

## Calculation of the Structure of Carbon Clusters Based on Fullerene-Like $C_{24}$ and $C_{48}$ Molecules

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**Abstract**—Equilibrium structures obtained by linking with valence bonds the carbon carcasses of two fullerene-like molecules have been studied by molecular dynamics simulation. In free fullerene, carbon atoms form  $sp^2$  hybridized bonds, but at places of links between fullerenes,  $sp^3$  hybridized bonds are formed, which determines the changes in the properties of such structures. In the literature, the topology of diamond-like phases is described, but equilibrium clusters based on fullerene-like molecules are underexplored. The right angles between the C–C bonds are energetically unfavorable, and the reduction in the energy of clusters in the process of relaxation is connected with the optimization of valence angles, which leads to a reduction in the symmetry of clusters and, in a number of cases, even to disruption of some valence bonds. It is shown that different fashions of linking two fullerenes result in the formation of clusters with different structures and energies. Different initial conditions can lead to different configurations of clusters with the same topology. Among the analyzed clusters, a structure with the minimum potential energy per atom was found. The results of this work contribute to the study of the real structure of carbon clusters.

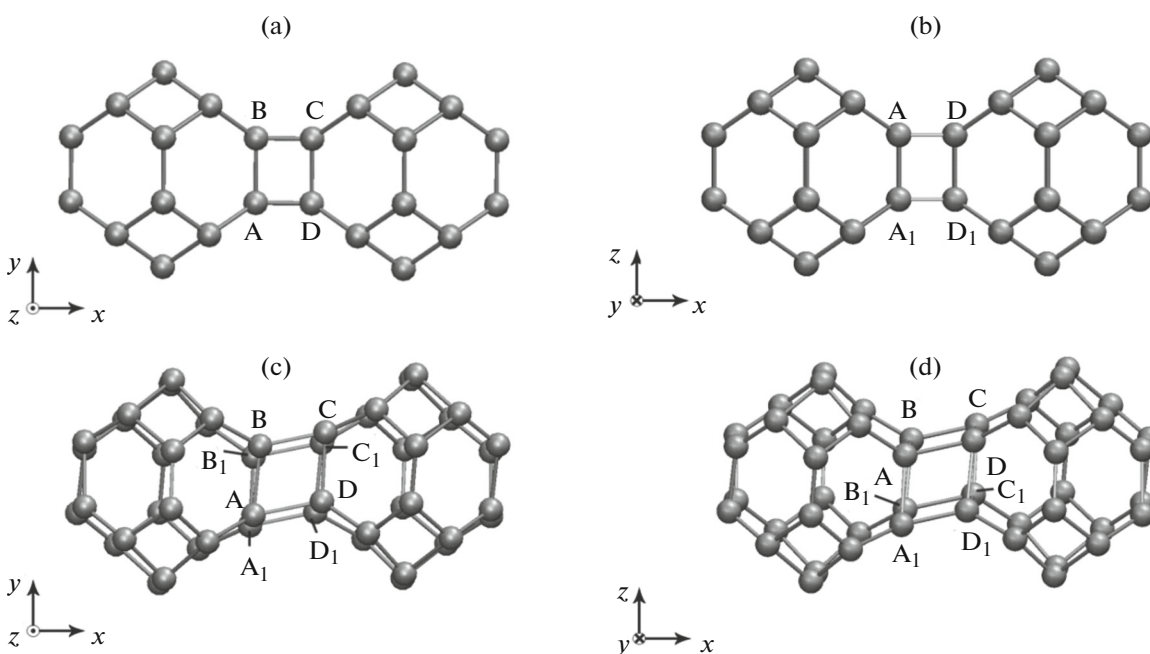
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### 1. INTRODUCTION

Fullerenes, whose 1985 synthesis [1] was awarded a Nobel Prize, possess unique physical properties, which open wide possibilities of their various application [2–6]. For example, fullerenes with metal inclusions (so-called fullerides) are magnetic dipoles, which may be used for the creation of new high-capacity information carriers. Compounds of fullerenes with radioactive elements can be used in medicine as anticancer drugs. A small addition of fullerene soot improves antifriction and antiwear properties of metals [7].

The discovery of new unusual properties of fullerenes extends the range of their application and, therefore, the demand for synthesizing novel materials on their basis [8–10]. An example is diamonds, in which one part of the carbon atoms have the coordination number  $k = 4$  and  $sp^3$  hybridization, inherent in crystalline diamond, and the other part of the carbon atoms have the coordination number  $k = 3$  and  $sp^2$  hybridization, inherent in graphite, fullerenes, carbon nanotubes, and graphene. There are different methods for the synthesis of nanodiamonds [11]. Nanodiamonds, which comprise clusters of fullerenes connected by valence bonds, can form various structures.

