



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

PhD position on the development of multilevel surrogate models for atomistic-continuum coupling for heterogeneous catalysis

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:

The position is framed within the DFG funded project "Kopplung Atomistischer und Kontinuums-skaliger Modelle der Heterogenen Katalyse mittels eines Reduzierten-Basen-Ansatz und Mehrlevel-On-the-fly-Dünngitter-Interpolation". The applicant will work at an interdisciplinary project involving the modeling and simulation of multiscale flow, transport and reaction processes in heterogeneous catalysis in cooperation with the Weierstrass Institute for Applied Analysis and Stochastics of the Leibniz Association (WIAS). Within this collaborative effort, the project at FHI focuses on the development of multilevel on-the-fly sparse grid interpolation approaches. These will be used to couple quantum chemistry derived kinetic Monte Carlo models with a novel reduced basis approach for reactive flow simulation, which will be developed at WIAS.

Additionally to the collaboration with WIAS, collaboration with experimental groups from Berlin and abroad is planned.

The position is funded for 36 month. This is a part time position (75%) and the salary is according to TVöD/E13. The project is supposed to start beginning/spring 2022.

Your profile:

The applicant should hold a master degree (or equivalent) in mathematics, physics or a related discipline. Knowledge of numerical mathematics and programming (preferably C++) are presumed. Experience with the more specific subjects of the project, such as sparse grids or stochastic simulation, 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)