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DESIGNING OF NEW 2D SEMICONDUCTING CARBON ALLOTROPE AS AN INVERSE PROBLEM

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

[1] Institute of Fundamental Technological Research, Polish Academy of Sciences,
Pawinskiego 5B, 02-106 Warsaw, Poland
e-mail: tburczynski@ippt.pan.pl

[2] AGH University of Sciences and Technology, Kraków, Poland
e-mail: amrozek@agh.edu.pl

[3] Silesian University of Technology, Gliwice, Poland
e-mail: waclaw.kus@polsl.pl

1 INTRODUCTION

A new, single-atom thick semiconducting 2D-graphene-like material, called Anisotropic-Cyclicgraphene, is generated by the two stage searching strategy linking molecular and ab initio approaches. The candidate is derived from the memetic based algorithm and molecular simulations as a solution of an inverse problem and next is profoundly analysed using first-principles density functional theory from the structural, mechanical, phonon, and electronic properties point of view.

2 COMPUTATIONAL METHODOLOGY

The structure of the two-dimensional graphene-like material is considered as a discrete atomic model, with imposed periodic boundaries. The behavior of such a system is investigated using one of the molecular methods. The potential energy of carbon atoms, the forces acting between them and the overall behavior is determined by the AIREBO potential, especially developed for hydrocarbons.

The memetic optimization algorithm based on global evolutionary and local gradient-based algorithms is used. The coupling of these two algorithms leads to amplifying advantages and reducing disadvantages in both of them. The objective function is formulated on the basis of energy of structure, energies of atoms, coordinates of atoms after deflection, and elastic parameters of the structure.

The goal of the inverse problem is to discover an atomic structure with stable configuration, predefined number of atoms and elastic material properties. The elastic properties are computed based on the molecular analysis of a structure with applied small strains. The atomic structures with orthotropic elastic material properties are taken into account. The objective function depends on the norm of differences between the vector of prescribed $\mathbf{C}_{\text{ref}}$ and computed $\mathbf{C}$ elastic properties [1].

First-principles calculations with the use of density functional theory (DFT) within the pseudopotential, plane-wave approximation (PP-PW) have been made using the Cambridge Serial Total Energy Package (CASTEP). For structural, mechanical and phonon calculations the modified Perdew-Burke-Ernzerhof generalized gradient approximation for solids was applied as an exchange-correlation functional whereas for band structure computations the hybrid exchange-correlation functional HSE06.

The material derived from the first stage is then profoundly analyzed using first-principles density functional theory from the structural, mechanical, phonon and electronic properties point of view. The proposed Anisotropic-Cyclicgraphene is mechanically, dynamically and thermally stable and can be semiconducting-like with a direct band gap of 0.829 eV [2].

3 FINAL REMARKS

The presented approach consists of two stages. In the first molecular stage the inverse problem is solved using the memetic algorithm. The second stage based on the first-principles density functional theory is used to examine results from the previous step. The proposed polymorph of graphene is mechanically, dynamically, and thermally stable and can be semiconducting 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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