For example, being deposited onto a substrate, they can form either unordered (amorphous) films or various densely packed lattices the main properties of which are a large number of atoms of an elementary cell, large lattice parameters, and significant molecular interstices. These materials attract attention as antifriction materials and oil additives and as materials for metal-diamond strengthening coating [12]. Nanodiamonds hold promise for application in medicine and biology. At present, several diamond-like carbon phases have been experimentally synthesized and theoretically studied, e.g., cubic diamond [13], the hexagonal polytype of diamond (the 2H polytype: lonsdaleite) [14], polymerized cubic fullerite  $C_{24}$  [15, 16], and the high-density  $C_8$  carbon phase [17]. In [18], a new scheme of the structural classification of carbon phases and nanostructures was proposed; it is based on the types of chemical bonds forming in the materials and the number of nearest atoms with which each carbon atom forms covalent bonds. A number of diamond-like phases were predicted as a result of theoretical analysis. For example, by the method of density functional theory, the optimized structure of ten carbon diamond-like phases was calculated and their parameters and some properties were determined [19,



**Fig. 1.** Initial (a, b) and equilibrium (c, d) structures of the CA4 phase formed by linking fullerenes  $C_{24}$  in projections onto the planes  $xy$  (a, c) and  $xz$  (b, d).

20]. Stable structures of diamond-like phases obtained from nanotubes and bulk graphites were calculated from the first principles [21]. In [22], for the first time, it was suggested to obtain the nanodiamond phase from polymerized nanotubes (4, 0), i.e., covalent-bound nanotubes (4, 0). As a result of calculations, it was established that a crystal of polymerized nanotubes is a semiconductor with a band gap of 3.18 eV [22]. By the molecular dynamics methods, the structures of carbinoid layers, carbinoid nanotubes, and carbyne fullerenes were studied and their basic characteristics were obtained [23]. A number of structures were obtained by chemical synthesis: for example the dimer  $C_{120}$ , consisting of fullerenes  $C_{60}$ , and the dimer  $C_{130}$ , consisting of fullerenes  $C_{60}$  and  $C_{70}$  [24]. Polymers based on fullerene  $C_{60}$  are being actively studied [25, 26]. For example, the influence of hydrostatic pressure on the cluster formation from fullerenes  $C_{60}$  was studied and it was shown that application of pressure leads to formation of dimers, whereas an increase in temperature leads to their destruction [25].

Earlier, a hypothesis was asserted of the possible existence of diamond-like phases, which can be obtained by linking by valence bonds carbon carcasses of fullerene-like molecules, e.g.,  $C_{24}$  and  $C_{48}$ . Theoretical models of such phases and the conditions for their existence in a nonequilibrium state were considered in [15, 27, 28]. However, the equilibrium configurations of such structures are studied insufficiently and, therefore, it is an urgent problem to study them.

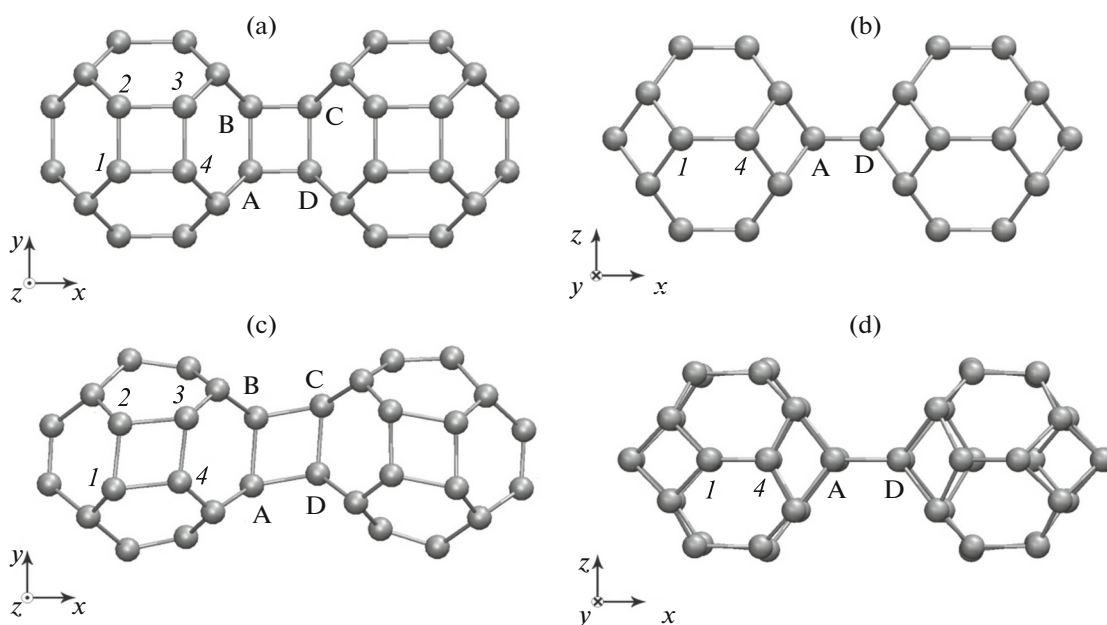
In the present work, with the aid of molecular dynamics (MD) simulation, we obtained equilibrium

