EAST EUROPEAN JOURNAL OF PHYSICS. **3.** 273-280 (2025)
DOI:10.26565/2312-4334-2025-3-24 ISSN 2312-4334

COMPUTER SIMULATION STUDY OF ADSORPTION PROCESSES OF C_{20}@C_n AND C_{60}@C_n (n=1-5) CARBON CLUSTERS ON RECONSTRUCTED SILICON Si(001) SURFACE

Ikrom Z. Urolov[a,b], Farid F. Umarov[c], Ishmumin D. Yadgarov[a]*, Ganiboy T. Rakhmanov[b], Khayitmurod I. Jabborov[d,e]

[a]U.A. Arifov Institute of Ion-Plasma and Laser Technologies, Academy of Sciences of the Republic of Uzbekistan, 100125, Tashkent, str. Durmon Yuli, 33
[b]Mirzo Ulugbek National University of Uzbekistan, Republic of Uzbekistan, 100174, Tashkent, Universitetskaya str., 4
[c]Kazakhstan-British Technical University, Almaty, str. Tole bi 59, Kazakhstan
[d]Tashkent state technical university named after Islam Karimov, Tashkent, Uzbekistan
[e]Tashkent University of information technologies named after Muhammad al-Khwarizmi, Tashkent, Uzbekistan
**Corresponding Author E-mail: ishmuminyadgarov@gmail.com*

Received March 27, 2025; revised June 17, 2025; accepted June 23, 2025

In today's nanotechnology field, one of the requirements of the current direction is the ability of carbon nanostructures to have a strong bond with the substrate surface among the materials formed by the interaction of different substrates with the surface of various substrates. The study and identification of new structures with similar properties is one of the problems facing modern theoretical research. The current research work was carried out as one of the solutions to the above-mentioned problems, in which the adsorption of fullerene molecules on silicon substrates using the molecular dynamics (MD) method is a continuation of our work on the adsorption of fullerene C_{20} and C_{60} molecules on the surface of silicon Si(001) reconstructed by C_n (n=1-5) carbon clusters was simulated using the open source LAMMPS package based on the molecular dynamics method. Using the Tersoff interatomic potential, the interactions between the atoms of the substrate, Cn cluster, and fullerene molecules were expressed, and the adsorption energies of C_{20}@C_n and C_{60}@C_n carbon clusters, the length and nature of Si-C bonds, as well as stable adsorption states in trench and dimer rows were determined.

Keywords: *Fullerene molecule; Base; Cluster; Trench; Dimer array; Modeling; Potential; Bond; Simulation; Adsorption*
PACS: 61.48.-c, 02.70.Ns

INTRODUCTION

Carbon-based nanostructures have remained relevant for decades. Fullerenes, nanotubes, graphene and graphene-based derivatives, carbon-based quantum dots, and the like are being widely studied and are gaining popularity. It is worth noting that among these nanostructures, fullerenes stand out sharply with their unique physical and chemical properties, promising practical applications. In particular, C_{20} [1], which has the highest adsorption capacity on the surface of the substrate due to the largest number of bends among fullerenes, and C_{60} [2], which has the highest symmetry among fullerenes, are making a fundamental difference in the latest generation of computers - quantum computers [3-6]. Despite the fact that many experimental studies on the adsorption of C_{60} and C_{20} fullerene molecules on the surfaces of metal and semiconductor substrates have been carried out using STM, XPS and STS [7-14] and theoretical studies using DFT, ab-initio, MD [15-19] methods, the adsorption of fullerene molecules with C_n carbon clusters on the surfaces of semiconductors, especially the interaction processes on the surfaces of silicon substrates, have been studied very little both theoretically and experimentally. It is known that the structures arising from the adsorption of fullerene molecules on the surfaces of various substrates are one of the current directions of scientific research due to their promising practical importance [20-29]. Also, in today's nanotechnology field, strong and stable binding of fullerene molecules to the surface is of great practical importance [30]. In particular, the binding of fullerene molecules on the surface of graphene substrates via C_n (n=1-5) clusters are distinguished by its stability from the cluster-free adsorption of these molecules [31]. As a result of the high importance of stable adsorption states of fullerene molecules on silicon substrates in the production of molecular devices that replace semiconductor devices [32], it is important to study the adsorption of C_{60} and C_{20} molecules on the surface of reconstructed silicon Si(001) substrates via Cn clusters.

