

In the field of Applied Computational Catalysis at the Institute of Catalysis Research and Technology (IKFT) we are currently seeking to recruit, limited to three years, a

PhD student

Theoretical Modeling of dynamical metal support interaction of promoted copper catalysts for methanol synthesis

The group theory and model system of Prof. Studt focuses on the theoretical description of surface processes relevant for heterogeneous catalysis using density functional theory calculations and microkinetic modeling (<https://www.ikft.kit.edu/english/232.php>). A particular of the group is on topics related to chemical energy storage as liquid fuels such as e.g. methanol, which are important energy carriers in the context of the German energy transition (“Energiewende”).

By using theoretical calculations we aim at a detailed understanding of how catalysts work at the atomic scale. This PhD position requires interdisciplinary cooperations with groups from the fields of synthesis and characterization in the framework of the priority program SPP 2080 “Catalysts and reactors under dynamic reaction conditions for energy storage and conversion” (www.spp2080.org).

Responsibilities involve:

- Calculations of transition states of the reduction/oxidation of ZnO on copper surfaces
- Kinetic modeling of the dynamics of the ZnO_x layer on copper surfaces
- Calculations of the important intermediates of methanol synthesis and estimation of reaction rates
- Determination of spectroscopic parameters of adsorbates on surfaces
- Modeling of the influence of promoters on the stability of the active site

You hold a very good master’s degree in chemistry, chemical engineering, and physics or in a related area. Basic knowledge and experience in physical and technical chemistry, as well as in catalysis are desired. Besides the professional qualification, strong commitment, independent and self-responsible working including fluent verbal and written English skills are expected.

We offer you an attractive and modern workplace with access to the excellent facilities of the KIT, a diverse and responsible job and a wide-ranging offer of advanced training possibilities. Supplementary pension line according to VBL, flexible working time models and support of the JobTicket (BW) are also provided.

We aim for an equal filling of jobs with female and male employees. Therefore, we would be especially glad about applications from women for this position. If qualified, handicapped applicants will be preferred.

Please apply online at felix.studt@kit.edu