structures of diamond-like phases synthesized on the basis of fullerene-like molecules  $C_{24}$  or  $C_{48}$ , named, for brevity, fullerenes. It should be noted that, nowadays, the method of MD simulation is widely used for studying the structure and properties of metallic and nonmetallic nanodimensional materials [29–34], including fullerenes, carbon nanotubes, and graphene sheets [35–39].

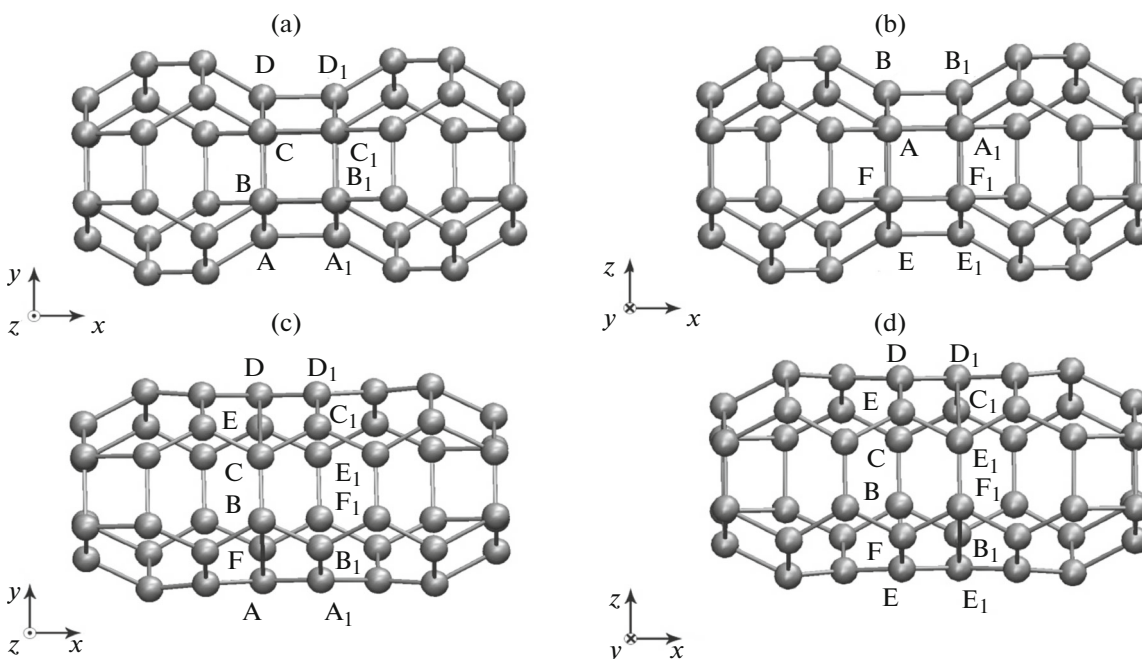
## 2. METHODS

According to [28], the same fullerene can be used for creating different cluster structures. In the present work, we consider three variants of linking by valence bonds fullerene-like molecules  $C_{24}$  and two variants of linking  $C_{48}$  molecules.

