

PhD SCHOLARSHIP

SONATA-BIS (ST): Investigation of the bio-active properties of new two-dimensional structures of the transition metal carbides

RESEARCH TOPIC:

The main topic of doctoral thesis is to develop numerical scheme allowing for quantitative predictions of toxicity of synthesized nano-crystals and their properties such as morphology, shape, dimensions, based on the machine learning methods and descriptors. The second aim during the PhD work is to perform the atomistic calculations of the molecular adsorption to the surface of 2D nano-crystals in the presence of electrolyte. This part of the project's tasks will be realized by the consortium partner, in the Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, under supervision of the project co-leader **Dr. Magdalena Popielska (Birowska)**.

Requirements:

The candidate should fulfill the following conditions:

- To finish the studies in the field of physics, quantum chemistry, biophysics, or electrical engineering and possess master degree (or equivalent).
- To possess interdisciplinary knowledge in the field of physics, biology and chemistry.
- To possess good knowledge of programming language(s) (e.g. C/C++, Fortran, Matlab, Mathematica, SQL).
- To possess command of English allowing for easy communication and writing of scientific reports.

Tasks in the project:

- Performing Molecular Dynamics (MD) calculations with effective valence force field potentials (VVF).
- Performing *ab initio* calculations based on the DFT for the simplified structures in order to verify effective potential calculations.
- Implementation of machine learning algorithms allowing to quantify the relationship between morphology, structure and physico-chemical properties of 2D nano-crystals of MXenes phases from biological media.

Required documents:

(i) Motivation letters, (ii) CV; (iii) copy of the master diploma; (iv) agreement to process personal data for the purposes of the recruitment.

Employment conditions

The PhD scholarship is planned for the period of 48 months. During his/her participation in the project, the PhD will obtain the tax-free scholarship from National Science Center project funding.

Recruitment procedure

In addition to the careful assessment of the sent documents, interview with selected candidates is planned (over skype). The chosen candidates will be personally informed about the time of interview by email. All required documents have to reach the recruitment commission by 7 June, 2018.

These documents can be delivered either personally or per surface mail to the Secretary Office of the Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, ul. Pasteura 5, PL-02-093 Warszawa, Poland. They can be also delivered in the PDF format electronically per email to Magdalena.Birowska@fuw.edu.pl (quoting the subject **PhD position SONATA-BIS**). Each candidate will be informed personally per email about the results of the recruitment procedure. All further information can be achieved from Dr. Magdalena Popielska (Birowska).