Department Chemie und Pharmazie

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG

NATURWISSENSCHAFTLICHE FAKULTÄT

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Department Chemie und Pharmazie

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Job Advertisement

At the Chair of Theoretical Chemistry of the Friedrich-Alexander-University Erlangen-Nuremberg **one Postdoc position** (13 TV-L, 1.0) and **one PhD position** (13 TV-L, 0.5) are to be filled.

Both positions are associated with the recently established Collaborative Research Center CLINT (Catalysis at Liquid Interfaces, SFB 1452). CLINT is a consortium of 21 reasearch groups at the University of Erlangen-Nuremberg funded by the German Sciecne Foundation (DFG) that will explore the highly dynamic, anisotropic environment of liquid interfaces to create, taylor, and stabilise catalytically active sites with unique reactivity and performance. The openings are in the work goup of Prof. Dr. A. Görling, one of the four theory groups in CLINT. Responsibilities in both positions comprise the use of electronic structure methods, in particular density-functional methods, to contribute to the research program of CLINT in close collaboration with the experimentally working groups as well as in cooperation with the other theory groups. Typically, slab models for surfaces including catalytic sites will by studied to unravel reaction mechanisms and predict promising catalytic setups. Ab-initio molecular dynamics simulations will be employed to get insight into the behavior of Supported Catalytically Active Metal Solutions (SCALMS) that represent a new novel catalyst concept developed in recent years at the University of Erlangen-Nuremberg. Some projects in CLINT consider electrocatalysis. Therefore questions related to electrochemistry have to be considered as well by means of theory. Within CLINT a broad range of spectroscopic methods are employed, comprising, amongst others, neutron scattering, various infrared and Raman techniques, or X-ray photoelectron spectroscopy. Simulation of spectroscopic data in order to help analysing experimental results is part of the responsibilities. Together with the other theory groups in CLINT a multiscale modelling workflow for catalytic processes at liquid interfaces shall be established.

Successful candidates for the Postdoc position should hold a PhD obtained in a pertinent field and have experience in electronic structure calculations with density-functional methods. Experience with molecular modeling is helpful but not mandatory. Employment will be for one year at first but can be prolonged on a yearly basis. Candidates for the PhD position should have a Master degree in chemistry, physics, or materials science and a solid knowledge in quantum mechanics, quantum chemistry or solid state physics, as well as an affinity to computer related work. According to the hiring praxis of PhD students at the University of Erlangen-Nuremberg an initial employment within an orientation phase is for one year. This can be followed by a three year employment.

Please send your application with the usual documents to Prof. Dr. Andreas Görling by email (andreas.goerling@fau.de).