



Postdoc / Research Software Engineer (m/f/d)

The Institute of Physical and Theoretical Chemistry at Technische Universität Braunschweig is looking for a

Postdoc / Research Software Engineer (m/f/d)

for a DFG-funded project in its Theoretical Chemistry group in a full-time (100 %) position for a period of three years (according to WissZeitVG).

With 18,500 students and 3,700 staff members, Technische Universität Braunschweig is the largest Institute of Technology in Northern Germany. It stands for a strategic and achievement-oriented way of thinking and acting, relevant research, exceptional teaching and the successful transfer of knowledge and technologies to industry and society. We consistently advocate family friendliness and equal opportunities. Our campus is located at the heart of one of Europe's most active research regions. We cooperate closely and successfully with more than 20 research institutions right on our doorstep and maintain strong relationships with our partner universities all over the world.

In the Theoretical Chemistry Group (see: <http://christophjacob.eu/>) at the Institute of Physical and Theoretical Chemistry we develop quantum-chemical methods for the description of complex chemical systems – ranging from biomolecules to materials. We apply these methods to study spectroscopic properties and to design functional chemical systems – for energy conversion, for catalysis, and for drug discovery.

Within a project funded by the DFG within the program “Quality Assurance of Research Software”, you will be responsible for improving the research software “Vibrations” for the calculation of anharmonic vibrational spectra, which was previously developed in the Theoretical Chemistry Group (see, e.g., [DOI: 10.1063/1.4947213](https://doi.org/10.1063/1.4947213) and [DOI: 10.1021/acs.jpcllett.6b01451](https://doi.org/10.1021/acs.jpcllett.6b01451)), with the goal of making it useable for a broad scientific community. This includes the further scientific development of “Vibrations”, the maintenance and quality assurance of the source code (including documentation, testing, packaging etc.), the support of external users, and building and fostering a community of external contributors.

Your profile:

- Ph.D. in theoretical chemistry or in a related field (e.g., numerical physics, simulation sciences, etc.).
- Experience in scientific software development, in particular in Python.
- Willingness to familiarize yourself with the methods and algorithms of theoretical vibrational spectroscopy.
- Good knowledge of modern methods of scientific software development, such as version control and continuous integration.

- Fluency in English and experience in writing scientific and technical texts, such as software documentation. German language skills are welcome, but not required.
- Ability to work within a team and good communication skills.

The salary depends on the assigned tasks and fulfilment of personal requirements and ranges up to salary group E 13 TV-L. The position is generally suitable for part-time employment but should be staffed 100 percent.

Candidates with disabilities will be preferred if equally qualified (in that case, please attach proof of disability). Applications from international candidates are welcome. TU Braunschweig seeks to reduce underrepresentation in the sense of the NGG in all areas and positions. Therefore, applications from women are highly welcome.

Please submit your application in a single PDF document (including CV, academic certificates, and naming two references) until 20. August 2021 by E-Mail to Prof. Dr. Christoph Jacob, c.jacob@tu-braunschweig.de, who will also be happy to provide further information on the advertised position.

Please note that personal data will be stored for the purpose of the application process. Please note that application costs cannot be refunded.