In this work, the adsorption processes of fullerene C_{20} and C_{60} molecules on the reconstructed silicon Si(001) surface through C_n (n=1-5) carbon clusters exodrilled to fullerenes were studied based on the molecular dynamics (MD) method. In these processes, the adsorption energies of the C_n@C_{20} and C_n@C_{60} structures were determined to a first approximation, and the lengths of the Si-C bonds representing the interaction of the Cn carbon clusters with the substrate were found, conclusions were drawn about the nature (physical or chemical bond), and stable adsorption states and locations were determined by analyzing the results obtained.

DESCRIPTION OF RESEARCH METHODOLOGY AND OBJECTS

One of the most important aspects of fullerenes is their 0D materiality, and this property has attracted attention in various fields since their discovery. The first representative of fullerenes, C_{60}, consisting of 60 carbon atoms, the

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Cite as: I.Z. Urolov, F.F. Umarov, I.D. Yadgarov, G.T. Rakhmanov, Kh.I. Jabborov, East Eur. J. Phys. 3, 273 (2025), https://doi.org/10.26565/2312-4334-2025-3-24

buckminster fullerene [33], discovered by Croto and his team, has gained a sharp recognition compared to other fullerene representatives. In this regard, the C_{60} fullerene molecule, together with C_{70}, is distinguished from fullerenes with a small atomic number by its strength and stability [34]. When talking about the fullerene C_{60}, it is certainly important to emphasize its symmetry. The C_{60} molecule has 120 different symmetries with self-return properties with respect to different axes and planes [35]. This feature makes it the most symmetrical molecule among molecules and fullerenes found in nature. Each carbon atom in it forms hybrid sp2 bonds with three side atoms, C_5-C_5 with a length of 1.45 Å and C_6-C_6 with a length of 1.40 Å [2, 16, 17].

The C_{20} fullerene molecule is the smallest or least carbon-containing member of the fullerene family [36], consisting of 12 pentagons and 30 C_5-C_5 bonds, according to Euler's theorem. C_{20} also has 120 different symmetries, making it the only fullerene with less than full icosahedral symmetry than C_{60}. [40]. C_{20} has a number of practical applications in many fields, including high-temperature superconductivity, as has been theorized by Y. Miyamoto and M. Saito, I. Spagnolatti, and others [37-39].

Silicon has an atomic mass of 28, a valence of 4, and is the second most abundant chemical element on Earth (25.7%) after oxygen. It does not occur in free form, i.e., pure silicon, in nature [41]. Silicon monocrystal has diamond structure (fcc-face centered cubic), with a lattice constant of 5.43 Å and a shortest distance between atoms at lattice sites of 2.35 Å [42].