In the first case, we mean the structures CA4 (Figs. 1a, 1b), CA6 (Figs. 2a, 2b), and CA9 (Fig. 3a, 3b) and, in the second case, CA4 (Fig. 4a, 4b) and CA7 (Fig. 5a, 5b). The name of a structure corresponds to the type of interconnection of fullerenes; for example, the CA4 structure is obtained by linking via a square face, CA6, by linking via an edge, CA7, via an octahedron, and CA9, via a hexahedron. The lengths of four carbon bonds ( $L_1, L_2, L_3, L_4$ ) of the clusters were taken from [28]. To obtain equilibrium structures of diamond-like structures and estimate their potential energies, we used the freely distributed LAMMPS program complex for MD simulation [40]. The atomic interaction was described by the AIREBO potential [41], which involves multiparticle valence interactions between carbon atoms and the Van der Waals long-



**Fig. 2.** Initial (a, b) and equilibrium (c, d) structures of the CA6 phase formed by linking fullerenes  $C_{24}$  in projections onto the planes  $xy$  (a, c) and  $xz$  (b, d).

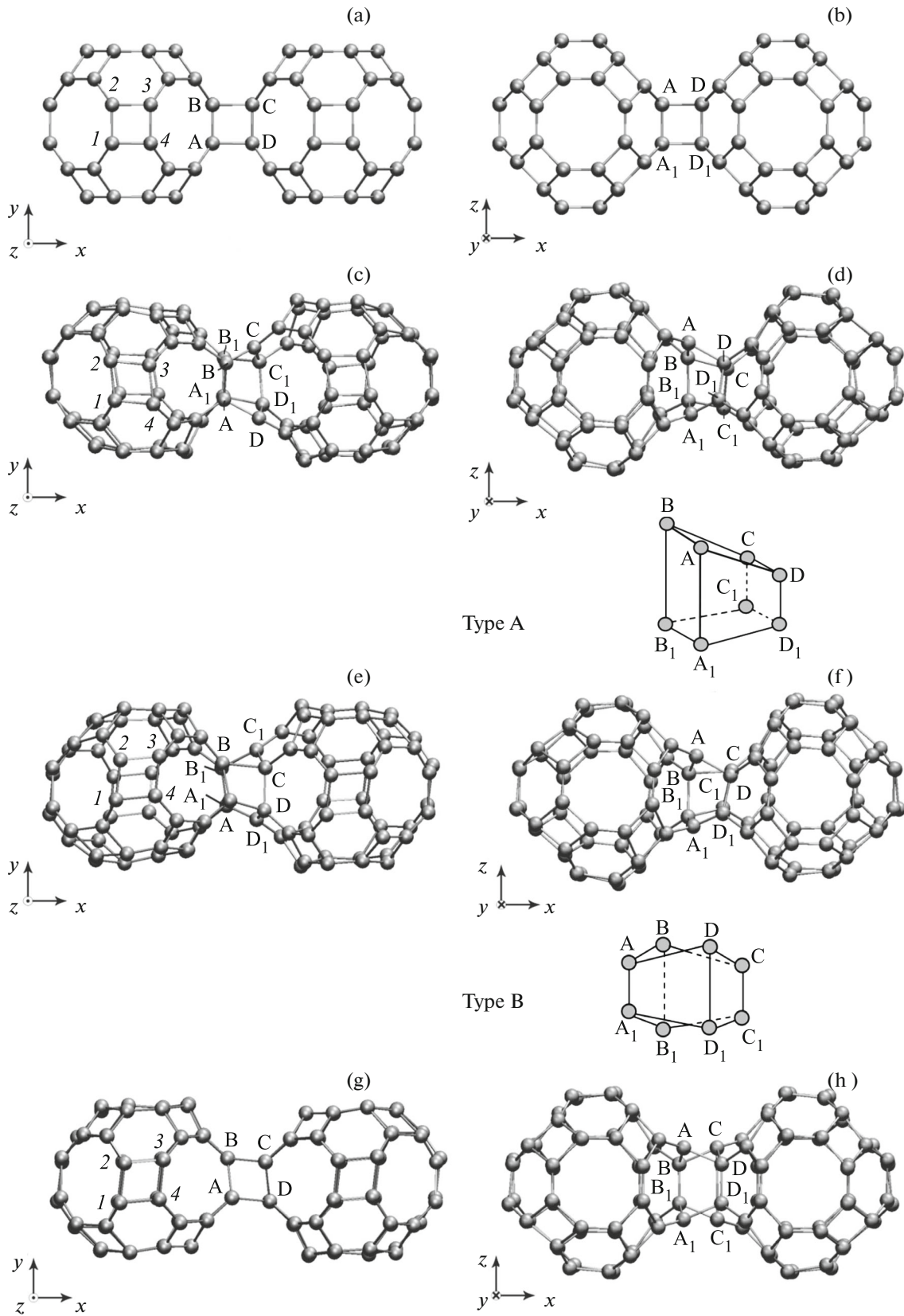


**Fig. 3.** Initial (a, b) and equilibrium (c, d) structures of the CA9 phase formed by linking fullerenes  $C_{24}$  in projections onto the planes  $xy$  (a, c) and  $xz$  (b, d).

