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ADSORPTION OF C_{60} FULLERENE ON DEFECT-FREE GRAPHENE

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Нуқсонсиз графен сиртига фуллерен C_{60} нинг турли усулидаги адсорбцияси Бреннер потенциали доирасида компьютерда моделлаштириш методи билан тадқиқ этилди. Адсорбция оралиғи ва энергия боғланишлари олинди. Шунингдек фуллерен адсорбция-сининг геометрик ўзгариши адсорбцияланиш усулига боғлиқлиги тадқиқ этилди.

Методами компьютерного моделирования в рамках потенциала Бреннера исследованы разные способы адсорбции фуллерена C_{60} на поверхности бездефектного графена. Были получены энергии связи и дистанция адсорбции, а также исследовано изменение геометрии адсорбированного фуллерена в зависимости от способа адсорбции.

Different ways of C_{60} fullerene adsorption on surface of defect-free graphene have been studied by the methods of computer simulation within the framework of the Brenner potential. The energies of binding and distance of adsorption have been obtained. It has been also studied how geometry of adsorbed fullerene depends on a way of adsorption.

Fullerenes are an independent allotropic form of carbon as isolated molecules of that are self-organized in the form of convex closed polyhedrons composed from the even number of three-coordinated atoms of carbon. Defect-free fullerenes consist of geometrically regular hexagons (Fig. 1*a*) and geometrically regular pentagons (Fig. 1*b*) and defect-free graphene is composed of hexagons only (Fig. 2).

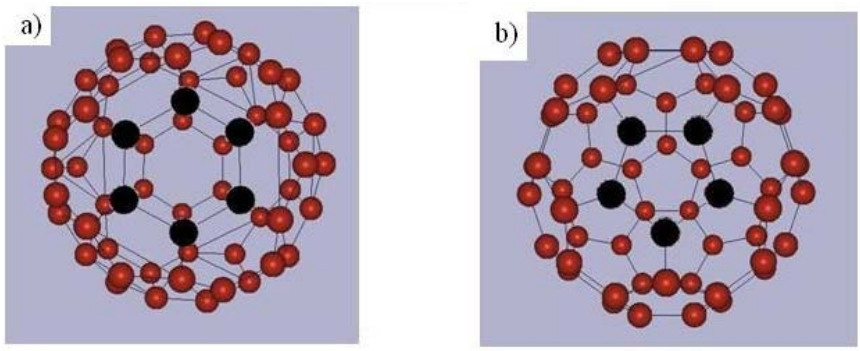


Fig. 1. Atomic structures as an example of C_{60} fullerene: hexagon (*a*) and pentagon (*b*) marked by black circles.

The number of carbon atoms (n) in fullerene obeys some regularity, namely n = 32, 44, 50, 58, 60, 70, 72, 78, 80, 82, 84 etc. The most stable fullerene has 60 atoms of carbon and is denoted as C_{60}. The fullerene C_{70} differs from C_{60} fullerene by inserting 10 carbon atoms into the equatorial region of C_{60}; as a result, the C_{70} molecule becomes elongated

and like a rugby ball. The fullerenes containing the greater number of carbon atoms (up to 400) are formed in much smaller amounts and often they have a rather complex isomeric composition.

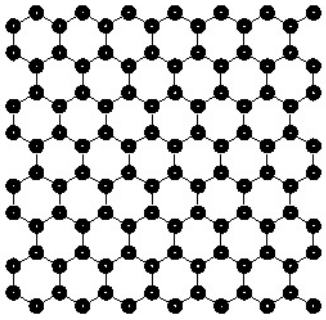


Fig. 2. Atomic structure of defect-free 112-atomic rectangular graphene consisting of just hexagons under periodical boundary conditions.

Among fullerenes, C_{60} has the highest symmetry and the highest stability. It is formed by 20 hexagons and 12 pentagons with carbon atoms at their vertices. Another structural feature of this fullerene is that it has an internal cavity whose diameter, taking into account the size of the carbon atoms, is about 5 Å; owing to that the atoms of other elements or even small molecules can be inside the fullerene.

The unique possibility of fullerene is broadening when fullerene is combined with other atoms and molecules, and endofullerenes are of special interest when additional atoms, for example, alkali metal ones, are in the inner cavity of fullerene. However, the practical application of fullerenes and endofullerenes in nanoengineering is depends on what substrate will be used for fullerene structures. Such substrates can be the surfaces of silicon carbide crystals, silicon, diamond and graphene Latter, in view of miniaturization, is more successful since its thickness is one atomic layer. In addition, defect-free graphene having a two-dimensional hexagonal carbon crystalline lattice (Fig. 2) is a unique object with distinctive physical properties [1] and can be selected as a substrate for integrated chips. In the present work, the adsorption of fullerene C_{60} onto the surface of defect-free graphene is studied by computer simulation within the framework of classical molecular dynamics.

