

Postdoctoral position at Slovak University of Technology in Trnava, SLOVAKIA

Title of the position: postdoctoral fellow in development and application of a new interface for quantum-mechanical solid-state modelling

Project & Job description: The postdoc will work on development of a high-performance Phase Diagram Calculator for crystalline matter. He/she will subsequently apply the new tool to study structural and dynamical behaviour of novel magnetic inorganic compounds with transition metals in pursuit for new materials for electronics and spintronics. This Calculator will be a computational interface that will combine already existing programs for quantum-mechanical calculations of electronic structure and lattice thermodynamics and its role will be to calculate thermodynamic stability of a given chemical system in function of pressure and temperature. The new platform will enable highly effective mapping of new inorganic compounds and alloys as well as their phase transitions over a wide range of temperatures and pressures. This project will be realized in cooperation with other group members and international collaborators involving both theoretical and experimental researchers. Short scientific stays at cooperating international institutions may apply.

Department information/Research group: The postgradual fellow will be a member of newly created research group dedicated to predictive computational materials modelling from first principles lead by dr hab. Mariana Derzsi. The group is situated at the [Advanced Technologies Research Institute ATRI](#) in Trnava near Bratislava (Slovakia), which is part of the Faculty of Materials Science and Technology of the Slovak University of Technology. The activities of the group will focus on development and application of computational tools for crystal structure and properties predictions aimed towards molecular design of new electronic and multifunctional materials from ab initio. The group will provide theoretical support for experimental quest for novel functional materials at the home Advanced Technologies Research Institute dedicated to [ion-beam nanomaterial engineering](#). The newly established research group will have an active collaboration with inorganic synthetic [Laboratory of Technology of Novel Functional Materials](#) at the University of Warsaw, Poland as well as with several other international experimental and theoretical materials research groups. The ATRI institute is a new research centre formed by young and enthusiastic researchers highly dedicated to new directions in scientific and technological innovations.

What we offer: We offer postdoc contract for 2+1 years with initial monthly salary of 1180-1270EUR (with possible contract extension and salary increase based on performance and funding), young and highly creative interdisciplinary research environment, free services of the University campus including sport facilities, possibility of housing&dining at the campus, assistance with all agenda related to new place of work&living. The host Institute will provide full support in the candidate's professional growth and formation of own research directions.

Eligibility: The candidate must hold PhD from physics, chemistry, computational material sciences or related field obtained no more than three years prior the application deadline. He/she must have programming skills and should have experience with quantum-physics/chemistry programs. The ideal postdoc is a team player, enjoys creative work, works independently, has good communication skills and is motivated to interact with scientists from other research fields. *We are highly committed to building a diverse research environment, and women, minorities and disabled persons are strongly encouraged to apply.*

How to apply: The applications should send (1) Curriculum Vitae including short summary of accomplishments and publication list, (2) contact information of two references (including email and possibly Scopus, Google Scholar or related identifier) to mariana.derzsi@stuba.sk.

Application deadline: The position is available immediately until a suitable candidate is found but must be filled prior the end of the year 2018. The applications are reviewed immediately.