





Bayerisches Geoinstitut at the University of Bayreuth (Germany) invites applications for a

Ph.D. position in Computational Mineral Physics

This doctoral research project will look at the effect light elements on the state and evolution of Earth's outer core and core-mantle interactions using ab-initio simulations. Due to the complexity of the chemical systems involved (liquid iron-based alloys and silicate liquids and solids), molecular dynamics simulations on two-phase configurations and thermodynamic integration will be performed using machine-learning (ML) potentials. Results will be integrated into thermodynamic models to quantify geochemical processes and address some geophysical questions associated with the geodynamo, creating and maintaining Earth's magnetic field over geological time.

This project is part of the priority program "Reconstructing the deep dynamics of planet Earth over geological time" (DeepDyn, <u>https://deepdyn.geophysik.uni-muenchen.de/</u>) and offers the possibility to interact with other projects in the program. In particular, it is closely related with a project at the group of Ronald Redmer at the University of Rostock (<u>https://www.statistische.physik.uni-rostock.de/</u>), with joint development and refinement of the ML potentials used, and the exchange and discussion of results.

The ideal candidate for the position should have a strong background (and a M.Sc. degree) in physics, chemistry or a related field. Prior experience with numerical methods and high-performance computing, ideally with molecular dynamics simulations, is highly desirable, and programming skills for data processing are expected.

The application should include a CV, synopsis or abstract of M.Sc. work, copies of degree certificates and transcripts, a statement of research interests and names and contact information of two potential referees. It should be sent (in a single pdf-file) to Gerd Steinle-Neumann (<u>g.steinle-neumann@uni-bayreuth.de</u>). The position is funded for three years and the starting date is flexible. Application deadline is September 15, 2023.