PhD position: Computational studies of molecular properties of N-heteropolycycles

Job description: The PhD position is available in the collaborative research center (CRC) 1249 “N-Heteropolyzyklen als Funktionsmaterialien” (Link) within research project B07 “Theoretical modeling of energy transport in small molecular clusters of N-heteropolycycles” (Link). The long term scientific aim of the collaborative research center is the rational development of new organic semiconductors focusing on a large and widely variable class of compounds, N-heteropolycycles, which derive from a limited number of fundamental structural building blocks. A precondition for the implementation of this research program is the detailed understanding of the underlying elementary processes. The aim of research project B07 is the quantum chemical computation of molecular properties to understand energy transport in bulk and interfaces in compounds relevant to CRC 1249.

The main objective of the PhD project is to obtain a solid understanding of the electronic properties of N-heteropolycycles and their complexes employing a broad spectrum of computational chemistry methods. A second objective is to extend existing quantum chemistry methods for particular computational cases when needed.

Qualification: • M.Sc. degree in chemistry with special interest in computational chemistry.
• Expertise in electronic structure methods
• Experience in using major quantum-chemical packages (Turbomole, Molpro, etc.)
• Experience scripting in Linux/Unix environment for job automation and data analysis/workup

Salary: The remuneration occurs on the basis of the wage agreement of the civil service in TV-L.

Institute: Institute of Physical Chemistry (IPC)

Contract duration: Limited until 31.12.2020
Starting date: As soon as possible
Application up to: 31.06.2018
Contact person in line-management: For further information, please contact Dr. Höfener, web: www.ipc.kit.edu/theochem, e-mail: sebastian.hoefener2@kit.edu.

Application: Application can be submitted to Karlsruhe Institute of Technology (KIT), Dr. Höfener, e-mail: sebastian.hoefener2@kit.edu

KIT is an equal opportunity employer. Women are especially
encouraged to apply. Applicants with disabilities will be preferentially considered if equally qualified.

KIT is certified as a family-friendly university (familienfreundliche Hochschule) and offers part-time employment, leaves for family-related reasons, dual career options, and individual coaching for family-work balance.