All simulations in the study were performed in the open source LAMMPS package based on the MD method [43]. The potential energies resulting from the interactions between the $C_{20}@C_n$ and $C_{60}@C_n$ carbon clusters and the atoms forming the substrate were expressed using the Tersoff interatomic potential [44]. The coordinates of the atoms of the silicon substrate, which were one of the objects of the study, were generated using the LAMMPS package and reconstructed by energy minimization. The reconstructed silicon monocrystal used as the substrate consists of 1083 atoms and has a size of 34×34×15.2 Å (Fig. 1, a). Also, in order to check whether the size effects can be observed in the results determined in the study, the interaction of randomly selected $C_{20}@C_n$ and $C_{60}@C_n$ cluster samples with reconstructed silicon monocrystalline substrates consisting of 1927, 5692 and 18630 atoms was studied. As a result, it was confirmed that size effects are not observed. The coordinates of C_{20} and C_{60} fullerene molecules were obtained using the nanotube modeler computer program (Fig. 1, b, c) and C_n carbon clusters were created in the JMOL computer visualization program [45]. The coordinates of the structures formed by these clusters with C_{20} and C_{60} fullerene molecules with a given configuration were also performed using the same program. The Si-C bond lengths were also measured in the JMOL program, visualizing the adsorption of $C_{20}@C_n$ and $C_{60}@C_n$ clusters with the substrate, and precisely when the interaction reached an equilibrium state. A Noze-Hoover thermostat [46] was used to maintain the selected temperature for the NVT ensemble. The selected temperature for all simulations was 0 K. The Verlet-velocity time scheme was integrated with a time step of 1.0 fs. The center of mass of the system was kept fixed during the simulation to avoid any translational motion. Each simulation was continued for a time period of 10 ns to 50 ns until an equilibrium state was reached. All results were determined based on the energy minimization method. Figure 1d) shows examples of different shapes of C_n carbon clusters for the case of n=2-5, and bonds of this shape are found in all adsorptions of $C_{20}@C_n$ and $C_{60}@C_n$ clusters and are distinguished by their stability compared to other shapes.

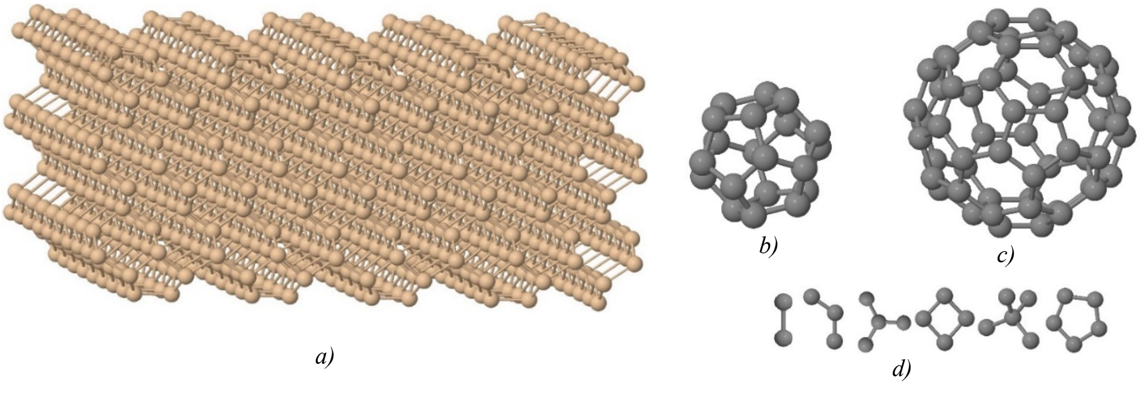


Figure 1. a) A silicon substrate with dimensions of 34×34×34×15.2 (Å);
a) and b) fullerene C_{20} and C_{60} molecules, respectively; d) C_n carbon cluster samples