First, a computer model of a single defect-free C_{60} fullerene was built by the energy minimization method using the second-generation Brenner potential (REBO) well describing the carbon structures [2]. It was found that the cohesive energy of each carbon atom in the fullerene is equal to 6.8 eV. Then, a computer model of defect-free rectangular graphene consisting of 112 carbon atoms was constructed (Fig. 2, the details and model validation see [3]) by the same method of energy minimization using the Brenner potential with periodic conditions for boundary atoms. As a result, a computer model of graphene with cohesion energy of 7.4 eV was obtained; that cohesion energy value is more than that of fullerene atoms, which indicates that graphene is a "stronger" structure than fullerene.

After the computer models of single defect-free fullerene C_{60} and graphene were obtained, the adsorption of this fullerene on graphene was studied as well as how these structures change as a result of adsorption. For this purpose, the models obtained were disposed at a necessary distance with a different set of fullerene locations with respect to the central part of the graphene surface. A method of energy minimization with the Brenner potential and periodic boundary conditions were used for calculation. It was found that the adsorption of fullerene C_{60} on graphene can be realized in different ways. Here only 5 selected adsorption methods are listed [4]:

I) interaction of one fullerene atom and one graphene atom (C-ATP);

II) interaction of fullerene hexagons and graphene hexagons (C-RING);

III) interaction of two neighboring atoms of fullerene and two neighboring atoms of graphene (BRI);

IV) interaction when the fullerene hexagon center is located over the graphene atom (C-RING2);

V) interaction of two non-neighboring atoms of fullerene and two non-neighboring atoms of graphene.

The geometric characteristics of adsorbed fullerene obtained by analyzing the results of computer simulation of the above 5 ways of adsorption are presented in Table 1.

Table 1. Geometric characteristics of C_{60} fullerene adsorbed on graphene.

	Way of adsorption				
	I C-ATP	II C-RING	III BRI	IV C-RING2	V
Radius averaged, Å	3.60	3.61	3.60	3.61	3.60
Radius maximal, Å	3.91	3.98	3.91	3.88	3.88
Radius minimal, Å	3.53	3.50	3.50	3.48	3.47
Ratio of maximal radius to minimal one	1.108	1.137	1.117	1.115	1.118

Since the radius of free fullerene C_{60} is equal to 3.60 Å and owing to spherical symmetry the maximal and minimal radii are equal (their ratio is 1), then according to Table 1 and as a result of adsorption, the spherical symmetry of C_{60} fullerene violates and this violation of symmetry depends on a way of adsorption.

The values binding energy and adsorption distance for adsorbed C_{60} fullerenes were obtained and they were compared with the available experimental and theoretical results (Table 2). In [5], no taking into account a way of adsorption, it was experimentally obtained that the energy of binding C_{60} fullerene with graphene is 0.85 eV and the least distance between the atoms of C_{60} fullerene and those of graphene is 2.9 Å. This distance

Table 2. Comparison of the results obtained with Brenner potential and with the first-principle calculations and experimental data.

	Way of adsorption	Calculation method				Exp. [5]
		Brenner potential	First-ptinciple [4]			
			PBE	PBE-D2	optB86b	
Bounding energy, эВ	I) C-ATP	1.08	0.15	0.91	1.28	0.85 eV
	II) C-RING	0.77	0.13	0.83	1.17	
	III) BRI	1.07	0.13	0.84	1.20	
	IV) C-RING2	0.06	0.13	0.90	1.23	
	V)	0.84	-	-	-	
Adsorption distance, Å	I) C-ATP	2.62	3.50	2.82	2.81	2.9 Å
	II) C-RING	2.69	3.79	3.32	3.35	
	III) BRI	2.69	3.57	3.10	3.14	
	IV) C-RING2	2.19	3.53	3.15	3.16	
	V)	2.22	-	-	-	

is considered as an experimentally measured value of the adsorption distance. In [4] by the three first-principle methods PBE, PBE-D2, optB86b the binding energy and adsorption distance were obtained for the ways of adsorption from I to IV (adsorption way V and geometrical changes of adsorbed C_{60} fullerene are not presented in this work).

As seen from Table 2, our results are in agreement with experimental data and with the results of first-principle methods PBE-D2, optB86b. It should be noted that the best way of adsorption is way I because adsorbed fullerene has the highest energy of binding with graphene and fullerene is less deformed as a result of its interaction with graphene.

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REFERENCES

1. A.K. Geim, K.S. Novoselov, Nature Mater. **6**, 183 (2007).
2. D.W. Brenner, O.A. Shenderova, J.A. Harrison, S.J. Stuart, B. Ni, S.B. Sinnot, J. Phys: Condens. Matter. **14**, 783 (2002).
3. A.A. Dzhurakhalov, F.M. Peeters, Carbon **49**, 3258 (2011).
4. S. Laref, A.M. Asaduzzaman, W. Beck, P.A. Deymier, K. Runge, L. Adamowicz, K. Muralidharan, Chemical Physics Letters **582**, 115 (2013).
5. H. Ulbricht, G. Moos, T. Hertel, Phys. Rev. Lett. **90**, 095501 (2003).