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# Computer Simulation of the Interaction of Ring like Carbon Clusters with Nanographene

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***Abstract***. *Various cases of interaction of ringlike carbon clusters $C_7$, $C_{12}$ and $C_{13}$ with one of nanographene - a rectangular plot of graphene consisting of 272 atoms were considered by us. By energy minimization method using second-generation Brener interatomic potential these clusters and this nanographene been previously modeled. Then, by defining various initial location of ringlike carbon clusters relative to nanographene different configurations of these clusters, interacting with nanographene, in the same manner have been found. As a result of the interaction of these clusters with nanographene form of clusters and cohesive energy of cluster atoms were changed.*

## 1. Introduction

Graphene term was originally used to refer to an abstract model, namely, a single layer of graphite atoms which do not interact with other objects. () Even at those theoretical studies, it was clear that graphene, whether in reality, would have the number of unique properties, such as high electrical and thermal conductivity. In 2004, Novoselov and Geim experimental for the first time received graphene in the laboratory, thus the term graphene has become point not only to an abstract model, but also on the nature of the real object.() As the real object of nature graphene interacts with the environment, and in particular with atoms and molecules (clusters).

There are a large number of works dealing with the interaction of graphene with atoms (molecules, clusters). Using different methods, this interaction was studied in different aspects. Nevertheless, the very first question that you need to decide - this question how mathematically infinite graphene according to his ideal model to result in an object suitable for computer simulation. Usually use two approaches: periodic boundary conditions was imposed on the final size of the graphene and thus it is defined as an infinite, or piece of graphene was taken. We use the second approach - working with the final piece of graphene and any such piece of graphene later in this article will be called nanographene.

With regard to research methods, either the classical molecular dynamics method with the corresponding interatomic interaction potentials: Brenner potential, Tersofa potential, UUF or methods ab-inito (Metod of Hartree-Fock-Roothaa, Perturbation theory of Meller Plessis, theory of the combined clusters and so on) are commonly used.

The choice of methods ab-inito inevitable if you need to determine the parameters that can not be determined using classical molecular dynamics, for example, spin, magnetic moment, etc. But if you focus on the configuration of the atoms and the cohesive energy of the atoms, the classical molecular dynamics of can give results closer to the experimental than methods ab-inito provide. We note that the ultimate goal of studies of the interaction of atoms (molecules, clusters) with graphene can be different. Some authors consider the graphene is bent or rolled in a tube (for example, by deposition of particles along a single line) as a result of this interaction.

In other cases, the local change of graphene, including the question of transition of graphene in graphane was reviewed. As for the atoms (molecules, clusters), which interact with graphene, the H, F, O and C atoms , metal atoms, the molecules of organic substances and clusters of metals are more often more choosen.

Our work focuses on the change in the shape of clusters $C_7$, $C_{12}$ and $C_{13}$ by reacting with nanographene and on the change cohesive energy of clusters with nanographene.

## 2. Method

The method of energy minimization is common technique to calculate the equilibrium configuration of molecules and clusters. The basic idea - a stable state of a molecular system corresponds to a local minimum of the potential energy [20]. The state with the lowest energy corresponds to the ground state, while other local minima is metastable states. In this paper we use the so-called Brenner second-generation reactive empirical bond order (REBO) potential, which is specifically parametrized for the carbon and hydrogen-carbon systems [25] How well REBO describes some characteristics of carbon carbon clusters, graphene and graphane shown in [.....]. In the same work * it was showed that the most stable cluster of seven atomic carbon clusters is ringlike cluster as well as ringlike clusters $C_5$, $C_6$, $C_8$, $C_9$ and $C_{10}$ are the most stable among the clusters of different configurations with the same number of atoms. Using the method of energy minimization models circular carbon cluster $C_7$, $C_{12}$ and $C_{13}$ were prepared, their radii and the cohesive energy of their atoms are shown in Table 1.