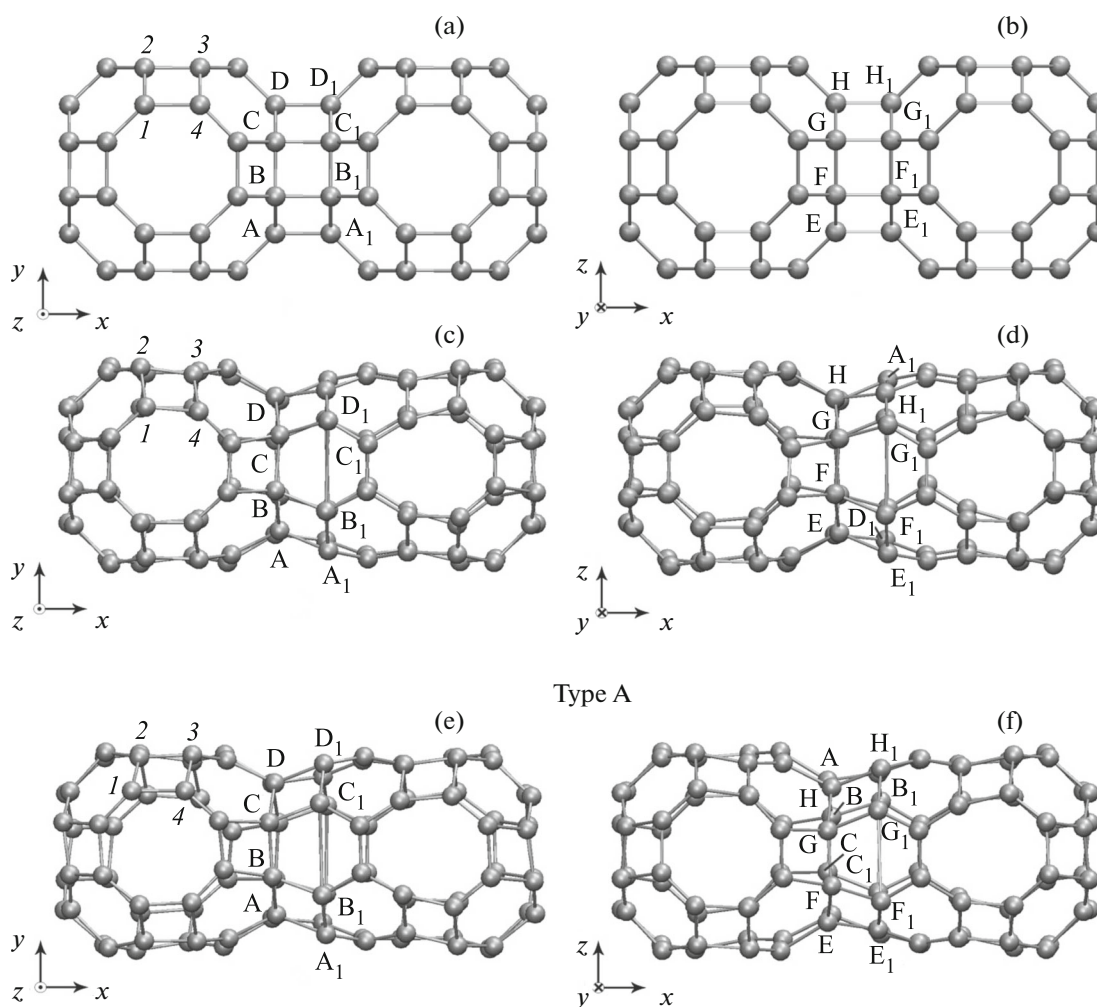
range interactions described by the Lennard–Jones pair potential. These potentials remove some errors of the REBO potential [42], earlier applied for the MD simulation of elastic and plastic deformation of graphene, fullerenes, and carbon nanotubes. The AIREBO potential is widely used for simulation of deformation processes of single- and multilayer

graphene sheets [43, 44], contorted graphene [36, 45], carbon nanotubes [37, 46], and fullerenes [35, 36]. The data obtained with this potential agrees well with the results of experiments and ab initio calculations.

