Computational design of new 2D nanostructures

***Tadeusz Burczyński[1], Wacław Kuś[2], Marcin Maździarz[1], and Adam Mrozek[3]**

[1]Institute of Fundamental Technological Research of Polish Academy of Sciences, Warsaw, Poland
[2]Silesian University of Technology, Gliwice, Poland
[3]AGH University of Science and Technology, Kraków, Poland

*Presenting and corresponding author: tburczynski@ippt.pan.pl

Abstract

New 2D nanostructures based on carbon are generated by the two-stage searching strategy combining molecular computing and ab initio methods. The two candidates X and Y are obtained from molecular model by the memetic base algorithm which combines the evolutionary algorithm and the conjugate-gradient optimization technique [1]. The main goal of the optimization is to find stable arrangements of carbon atoms under certain imposed conditions. The fitness function is formulated as the total potential energy of an atomic system. The optimized structure is considered as a discrete atomic model and interactions between atoms are modeled using the AIREBO potential [2]. The parallel approach used in computations allows significant reduction of computation time. Validation of the obtained results of the new 2D nanostructures X and Y obtained using the described algorithm are presented, along with their mechanical properties.

In the second stage the two candidates X and Y are then in depth analyzed using first-principles Density Functional Theory (DFT) from the mechanical, structural, phonon and electronic properties point of view. Both proposed polymorphs of graphene are mechanically and dynamically stable and can be metallic-like [3].

Optimal searching for the new stable atomic arrangements with predefined mechanical properties is also considered using the described memetic algorithm. The main goal of the optimization is to find stable arrangements of carbon atoms placed in the unit cell with imposed periodic boundary conditions, which reveal desired mechanical properties. One example of the newly obtained model of the flat carbon material is presented [4]. Its mechanical properties are additionally validated during the simulation of the tensile tests using molecular dynamics. The material derived from the first stage is then profoundly analyzed in the second stage using the first-principles DFT. The proposed 2D-graphyne-like material called AC is mechanically, dynamically and thermally stable and can be semiconducting-like with a direct band gap of 0.829 eV.

Keywords: **Nanostructures, Graphene-like materials, Molecular Computing, DFT**

References

[1] Mrozek A., Kuś W., and Burczyński T. (2015) Nano level optimization of grapheme allotropes by means of a hybrid parallel evolutionary algorithm. *Computational Materials Science*, 106, 161-169.

[2] Stuart S.J, Tutein J.A., and Harsison A. (2000) A reactive potential for hydracarbons with intermolecular interactions. *J. Chemical Physics,* 112, 2000, 6472-6486.

[3] Maździarz M., Mrozek A., Kuś W., and Burczyński T. (2017) First-principles study of new X-graphene and Y-graphene polymorphs generated by the two stage strategy. *Materials Chemistry and Physics*, 202, 7-14.

[4] Mrozek A., Kuś W., and Burczyński T. (2017) Method for determining structures of new carbon-based 2D materials with predefined mechanical properties. *Inter. J. Mulstiscale Computational Eng.*, 15(5), 379-394.