



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

### Opening for Doctoral Position (PhD)

Applications are invited for a three-year, DFG-funded doctoral position (TVL-13/0.75), under the supervision of Prof. Peter Deák and Prof. Thomas Frauenheim. The position is available immediately.

The recruited PhD student will carry out defect calculations in Ga-based semiconductors, using the HSE hybrid functional with the VASP and with the CP2k electronic structure packages. The mixing and screening parameters of the functional have to be optimized in each material, mapping the field of optimal parameters in a series of semiconductors, used in micro/optoelectronics and photovoltaics. The results should be the basis for developing an improved highly transferable hybrid functional.

Candidates should have completed an MSc in physics, chemistry or materials science, and should have preliminary experience with electronic structure calculations, preferably with one of the aforementioned computer packages. Good programming skills are also necessary. Knowledge of solid state and defect physics is an advantage. The working language is English.

Interested candidates should send a copy of their CV (including a list of publications and references) to Peter Deak (email: deak at [uni-bremen.de](mailto:deak@uni-bremen.de)), and to Thomas Frauenheim (email: frauenheim at [uni-bremen.de](mailto:frauenheim@uni-bremen.de)), simultaneously.