To obtain the equilibrium state of the considered structure, the energy of the system was minimized by



**Fig. 4.** Initial (a, b) and equilibrium (c, d) structures of the diamond-like cluster CA4 obtained by linking fullerenes  $C_{48}$  in projections onto the planes  $xy$  (a, c) and  $xz$  (b, d). The relaxed structure of cluster CA4 of type A (e, f) and type B (g, h) in two projections.



**Fig. 5.** Initial (a, b) and equilibrium (c, d) structures of the diamond-like cluster CA7 obtained by linking fullerenes  $C_{48}$  in projections onto the planes  $xy$  (a, c) and  $xz$  (b, d). Equilibrium modified structure CA7 of type A (e, f) in two projections.

the multiple correction of coordinates of atoms by the gradient descent method, which terminated if the variation in the energy or force was less than a given small value. At this moment, the system reached its local or global minimum of the potential energy; the result may depend on the initial configuration of the system.

### 3. RESULTS

#### 3.1. Diamond-Like Clusters

##### Based on Fullerene-Like $C_{24}$ Molecules

Let us consider a CA4 molecule formed by linking two  $C_{24}$  fullerenes via a square face. Figure 1 shows the structure of the molecule before (Figs. 1a, 1b) and after (Figs. 1c, 1d) relaxation in projections onto the planes  $xy$  (Figs. 1a, 1c) and  $xz$  (Figs. 1b, 1d). Carbon atoms A, B, C, and D (see Fig. 1a), which form four valence bonds, in the initial state, are bound to each other at a right angle [28], but, after relaxation, the angles between the valence bonds deflect from  $90^\circ$  (Figs. 1c, 1d).

Now let us consider a diamond-like cluster CA6 formed by linking two fullerenes  $C_{24}$  via the edges AB and CD of the hexahedron with the structure shown in Fig. 2 before (Figs. 2a, 2b) and after (Figs. 2c, 2d) relaxation in projections onto the planes  $xy$  (Figs. 2a, 2c) and  $xz$  (Figs. 2b, 2d). By analogy with the above-considered cluster CA4, in the structure of CA6, after relaxation, the square ABCD is transformed into a parallelogram (Figs. 2a, 2c). The initial structure of fullerene  $C_{24}$  also contains atoms (e.g., 1–4 in Fig. 2) linked by valence bonds at an angle of  $90^\circ$ . In the process of relaxation, these atoms shift and form a rhomb (Fig. 2c). A similar transformation of squares in fullerene  $C_{24}$  was observed in relaxation of the cluster CA4. In both cases, the transformation of the structure on relaxation results in a slight elongation (compression) along the axis  $x(y)$ .

Figure 3 shows the structural compound CA9 [28], formed by linking fullerenes  $C_{24}$  via hexahedra (in Figs. 3a and 3b, they are denoted by ABCDEF and

$A_1B_1C_1D_1E_1F_1$ ). Relaxation of the diamond-like cluster CA9 leads to disruption of two carbon bonds,  $B_1C_1$  and  $EF$ , and the initial structure is transformed to the phase presented in Figs. 3c and 3d, which have a symmetric structure. This structure can be classified as a carbon nanotube with closed ends, in which all carbon atoms have three  $sp^2$ -hybridized valence bonds.

### 3.2. Diamond-Like Clusters Based on Fullerene-Like $C_{48}$ Molecules

The structure of the diamond-like cluster CA4 obtained by linking fullerene  $C_{48}$  via the square phase is shown in Fig. 4 in the initial (Figs. 4a, 4b) and relaxed (Figs. 4c, 4d) states in projections onto the planes  $xy$  (Figs. 4a, 4c) and  $xz$  (Figs. 4b, 4d). By analogy with the diamond-like clusters CA4 (Fig. 1) and CA6 (Fig. 2), obtained by linking fullerenes  $C_{24}$ , carbon atoms forming squares, e.g., ABCD or 1234 (Fig. 4a), change their positions and form parallelograms (Fig. 4c). It should be noted that the equilibrium structure of the diamond-like cluster CA4 based on fullerene  $C_{24}$  (Figs. 1c, 1d) is more symmetric than the structure of the CA4 cluster based on fullerene  $C_{48}$  (Figs. 4c, 4d), although, in both cases, due to the transformation of the structure, relaxation leads to elongation (compression) of the cluster along the axis  $x(y)$ . However, in contrast to the CA4 cluster based on fullerene  $C_{24}$ , in the CA4 cluster based on  $C_{48}$ , the disruption of the carbon bonds CD and  $AA_1$  is observed (see Figs. 4c, 4d).