CALCULATION OF ADSORPTION ENERGY

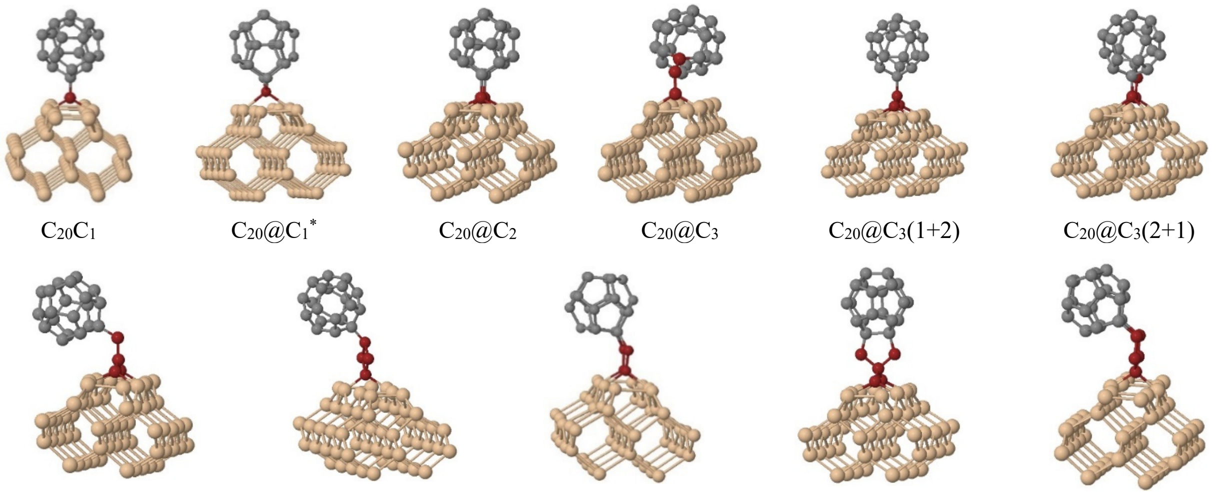
As mentioned above, the potential energies of the atoms constituting the objects, i.e. the total potential energies of the substrate and the $C_{20}@C_n$ and $C_{60}@C_n$ carbon clusters at the time of their unexposed and observed adsorption, were determined by energy minimization. After that, the adsorption energies of the $C_{20}@C_n$ and $C_{60}@C_n$ clusters were determined by the following traditional method [47-50]:

$$E_{\text{ads}} = E_{\text{ads/sub}}^{\text{tot}} - (E_{\text{sub}}^{\text{tot}} + E_{\text{ads}}^{\text{tot}}). \tag{1}$$

Here, E_{ads} is the adsorption energy of $C_{20}@C_n$ and $C_{60}@C_n$ carbon clusters on the substrate surface at the selected temperature, $E^{\text{tot}}_{\text{ads/sub}}$ is the total potential energy of the entire system at the time of interaction between the substrate and the $C_{20}@C_n$ or $C_{60}@C_n$ carbon clusters, i.e., the carbon clusters are adsorbed on the substrate, and $E^{\text{tot}}_{\text{sub}}$ and $E^{\text{tot}}_{\text{ads}}$ are the potential energies of the substrate and the $C_{20}@C_n$ or $C_{60}@C_n$ carbon clusters, respectively, determined by separately simulating and minimizing the energy. All energy values are determined at a temperature of 0 K.

DESCRIPTION AND ANALYSIS OF RESEARCH RESULTS

In the research work, the adsorption of C_{20} and C_{60} fullerene molecules by C_n clusters on the reconstructed silicon Si(001) surface through the dimer array and trench by C_n carbon clusters was observed according to the structures and configurations that can occur depending on the number of atoms in the carbon cluster. For example, in the symbolism of the compound formed by the fullerene C_{20} molecule with the carbon C_3 cluster as $C_{20}@C_3(1+2)$, the carbon atoms in the cluster are attached to the fullerene molecule with a single carbon atom, which can be seen in Figure 2 below. Therefore, in the designations in the configuration column of the Table, the first of the numbers in parentheses indicates how many atoms the carbon cluster is attached to the fullerene molecule, and the last number indicates how many carbon atoms are present at the other end of the carbon Cn cluster. The symbols representing the configurations in the form $tC_{20}@C_n$ or $tC_{60}@C_n$ indicate that the adsorption of $C_{20}@C_n$ and $C_{60}@C_n$ carbon clusters, respectively, was observed in the trench.


