COMPUTATIONAL MODELS OF NEW GRAPHENE-LIKE NANO-STRUCTURES

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1. Introduction

The paper is devoted to creation of computational models of new stable atomic arrangements of two-dimensional graphene-like carbon nano-structures. Carbon atoms form various types of bondings and spatial configurations. This ability is determined by the atoms' hybridization states, which depend on their particular electronic configuration. This phenomenon is responsible for the existence of many different allotropes of the carbon. This is due to unique electronic, thermal and mechanical properties of such structures. Graphene-like materials can be classified as periodic, flat atomic networks, made of stable configurations of carbon atoms in certain hybridization states. Since the stable configurations of atoms correspond to the global minima on the Potential Energy Surface (PES), such a task can be considered as a special optimization problem. However, the number of local minima increases almost exponentially with the number of atoms in the considered structure, thus searching for the global minimum on a PES became a non-trivial, NP-hard problem. The proposed hybrid approach combines the parallel evolutionary algorithm and the conjugated-gradient optimization technique.

2. Hybrid evolutionary-gradient method for searching new carbon nan-structures

The hybrid algorithm, proposed and presented in this work, combines the parallel **E**volutionary **A**lgorithm (EA) prepared by the authors, and the classical **C**onjugated-**G**radient (CG) minimization of the total potential energy of the optimized atomic system. Since the processed structure is considered as a molecular-atomic model, the behavior and the potential energy of carbon atoms are determined using the **A**daptive **I**ntermolecular **R**eactive **E**mpirical **B**ond **O**rder (AIREBO) potential developed for molecular dynamics simulations of hydrocarbons [2].

Chromosomes represent design variables in the form of real-valued Cartesian coordinates of each atom in the considered unit cell of the newly created atomic lattice. Each chromosome represents a certain spatial arrangement of atoms. In the initial population, atoms have randomly generated coordinates and are placed in the area of the unit cell with periodic boundaries. Dimensions, the rectangular or triclinic type of the unit cell, as well as the number of atoms, are part of a set of parameters of the simulation. Such an approach allows to control the value of atomic density of the newly-created structure. The periodicity of the atomic structure significantly reduces the number of design variables.

The fitness function is formulated as the total potential energy of the considered atomic system, i.e., the total sum of all potential energies of particular atomic interactions. The AIREBO potential in the following form is used in computation:

$$FF = \sum_{i} \sum_{j \neq i} \left(E_{ij}^{REBO} + E_{ij}^{LJ} + \sum_{k \neq i,j} \sum_{l \neq i,j,k} E_{kijl}^{TORSION} \right) \tag{1}$$

where: E^{REBO} corresponds to the short range interactions between covalently bonded pair of atoms, E^{LJ} is responsible for the long range interactions and is computed in a simplified way, using

the Lennard-Jones-like function with additional distance-dependent switching functions and $E^{TORSIONAL}$ is torsional potential which depends on the neighboring atom's dihedral angles.
Detailed description of the proposed algorithm is presented in [1].

3. Validation and results for new graphene-like structures

In order to validate the accuracy of the results, certain arrangements of carbon atoms already known from literature have been examined, e.g. the supergraphene (triclinic unit cell containing 8 carbon atoms) and the graphyne (triclinic unit cell containing 12 carbon atoms). Since all the tests yield promising results, the proposed optimization algorithm has been applied to search for new stable configurations of a given number of carbon atoms in a unit cell of given size and periodic boundaries [1]. For 8 carbon atoms placed in the 4 Å ×7 Å rectangular unit cell obtained a stable flat network named X (Figure 1A) and for the same number of carbon atoms placed in the rectangular unit cell 4 Å ×6 Å obtained a stable flat network named Y (Figure 1B).

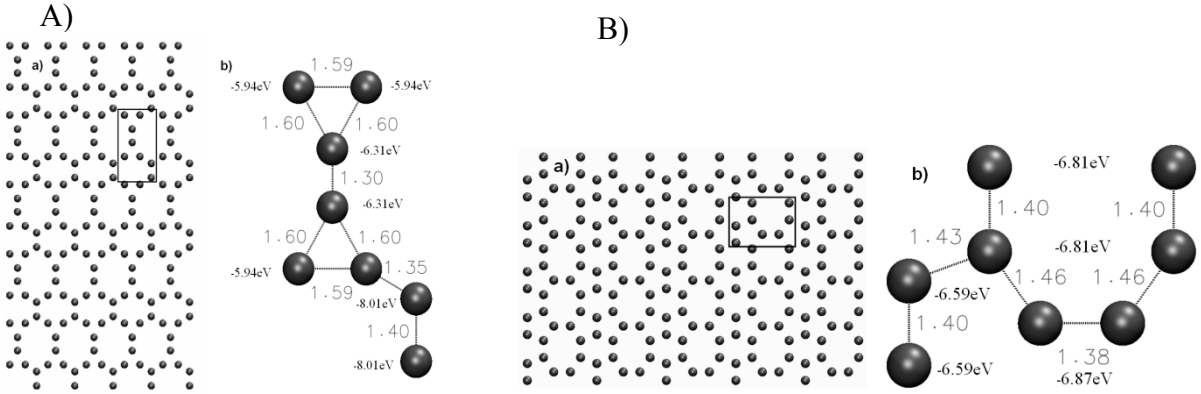

Figure 1. Layout of new stable carbon networks X (A) and Y (B) found by the hybrid algorithm

4. Conclusions

The main purpose of this paper was to present the computational models of new graphene-like nano-structures. The hybrid parallel algorithm was applied to searching for new 2D carbon nan-structures. The proposed method is able to find already-known structures like supergraphene and graphyne as well as new stable ones, named X and Y. Examples performed for new carbon networks clearly show that the final form and properties of optimized structures depend on the assumed size, type and atomic density of the unit cell. Thus, the considered problem can be reformulated and applied to searching for a molecular structure with predefined material properties, not only in the case of carbon-based structures.

5. References

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