



**University of Stuttgart**  
Institute for Theoretical Chemistry  
Computational Chemistry Group

## **Open Ph.D. Student Position: Simulation of Surfaces in Strong Electrical Fields**

Want to join the Computational Chemistry Group as a fully-funded doctoral researcher?

We search for highly motivated people with an MSc. degree in physics, chemistry, materials science, or related fields and an interest in chemistry and computing. The project is embedded in the collaborative research program SFB 1333 on "Molecular heterogeneous catalysis in confined geometries." You will use DFT and similar methods to simulate the molecular processes that lead to evaporation and fragmentation of molecules from surfaces under strong fields. That process is key to experimental atom-probe tomography, used by our cooperation partners to determine the 3D composition of materials with atomistic resolution. Your work will continue efforts like DOI [10.1021/acs.jpca.0c06887](https://doi.org/10.1021/acs.jpca.0c06887) or [10.1038/s41598-020-77130-x](https://doi.org/10.1038/s41598-020-77130-x).

To fit into the team, you should be willing to collaborate with experimentalists and theoreticians. Our team communicates in English. We offer the successful candidates an intellectually challenging position in the inspiring atmosphere of an interdisciplinary, diverse team connected to the SimTech cluster of excellence at the University of Stuttgart. We offer a structured doctoral training program within the SFB 1333, a research stay abroad in a cooperating group for three months, and participation at international conferences. Ample computer time is available.

We highly encourage applications from underrepresented groups, explicitly (but not exclusively) first-generation students, women, immigrants, parents, POC, LGBT\*IQ.

If you are interested, please send your application (CV, list of publications if applicable, contact details for references) via email to [kaestner@theochem.uni-stuttgart.de](mailto:kaestner@theochem.uni-stuttgart.de), Johannes Kästner, Institute for Theoretical Chemistry, University of Stuttgart, or informally contact him.