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COMPUTATIONAL STRATEGY IN DESING OF A NEW 2D SEMICONDUCTING CARBON ALLOTROPE

T. Burczyński[1], M. Maździarz[2], A. Mrozek[3] and W. Kuś[4]

[1] Institute of Fundamental Technological Research, Polish Academy of Sciences, Pawińskiego 5B, 02-106 Warsaw, Poland, E-mail: tburczynski@ippt.pan.pl, www.ippt.pan.pl/staff/tburczynski
[2] Institute of Fundamental Technological Research, Polish Academy of Sciences, Warsaw, Poland, E-mail: mmazdz@ippt.pan.pl
[3] AGH University of Science and Technology, Kraków, Poland, E-mail: amrozek@agh.edu.pl
[4] Silesian University of Technology, Gliwice, Poland, E-mail: Waclaw.Kus@polsl.pl

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Potentially new, single-atom thick semiconducting 2D-graphyne-like material called Anisotropic-Cyclicgraphene, is generated by the two stage searching strategy linking molecular and ab-initio approaches.

In the first stage optimal searching for new stable atomic arrangements of 2D carbon lattices with predefined mechanical properties is presented. The proposed method combines the evolutionary algorithm and the conjugate-gradient optimization. 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. The semi-empirical potential (AIREBO) is used in these molecular simulations [1].

The material derived from the first stage is then profoundly analyzed in the second stage using the first-principles density functional theory from the structural, mechanical, phonon and electronic properties point of view. The proposed methodology is similar to the ab-initio method, which was applied to study of X- and Y-graphene polymorphs [2]. The proposed Anisotropic-Cyclicgraphene is mechanically, dynamically and thermally stable and can be semiconducting-like with a direct band gap of 0.829 eV.

Some results in this paper are unique and we trust will be verified by other works. The synthesis of the proposed structure is a separate task and goes beyond the area of this work.

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REFERENCES

[1] A. Mrozek, W. Kuś, T. Burczyński, Method for determining structures on new carbon-based 2D materials with predefined mechanical properties, *International Journal for Multiscale Computational Engineering,* Vol. **15** (5) 379-394, 2017.

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