Graphene which hereinafter called nanographene was also was prepared by the method of minimizing the energy it is a rectangular portion 32.7x19.9Å, composed of 272 carbon atoms lying in the same plane. We note that the internal atoms of

nanographene have cohesive energy $E_h$=7.39 eV, whereas the boundary its atoms, the total number of which 48, have cohesive energy $E_{h<i>}$=4.9÷5.2 eV

After obtaining of nanographene and $C_7$, $C_{12}$ and $C_{13}$ clusters by minimizing the energy their possible interactions with each other was determined. Original location of $C_7$, $C_{12}$ and $C_{13}$ cluster was set vertically and at an angle to the nanographene: 15°, 30°, 45°, 60°, 75°, 90°, where the angles are measured from the normal to nanographene. The initial heights of ringlike clusters, which is defined as the smallest of the distances from the atom of cluster to the plane of nanographene are $h_7$ = 0.127Å, $h_{12}$ = 0.149Å and $h_{13}$ = 0.101Å. Here $h_7$, $h_{12}$ and $h_{13}$ are heights of ringlike clusters $C_7$, $C_{12}$ and $C_{13}$, respectively. Place of interaction of ringlike cluster is the center of nanographene, in order to influence ringlike clusters on the edge atoms of nanographene was minimal, which contributes to the fact that the overall results are similar to the interaction of these clusters with graphene.

When searching for the minimum energy there is a ban on breaking a large number of connections in the algorithm of the program that can be, for example, when any vacancy of atom is in nanographene. Therefore, there are some initial angles, which will be called a failure, in which the computer simulation does not determine the final configuration of the atoms. These unsuccessful angles for $C_7$, $C_{12}$ and $C_{13}$ clusters are 45°, 60° and 75°, respectively.

As a result of the interaction of ringlike clusters with nanographene geometry of these clusters is changing and often atoms of ringlike cluster do not lie in the same plane what is not observed in the interaction-free ringlike clusters. On the atomic scale nanographene and clusters are discrete and consisting of atoms, and the interaction of nanographene with cluster occurs through the formation of bonds of some of cluster atoms with atoms of nanographene. These bonds determine the cohesive energy of the entire cluster with nanographene, but these bonds are not uniquely determine the cohesive energy as in the case of the binding of a single atom with nanographene. If one atom cluster is binding with nanographene, then binding energy of this atom with nanographene good estimates cohesive energy of the entire cluster with nanographene.

If some cluster atoms of cluster bound to atoms of nanographene, we provide the maximum energy of the atom of cluster with nanographene and the sum of all the energies of atoms of cluster with atoms of nanographene, that allows us to give an estimate of the total energy of cohesion of the entire cluster with nanographene (see Table 2).

The shape of nanographene and binding energy of its atoms slightly changed as a result of interaction with ringlike clusters: form of nanographene becomes wavy, but such thing as a large bending or folding of nanographene is not observed.

## 3. Results and discussion

The free 272-atomic rectangular nanographene and circular carbon clusters $C_7$, $C_{12}$ and $C_{13}$ are presented in Fig. 1. As shown by computational simulation, the circular clusters interact with nanographene forming bonds either with one and two atoms of the cluster (see Fig. 2) or with over two atoms of the cluster (see Fig. 3). It should be noted that the cluster atoms that interact with nanographene can be none-neighboring atoms in the cluster. The characteristics of the free clusters $C_7$, $C_{12}$ and $C_{13}$ are presented in Table 1. The cohesion data of the clusters $C_7$, $C_{12}$ and $C_{13}$ interacting with nanographene are presented in Tables 2.

**Table 1.** The characteristics of the free clusters $C_7$, $C_{12}$ and $C_{13}$.

| Type of cluster | cluster radius (Å) | The cohesive energy of atoms in the cluster (эВ) |
|---|---|---|
| $C_7$ | 1.58 | 5.51 |
| $C_{12}$ | 2.59 | 5.90 |
| $C_{13}$ | 2.80 | 5.93 |

**Table 2.** The cohesion data of the clusters $C_7$, $C_{12}$ and $C_{13}$ interacting with nanographene.

| Type of cluster | Initial angle (degrees) | The maximum binding energy (eV) | The sum of binding energy (eV) | The number of atoms interacting with nanographene |
|---|---|---|---|---|
| $C_7$ | 0 | 0.78 | 1.41 | 2 |
| $C_7$ | 15 | 0.93 | 3.21 | 4 |
| $C_7$ | 30 | 1.37 | 4.66 | 4 |
| $C_7$ | 60 | 1.37 | 2.52 | 2 |
| $C_7$ | 75 | 1.38 | 2.12 | 2 |
| $C_7$ | 90 | 1.35 | 4.22 | 4 |
| $C_{12}$ | 0 | 1.51 | 2.32 | 2 |
| $C_{12}$ | 15 | 1.49 | 3.14 | 3 |

