Doctoral School of Information and Biomedical Technologies
Polish Academy of Sciences (TIB PAN)

SUBJECT:

Inter-atomic potentials for numerical optimization of 2D materials

SUPERVISOR:

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DESCRIPTION:

2D materials, built out of a single atomistic layer, are at the moment at the forefront of materials engineering research. They give us realistic chance to create the thinnest possible devices, with unique functional properties. The first material of this class, graphene, has already transformed our thinking about nano-electronics and that has lead to a recent Nobel prize in physics. In this project we aim for a numerically optimized search for a new allotropes of 2D materials. The specific task of the PhD student will be to devise and optimise inter-atomic potentials for various chemical content of the 2D sheet. He/she will invesitigate problems at the cross-roads physics, materials engineering and computational engineering, such as the nature of screening and the influence of spin-orbit coupling on the inter-atomic interactions. Knowledge of quantum mechanics is desired but not essential to develop these potentials. We are looking for a person with a keen interest to develop numerical methods that can be applied at the frontier of materials science.

BIBLIOGRAPHY:

1. Mrozek A., Kuś W., Burczyński T., Nano level optimization of graphene allotropes by means of a hybrid parallel evolutionary algorithm, COMPUTATIONAL MATERIALS SCIENCE, Vol.106, pp.161-169, 2015