Figures 4c and 4d show the equilibrium structure obtained by relaxation of the "ideal" structure of a higher symmetry. The new low-symmetric structure is formed due to the development of a small (within the rounding error) asymmetry of the molecule. To obtain other possible configurations, calculations with a varied initial geometry of the molecule were performed in order to find equilibrium configurations having the topology of the initial structure—in other words, to avoid the disruption of valence bonds in relaxation. For the diamond-like cluster CA4 based on fullerene  $C_{48}$ , before relaxation, the cubic structure of atoms ABCDA<sub>1</sub>B<sub>1</sub>C<sub>1</sub>D<sub>1</sub> is turned into a truncated pyramid (type A) or into a complex figure (type B). These deviations of atoms in the initial state is inherited in the relaxed structures shown in Figs. 4e, 4f and 4g, 4h, respectively, in the projections onto the planes  $xy$  (Fig. 4e, 4g) and  $xz$  (Fig. 4f, 4h). It turned out that the relaxation of modified structures CA4 of type A and type B also leads to disruption of bonds as on the relaxation of the initial structure (in Figs. 4f and 4h, we see a disrupted bond  $AA_1$ ). However, the diamond-like cluster CA4 of type B (Figs. 4g, 4h) has a more symmetric equilibrium form than that of the clusters presented in Figs. 4c, 4d and 4e, 4f. Thus, we failed to find an equilibrium configuration of the diamond-like cluster CA4 based on fullerene  $C_{48}$  preserving the ide-

alized topology shown in Figs. 4a and 4b. Nevertheless, in all relaxed structures, carbon atoms with four valence bonds remain. It should be noted that our calculations cannot prove the absence of equilibrium structures with the topology shown in Figs. 4a and 4b. Possibly, there is an initial configuration preserving this topology after relaxation. The search of the initial condition at which no disruption of bonds occurs requires further efforts.

The most complex structure as compared to the above-considered ones is the structure of the diamond-like cluster CA7, which has the maximum number of  $sp^3$ -hybridized carbon atoms at the place of linking of fullerenes  $C_{48}$  (Figs. 5a, 5b). Figures 5c and 5d show the equilibrium structure obtained as a result of relaxation of the initial structure CA7 with perturbations on the order of the rounding error. It is evident from the figure that, in contrast to the above-considered structures, the valence bonds making right angles and forming a square can transform not to a parallelogram but to an isosceles trapezoid as, e.g., the square BCC<sub>1</sub>B<sub>1</sub>. No disruption of valence bonds in the process of relaxation of the structure CA7 was observed. However, the deviation of the angles between valence bonds from  $90^\circ$  on relaxation is observed in all studied diamond-like clusters, due to which their structure is asymmetric. The variation in the initial conditions for the structure CA7 has not raised the symmetry in the equilibrium state. For example, the rotation of the plane ABCD with respect to  $A_1B_1C_1D_1$  by  $10^\circ$  (Figs. 5a, 5b) has influenced weakly the form of the equilibrium structure shown in Figs. 5e and 5f.

## 4. DISCUSSION

Since the equilibrium angles between  $sp^3$ -hybridized valence bonds in the diamond crystal equal  $109.47^\circ$ , it might be expected that, in the most stable configuration, the angles near atoms with four neighbors in the structures under consideration will tend to this value. The analysis of all analyzed structures has shown that the formation of stable configurations is connected with the reduction in the symmetry of the idealized structures and, moreover, can be accompanied by disruption of some valence bonds. Most frequently, the atoms remaining in the structure have four valence bonds, but the relaxation of the structure CA9 led to the formation of a structure similar to a carbon nanotube with closed ends, in which all atoms have three valence bonds (see Fig. 3).

