FRITZ-HABER-INSTITUT
MAX-PLANCK-GESELLSCHAFT

The Fritz Haber Institute (FHI) in Berlin-Dahlem is one of the most renowned institutes within the Max Planck Society (MPG), Germany's organization for basic research. At the FHI, scientists from all over the world are engaged in fundamental studies in the field of chemical physics at interfaces and surfaces, catalysis research and molecular physics.

The Multiscale Modeling from the Electron to the Reactor Group at the Theory Department of the Fritz Haber Institute is offering a

Postdoc position development of kinetic Monte Carlo software and multilevel strategies

The research of the group concentrates on the development coarse-graining strategies which allow to transfer the detailed information available from atomistic and electronic structure simulations to models of macroscopic behavior. A special focus is kinetic Monte Carlo simulations and their coupling with macroscopic models. Here, we have been developing new algorithms and corresponding software, both for the simulations as well as for analyses of their results. The group, the department and the FHI offer an excellent and inspiring environment for outstanding research.

The project:

Many processes in nature are controlled by rare-event dynamics, e.g. chemical reactions or diffusion in solids. Simulating the interplay between many of such rare event by the kinetic Monte Carlo methodology has become more and more popular during the last years. In the project, a simulation software tool for kinetic Monte Carlo models shall be developed and implemented. Besides efficiency, the focus will be on flexibility to be able to implement complex models and novel numerical/simulation strategies. One such strategy, which shall be addressed, is a multilevel extension of kinetic Monte Carlo for charge transport, which has the potential to significantly reduce the computational burden due to long range interactions.

The project will be part of department's research activities on battery materials and electrochemistry. Besides this, it will be involved in collaborative efforts within the Berlin applied mathematics and chemistry communities.

The project is initially limited to 2 years and may be extended upon review of the project status. The salary is according to TVöD/E13. The project is supposed to start beginning/spring 2022.

Your profile:

The applicant should hold a PhD in mathematics, physics or a related discipline and should have demonstrated a strong background in the development of simulation software. Proficient knowledge of numerical mathematics and low-level programming (preferably C++) are presumed. Experience with stochastic simulation, particularly kinetic Monte Carlo, is beneficial, but not required.

Applications for this position are only accepted via our online application portal www.fhi.mpg.de/open-positions. Closing date: Applications will be accepted until the position is filled. We thank all applicants for their interest; however, only those individuals selected for an interview will be contacted.

The FHI strives for gender equality and diversity. We welcome applications from all backgrounds.
The Max Planck Society is committed to increasing the number of individuals with disabilities in its workforce and therefore encourages applications from such qualified individuals. Furthermore, the Max Planck Society seeks to increase the number of women in research and therefore explicitly encourages women to apply.

In case of questions, please contact: Dr. Sebastian Matera (matera@fhi-berlin.mpg.de)