

## PhD position (75% TV-L E13): Systematically Improvable Modelling of Electrochemical Processes

### About us

In our IAC focus group consisting of Hans-Fischer Senior Fellow Prof. Heather J. Kulik (MIT), Prof. Christopher J. Stein and Prof. Jennifer L. M. Rupp (both TUM), we seek to model electrochemical processes in batteries and electro-catalysts both from first principles and with machine-learning techniques. Please check out <https://www.ias.tum.de/ias/research-areas/advanced-computation-and-modeling/systematically-improvable-modeling-of-electrochemical-processes/> for more details.

### Required qualifications

Prospective candidates

- completed their undergraduate studies (M.Sc. or equivalent) in chemistry, physics, or a related field with excellent grades
- are highly motivated to learn, advance and apply new theoretical methods
- are team players who are eager to communicate and learn from other group members and collaborators
- have at least rudimentary programming skills and prior experience with quantum-chemical software packages
- have excellent communication skills in English

### Tasks

The theoretical modeling of complex electrochemical processes requires fast yet accurate quantum-chemical models. Density-functional tight-binding (DFTB) models potentially fulfill this promise but require fast and automated parameter optimizations. The selected candidate will develop a parameter-optimization strategy with uncertainty quantification based on density-dependent metrics. Reference data for this optimization will be generated by accurate embedding models that will also be developed and applied as part of the PhD program. Finally, the new approach will be combined in a fully automated workflow for catalyst and battery material screening.

### We offer

The position is fully funded, available immediately and limited to three years. The selected candidate will for the most part be hosted in the group of Prof. Stein but an extended visit of about 6 months in the group of Prof. Kulik at MIT is part of this position. In addition, frequent exchange and potential lab visits in the group of Prof. Rupp are expected. TUM strives to raise the proportion of women in its workforce and explicitly encourages applications from qualified women. Applications from disabled persons with essentially the same qualifications will be given preference.

### Application

Please send your CV, meaningful letter of motivation detailing your interest in the field of simulation and modeling of catalytic processes, two recommendation letters and degree certificates or transcripts of record to Prof. Stein ([recruitment.stein@tum.de](mailto:recruitment.stein@tum.de)) and Prof. Kulik ([hjkulik@mit.edu](mailto:hjkulik@mit.edu)). Only complete applications will be considered. The application deadline is October 19<sup>th</sup>, 2023 but the position will be reopened until a suitable candidate has been identified.

### Technische Universität München

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