For all analyzed clusters consisting of  $N$  atoms, the total potential energy  $P_\Sigma$  after relaxation of the structure was found. In addition, the energy of one C–C bond in diamond,  $P_0 = 3.725$  eV, has been calculated. For the analyzed structure, the table presents the values of  $P_\Sigma$  and  $P = P_\Sigma/N - 1.5P_0$ , where  $1.5P_0$  is an estimate of the energy of one atom having three C–C valence bonds. Thus, the quantity  $P$  characterizes the

Potential energy of the system after relaxation of diamond-like phases

Fullerene	Diamond-like structure		$P_{\Sigma}$ , eV	$N$	$P = P_{\Sigma}/N - 1.5P_0$ , eV/atom
$C_{24}$	CA4	Initial structure	280.29	48	0.252
	CA6	Initial structure	282.38	48	0.296
	CA9	Initial structure	308.21	48	0.834
$C_{48}$	CA4	Initial structure	589.31	96	0.682
		Type A	589.08	96	0.680
		Type B	589.80	96	0.687
	CA7	Initial structure	600.61	96	0.802
		Type A	600.40	96	0.800

difference specific potential energy of cluster with respect to diamond. The comparison of the values of the potential energy per atom for diamond-like clusters obtained from  $C_{24}$  shows that the minimum energy  $P$  is inherent in the structure CA4 and the maximum energy, in CA9 ( $P_{CA4} = 5.839$  eV/atom and  $P_{CA9} = 6.421$  eV/atom, respectively). From the comparison of the potential energies per atom of the diamond-like cluster of fullerene  $C_{48}$ , we see that the structure CA4 also possesses the minimum value of  $P$ . It should be noted that the potential energy  $P$  for CA4 and CA7 obtained by linking of  $C_{48}$  is almost independent of the topology.

## 5. CONCLUSIONS

Equilibrium diamond-like clusters with the structures CA4, CA6, CA7, and CA9, obtained by linking fullerenes  $C_{24}$  and  $C_{48}$  were studied by molecular dynamics methods.

It has been found that the relaxation of idealized initial forms of diamond-like clusters CA4 and CA6 obtained by linking fullerenes  $C_{24}$  does not lead to the disruption of valence bonds but leads to a reduction in the symmetry due to deviation of the angles between valence bonds from  $90^\circ$  (see Figs. 1 and 2). The formation of an equilibrium structure in the process of relaxation of the diamond-like cluster CA9 also obtained by linking fullerenes  $C_{24}$  leads to the disruption of some valence bonds between atoms with the coordination number  $k = 4$  and to formation of a symmetric cluster in which all carbon atoms have three valence bonds (see Fig. 3).

On the relaxation of the diamond-like molecule CA4 obtained by linking fullerenes  $C_{48}$  via square face, the disruption of several bonds between atoms with the coordination number  $k = 4$  always occurs but a fraction of atoms preserves four valence bonds (see Fig. 4). No disruption of valence bonds was observed in the equilibrium structure CA7, obtained by linking fullerenes  $C_{48}$  via octahedra (see Fig. 5).

In the initial idealized structure of all analyzed diamond-like clusters, some valence bonds make

right angles with one another but the relaxation of such a structure has led to a deviation of all these angles from  $90^\circ$ . Square faces can transform either into parallelograms or into isosceles trapezoids. The analysis has shown that, after relaxation of the structure, the minimum potential energy per atom is inherent in the diamond-like clusters CA4 obtained by linking fullerenes  $C_{24}$  or  $C_{48}$  via an edge and, therefore, such linking of fullerenes is more energy favorable than the linking via any face.

It should be noted that different fullerenes can be linked by valence bonds for the creation of two- and three-dimensional quasi-periodic structures, forming so-called diamond-like structures. The data obtained in this work give an idea of possible ways of relaxation of such structures on the example of paired clusters. The properties of bulk systems based on fullerenes are known sufficiently well, but the functional properties of the structures in which fullerenes and fullerene-like molecules are connected by a covalent rather than Van der Waals bond can strongly differ from the properties of traditional fullerenes. Interesting properties of such diamond-like phases are a large surface area and porosity, which promise their application as material for catalysis, storage, and transportation of hydrogen. The results of this work are preliminary. A more accurate calculation of equilibrium diamond-like structures should be carried out by a more computation-expensive method based on the density functional theory. The comparison of the results obtained in this work with the results of the first-principle calculations will enable one to make conclusions on the accuracy of the AIREBO interatomic potential. However, the data of this work agree well with the experimental results known from the literature, obtained for other fullerenes, e.g.,  $C_{60}$  [24, 25]. In the experimental works, stable dimers of fullerenes and other stable structures based on fullerenes have been obtained. Intensive experimental studies of such structures have been performed in the last decades, but concern only the well-known fullerenes  $C_{60}$  and  $C_{70}$ . Therefore, theoretical studies of dimers of other fullerene-like molecules are an important and urgent problem.

## ACKNOWLEDGMENTS

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