| | | | | |
|---|---|---|---|---|
| $C_{12}$ | 30 | 1.59 | 1.27 | 1 |
| $C_{12}$ | 45 | 0.84 | 3.82 | 5 |
| $C_{12}$ | 75 | 1.51 | 2.34 | 2 |
| $C_{12}$ | 90 | 1.49 | 3.35 | 3 |
| $C_{13}$ | 0 | 0.57 | 1.10 | 2 |
| $C_{13}$ | 15 | 1.27 | 5.45 | 4 |
| $C_{13}$ | 30 | 2.93 | 2.29 | 2 |
| $C_{13}$ | 45 | 1.76 | 3.16 | 2 |
| $C_{13}$ | 60 | 1.11 | 2.65 | 4 |
| $C_{13}$ | 90 | 2.02 | 5.89 | 5 |

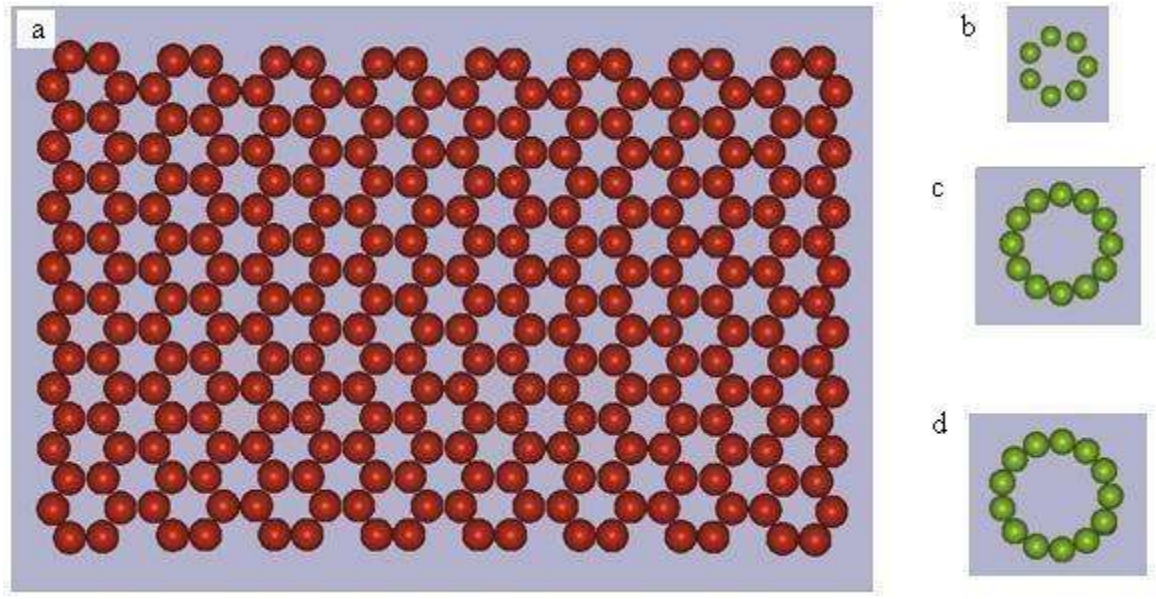


Figure 1 (Color on-line) 271-atomic rectangular nanographene and circular carbon clusters $C_7$, $C_{12}$ and $C_{13}$ are shown in plane.
It is shown in a plane: a - free 272 atomic rectangular nanographene, b - free ringlike e 7-atom carbon cluster, c - free ringlike 12-atom carbon cluster, d - free ringlike 13-atom carbon cluster.

Показано в плане: a – свободный 272 атомный прямоугольный нанографен, b – свободный круговой 7-атомный углеродный кластер, c - свободный круговой 12-атомный углеродный кластер, d - свободный круговой 13-атомный углеродный кластер.

