**Are you looking for a new professional challenge?
Then this is the place to be!
Become part of our international team!**

ZIB
ZUSE INSTITUTE BERLIN

November 7, 2024

The Zuse Institute Berlin (ZIB) is a non-university research institute under public law of the state of Berlin. Within the department "Supercomputing", we are offering at the earliest possible date until September 30, 2026, with the option of extension subject to the approval of further funding, a

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**Postdoctoral Researcher (m/f/d)
Reference Code: IWA 51/24
Pay Grade 13 TV-L (100 %)**

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The Supercomputing department performs research and development work on heterogeneous compute and storage architectures in context of high-performance computing (HPC) and data analytics (HPDA). As a member of the nationwide HPC initiative "Nationales Hochleistungsrechnen" (NHR), ZIB operates compute and storage resources at a top level. Currently, our HPC system "Lise" comprising over 120,000 CPU cores, 200 GPUs in total as well as more than 10 PB persistent online storage.

We are looking for a candidate with a strong background in computational chemistry and basic experience in machine learning and who is highly motivated to work in the interdisciplinary fields of high performance computing. Within a NHR funded project you will work in concert with NHR resources and personnel to develop deep neural network models for predicting chemical structures from measured spectroscopic data, as well as a comprehensive, open source code-base to provide a future research platform for the NHR and scientific communities at large.

Your tasks

- Training/validation/testing of neural network models with various modern neural network architectures
- Managing and preprocessing large databases
- Contribution to the development of an open source code
- Collaboration within an interdisciplinary team of physicists, chemists and computer scientists to tackle complex challenges in chemical structure prediction
- Participation in active, collaborative open source software development, including code review, documentation and deployment

Your profile

- Master's/diploma degree (PhD is favorable, but not necessary) in the fields of physics, computational chemistry, biophysics or related fields
- Good experience with computational quantum chemistry codes

- Experience in machine learning, preferably deep learning
- Basic experience with a modern deep learning framework is desirable, for example PyTorch (preferred), TensorFlow, or JAX
- Some experience with managing large scale, distributed computational workloads on HPC systems
- Good teamwork skills and friendly professionalism
- Good English skills (German is beneficial)

We are offering a friendly working atmosphere with flexible work and meeting times, excellent equipment, and a challenging professional environment

as well as

- comprehensive training in a competent and cooperative team,
- an additional pension scheme (VBL),
- 30 days annual leave, additionally free from work on December 24th and 31st,
- compatibility of work and family through flexible working hours, e.g. (flexitime),
- a salary in accordance with TV-L (Collective Agreement for the Public Service of the Federal States), taking into account the relevant professional experience,
- capital allowance of up to €150 per month, alternatively a discounted BVG (public transport) ticket + difference amount,
- an end-of-year bonus,
- the use of canteens and sports programs of the Freie Universität Berlin (FUB) at reduced rates.

Female applicants are highly encouraged to apply. Since women are underrepresented in information technology, the ZIB is trying to increase the proportion of women in this research area.

Applicants with disabilities will be given preference if equally qualified.

Please send your application, quoting the reference code **IWA 51/24**, including a cover letter, your CV and the standard supporting documents as **one PDF file** by November 13, 2024 (date of receipt) to: jobs@zib.de.

For further information about this vacancy, please refer to our website www.zib.de or contact Dr. Nicholas Charron (charron@zib.de) or Dr. Anita Ragyanszki (ragyanszki@zib.de).

Our private policy statement regarding application data is available at www.zib.de/impressum.

For further job offers please visit our website at https://www.zib.de/jobadvertisement.