



At the Computational Materials Science Group (Prof. Dr. T. Frauenheim), Bremen Center for Computational Materials Science (BCCMS), Department of Physics, University of Bremen the position of a

Research Fellow / Postdoc Position

is open to work in the field of modeling charge assisted surface reactions. (Subject to personal qualification employees are remunerated according to the salary group E 13 TV-L).

The position is under the supervision of Dr. Bálint Aradi and Prof. Peter Deák at the BCCMS, University of Bremen and of Dr. Dario Rocca and Dr. Sébastien Lebègue at the University of Lorraine (Nancy, France). The position will start at the earliest possible date and is limited for 3 years. The period of employment is governed by the Fixed Term Research Contracts Act (WissZeitVG).

Tasks: The recruited postdoc will work on *ab initio* simulations of photocatalytic charge transfer processes on the TiO_2 surface. A crucial part of the project is the development of a general and self-consistent charge correction scheme for low dimensional periodic systems. This part of the project will be guided by the *University of Lorraine where the applicant must spend the first 6 months of the project*. The methodological development will have to be implemented into the plane-wave code Quantum Espresso. The postdoc will then move to the University of Bremen and, parallel with testing different stages of the development, will investigate the photocatalytic oxidation of CO and reduction of NO_2 on the anatase (101) surface, with special emphasis on electron- and hole-scavenging by O_2 and H_2O , respectively.

Requirements: PhD degree in physics, (quantum) chemistry, or materials science, with background in the theory of electronic structure calculations. Since the project will involve an extensive part of method development, good Fortran programming skills are necessary. Experience with solid state calculations using plane wave codes is required. The working language is English.

We target at a top-notch dedicated and proactive young scientist with excellent communication and writing skills who plans to make her/his mark in science.

Please visit <http://bccms.uni-bremen.de/> for more information on our activities. Applications from women are particularly welcome. The same applies to people with disabilities.

Applicants should send their complete application documents, including a letter of motivation, Curriculum Vitae, the complete publication record by email until **15.06.2017** as a single pdf file to Peter Deak (email: deak@uni-bremen.de) and to Dr. Dario Rocca (email: dario.rocca@univ-lorraine.fr), simultaneously.

