PhD position: Quantum chemical studies of degradation mechanisms in organic electronics

Job description

The PhD position is available in the Research Training Group (RTG) 2450 "Tailored Scale-Bridging Approaches to Computational Nanoscience" (www.compnano.kit.edu) within Research Project P2 "Degradation Mechanisms in Organic Electronics". The quantum chemical aspect of Research Project P2 is the modeling of excited states of relevant (charged) molecular building blocks by employing a range of quantum-chemistry methods such as time-dependent density-functional theory, the Bethe-Salpeter equation, and approximate linear-response coupled-cluster theory, embedded in the environment of the organic-electronics material, to understand the degradation which leads to reduced lifetimes of the materials.

The objectives of the PhD project are twofold. One objective is to develop further the *ab initio* methods required for RTG-specific computations with the TURBOMOLE package of programs, with emphasis on time-dependent density-functional theory applied to molecular systems with emphasis on energy- and charge transport and their degradation mechanisms. The second objective is to apply a wide range of computational chemistry methods and program packages for the cross-sectional support of other research projects of the RTG.

Personal qualification

M.Sc. degree in chemistry with emphasis on method and code development in the area of *ab initio* quantum chemistry. Detailed knowledge of the TURBOMOLE program package and solid programming experience in FORTRAN are required.

Organizational unit

Institute of Physical Chemistry (IPC)

Salary

The salary is based on the wage agreement for public service in the state Baden-Württemberg (TV-L, 75% E 13).

Starting date

01.04.2019

Contract duration

Limited to 3 years.

Application up to

31.01.2019

Contact person in line management

For further information, please contact Dr. Höfener, phone: 0721 608-43321, e-mail: sebastian.hoefener2@kit.edu or Prof. Dr. Klopper, phone: 0721 608-47263, e-mail: willem.klopper@kit.edu.

Application

Please send your application until **January 31st, 2019** as a single pdf file **by email to** sabine.holthoff@kit.edu. See http://www.compnano.kit.edu/26.php for further information about what this pdf file should include.

We prefer to balance the number of female and male employees. We therefore kindly ask female applicants to apply for this job.

If qualified, handicapped applicants will be preferred.

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.