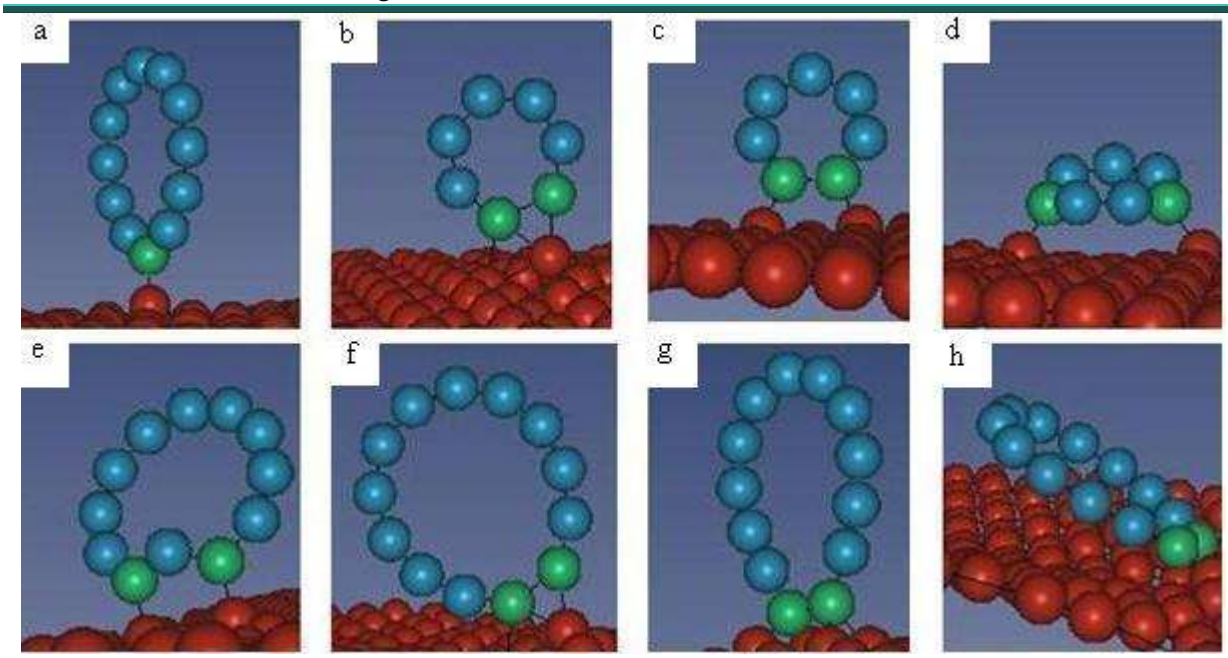


Figure 2 (Color on-line)
Interaction of clusters $C_7$ $C_{12}$ and $C_{13}$ clusters through its one or two atoms. Red circles are atoms of nanographene, blue circles are cluster atoms, green circles are cluster atoms that interact directly with nanografenom. The letters in the figures indicate the following types of clusters and initial angles of clusters α: a - $C_{12}$ и α=30°, b - $C_7$ и α=0°, c - $C_7$ и α=60°, d - $C_7$ и α=75°, e – $C_{12}$ и α=75°, f – $C_{13}$ и α=0°, g – $C_{13}$ и α=30°, h – $C_{13}$ и α=45°.

Взаимодействие кластеров $C_7$ $C_{12}$ и $C_{13}$ посредством своего одного или двух атомов. Красные кружки – атомы нанографена, синие кружки атомы кластеров, зеленные кружки – атомы кластера, непосредственно взаимодействующие с нанографеном. Буквы на рисунках указывают на следующие типы кластеров и первоначальные углы наклона кластеров α: a - $C_{12}$ и α=30°, b - $C_7$ и α=0°, c - $C_7$ и α=60°, d - $C_7$ и α=75°, e – $C_{12}$ и α=75° и $C_{12}$ и α=75° и , f – $C_{13}$ и α=0°, g – $C_{13}$ и α=30°, h – $C_{13}$ и α=45°

