM-786

City: Berlin; Starting date (earliest): At the earliest possible; Duration: befristet auf 4  
Jahre; Remuneration: Entgeltgruppe 13 TV-L FU; Reference number: DM-786

**Tasks**

**Who We Are**

Research Group

The Keller research group develops theoretical and data-driven methods for describing complex molecular dynamics across a wide range of time and length scales. Research interests include rare events and molecular kinetics in systems with multiple metastable states and complex timescale hierarchies.

**Planned Tasks**

- Molecular dynamics simulations using enhanced-sampling and dynamic-reweighting methods
- Development and validation of ML force fields based on DFT reference data
- Use of high-performance computing resources
- Collaboration with experimental research partners
- Continuous documentation of research results in the form of reports and presentations, and preparation of scientific publications for peer-reviewed journals

**What You Can Expect in Your New Role**

Project

Recent advances in machine-learning force fields (ML force fields) now provide access to simulations of chemical reactions in complex molecular environments with near-quantum accuracy and atomistic resolution. However, many chemically relevant processes involve rare events and activated transitions that occur on timescales inaccessible to conventional molecular dynamics simulations. Overcoming this limitation requires combining ML-based potentials with advanced enhanced-sampling and dynamic-reweighting techniques. This project aims to develop and apply new simulation methods for studying rare events in molecular systems. The work will focus on activation

processes, free-energy barriers, and molecular kinetics that govern biomolecular dynamics and chemical reactivity. Research topics include the conformational dynamics of peptides and proteins using classical force fields, as well as the simulation of organic reactions using modern ML force fields. The project combines computational chemistry, multiscale modeling, and scientific machine learning to enable efficient simulations of complex molecular processes across realistic time and length scales.

<https://doi.org/10.48550/arXiv.2604.24245>

<https://doi.org/10.1146/annurev-physchem-083122-124538>

## Requirements

### Key Requirements

Completed Master's degree (or equivalent university degree) in chemistry, physics, or a related natural science discipline

### Desirable

Preferred Qualifications:

- Above-average academic performance (please provide supporting documents, e.g., transcript of records)
- Specialization in theoretical or computational chemistry
- Programming skills, preferably in Python
- Experience with machine-learning techniques, particularly ML force fields
- Experience in modeling and simulation of molecular systems
- Excellent written and spoken German and English skills

## What we offer

Modern workplace in the leafy suburb of Dahlem

- Job security
- Salary in line with the collective agreement for the civil service at the state level (TV-L FU), plus additional one-off annual payment
- Flexible working hours and mobile working by arrangement, where possible
- The compatibility of work and family life
- Thirty days of vacation (based on a five-day working week)
- Office closed on December 24 and December 31
- Numerous training and continuing education options for professional and personal development
- Opportunity to participate in University Sports Center courses and the health promotion program
- Free parking close to the office and good public transportation connections
- Discounted "Job Ticket" for public transportation
- Free use of the Freie Universität library system
- Employee discount in the cafeteria
- Exclusive deals for products and services through Corporate Benefits

## Application

If you are interested in what we have to offer,  
Then you can send your application materials including:

- Letter of motivation including information on previous research projects
- Curriculum vitae
- Academic transcripts
- Proof / self-assessment of language skills
- Master's thesis and
- Contact details of a previous supervisor.

Simply submit your application exclusively via our career portal by clicking the "Apply now" button. Unfortunately, we cannot consider applications by post or by e-mail. You can also get in touch with Prof. Dr. Bettina Keller / e-mail: [bettina.keller@fu-berlin.de](mailto:bettina.keller@fu-berlin.de)

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More information at <https://stellenticket.de/205726/BEUTH/>  
Offer visible until 12/08/26

