DESCRIPTION FOR THE GENERAL PUBLIC

Discovery of graphene in 2004 started a new era in solid-state physics. Intriguing properties of this purely carbonic two-dimensional material, e.g., extremely high velocity of electron traveling through the plane, caused increasing interest in other flat materials as well. Such 2D systems offer rich spectrum of properties and can be potentially engineered on-demand, which creates exciting prospects for using such systems in applications ranging from electronics, sensing, photonics, energy harvesting, catalysis, and flexible electronics. Therefore, **the main objective of the project is to gain deep understanding of the mechanisms that determine structure, stability, ordering phenomena in graphene-based materials containing carbon, boron and nitrogen, and investigation of properties resulting from varying concentrations and configurations of atoms in such C-B-N alloys.** However, the main complexity lies in the need to describe systems that inter alia:

(i) Usually lack the long-range order, i.e., dopants are not uniformly distributed within the material,
(ii) Exhibit a whole plethora of structural defects, e.g., vacancies,
(iii) Are available only in the form of ribbons or flakes, where edges play an important role.

Within this project, we want to prove the hypothesis, that by choosing suitable concentration of constituent atoms in the C-B-N alloys and by proper functionalization of them one can influence their properties to such an extent that new physical phenomena emerge and they can be utilized in novel functional devices. For this purpose, we will develop multi-scale theoretical scheme, based on well-known methods in condensed matter physics (empirical energy calculations, Monte Carlo optimization technique, determination of electronic structure), yet combined in an innovative way. Development of simulation technique will provide a valuable tool for quantitative predictions for large-scale multicomponent alloys, which is crucial for these materials as the existing **disorder** is clue to their properties.

The code developed during project, will serve us to **extract intrinsic properties of C-B-N 2D alloys with a special focus on investigation of disorder phenomena.** The aimed shape of the simulation program should open the door to investigation of other members of two-dimensional family in the same approach (including phosphorene, silicone, germanene, 2D chalcogenides, oxides etc.). The question of doping and ordering in those materials is equally as important as in graphene systems.

Finally, the knowledge gained through the realization of the project should contribute to the two most important problems of humanity nowadays, namely carbon capture and energy storage.