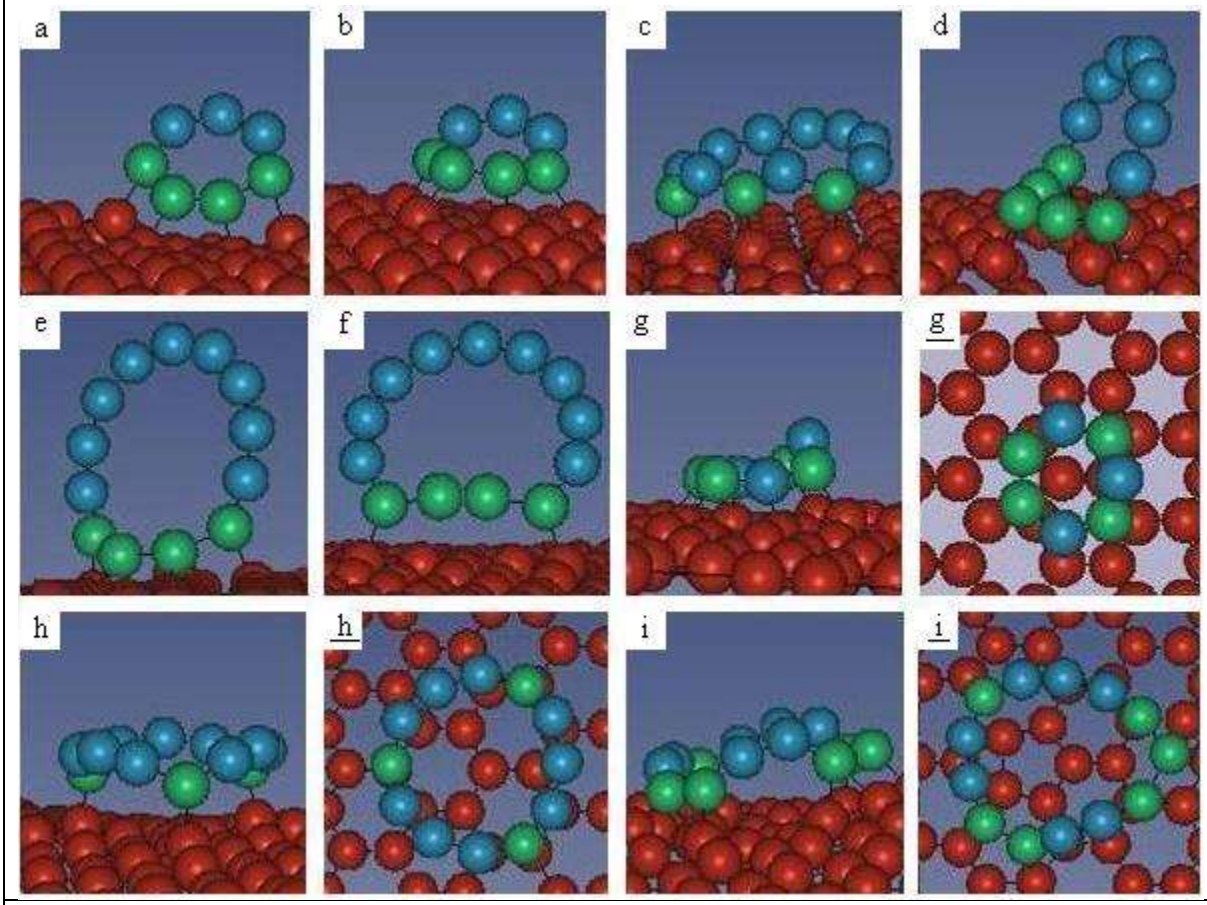


Figure 3 (Color on-line) Interaction of clusters $C_7$, $C_{12}$ and $C_{13}$ through its more than two atoms. Red circles are atoms of nanographene, blue circles are cluster atoms, green circles are cluster atoms that interact directly with nanografenom. The letters in the figures indicate the following types of clusters and initial angles of clusters α: a – $C_7$ и α=15°, b - $C_7$ и α=30°, c – $C_{12}$ и α=15°, d – $C_{12}$ и α=45°, e – $C_{13}$ и α=15°, f – $C_{13}$ и α=60°, g – $C_7$ и α=90°, h – $C_{12}$ и α=90°, i – $C_{13}$ и α=90°. Underlined g, h and i indicate that images of corresponding clusters is given in the plane

Взаимодействие кластеров $C_7$ $C_{12}$ и $C_{13}$ посредством своих более чем двух атомов. Красные кружки – атомы нанографена, синие кружки атомы кластеров, зеленные кружки – атомы кластера, непосредственно взаимодействующие с нанографеном. Буквы на рисунках указывают на следующие типы кластеров и первоначальные углы наклона кластеров α: a – $C_7$ и α=15°, b - $C_7$ и α=30°, c – $C_{12}$ и α=15°, d – $C_{12}$ и α=45°, e – $C_{13}$ и α=15°, f – $C_{13}$ и α=60°, g – $C_7$ и α=90°, h – $C_{12}$ и α=90°, i – $C_{13}$ и α=90° Подчеркнутые g, h и i указывают, что изображение соответствующих кластеров дано в плане

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