$C_{20}C_1$ $C_{20}@C_1{}^*$ $C_{20}@C_2$ $C_{20}@C_3$ $C_{20}@C_3(1+2)$ $C_{20}@C_3(2+1)$

$C_{20}@C_4(1+1+2)$ $C_{20}@C_4(1+2+1)$ $C_{20}@C_4(2+2)$ $C_{20}@C_5(2+1+2)$ $C_{20}@C_5(2+2+1)$

Figure 2. Adsorption states of $C_{20}@C_n$ (n=1-5) clusters in a dimer array on a silicon substrate surface: carbon atoms in C_n carbon clusters are shown in dark brown

By comparing the results obtained, it can be concluded that all the adsorptions of the $C_{20}@C_n$ cluster in the dimer row and trench are of a chemical adsorption nature, which indicates the stability of these bonds. According to the conclusion made in the research work of T. Sergeiva et al. [51], when the Si-C bond length is 1.93-1.94 Å or less, silicon-carbon bonds are considered covalent bonds. Also, when comparing the number of Si-C bonds formed during adsorption, it can be concluded that the adsorption energy is not strongly related to the number of bonds, which can be attributed to the presence of weak physical bonds in the bonds. When the adsorption energies and Si-C bond lengths of the $C_{20}@C_n$ carbon cluster in the dimer row and trench are compared in general, it can be seen from Table 1 that the adsorptions in the dimer row are relatively stable. This is because the double bonds in the reconstructed silicon atoms in the dimer series have the potential to become single bonds. Another reason for this is that the double-bonded Si-Si bonds in the dimer series have been completely broken.

The adsorption energies and lengths of Si-C bonds formed by the $C_{60}@C_n$ cluster on the silicon substrate surface in combination with the stable forms of the C_n carbon cluster are presented in Table 2. Comparing these results, we can also come to the same conclusions as above, namely, the adsorption energies of the $C_{60}@C_n$ cluster are relatively larger in the dimer series and, accordingly, the adsorptions in these cases are stable, and also the bonds observed in the dimer series consist mainly of pure chemical bonds or covalent bonds. Since the bonds with the $tC_{60}@C_2$, $tC_{60}@C_2(1+1)$ and $tC_{60}@C_3$ configurations occur with saturated, that is, silicon atoms forming four covalent bonds, their lengths also correspond to physical bonds and therefore the adsorption energies in them differ sharply from the adsorption energies in the trench. It can be seen from the tables that the adsorption energies observed in the dimer series with carbon clusters of the form $C_{20}@C_3(1+2)$, $C_{20}@C_4(1+1+2)$, $C_{20}@C_5(2+1+2)$ and $C_{60}@C_4(1+1+2)$ differ sharply from the binding energies observed in other states and forms. The reason for the observation of such states can be shown that two pairs of Si-Si bonds, which are the result of the reconstruction of these bonds in the dimer series, are broken and form double bonds with carbon atoms in the C_n cluster, and all of these bonds, except for the $C_{60}@C_4(1+1+2)$ cluster, are chemical bonds.

Table 1. Adsorption configurations, adsorption energies (eV) and Si-C bond length intervals (Å) of C_{20}@C_n carbon clusters

No.	configurations	E_{ads} (eV)	λ (Å)
1	C_{20}@C_1	-6.4493	1.86
2	C_{20}@C_1^*	-4.9343	1.91 – 1.92
3	C_{20}@C_2	-8.8248	1.94
4	C_{20}@C_3	-6.4395	1.86
5	C_{20}@C_3(1+2)	-11.6994	1.87
6	C_{20}@C_3(2+1)	-5.6031	1.95 – 2.06
7	C_{20}@C_4(1+1+2)	-11.6913	1.87
8	C_{20}@C_4(1+2+1)	-5.7340	1.89 – 1.90
9	C_{20}@C_4(2+2)	-6.4409	1.99
10	C_{20}@C_5(2+1+2)	-11.7498	1.87
11	C_{20}@C_5(2+2+1)	-5.0312	1.91
12	tC_{20}@C_1	-6.6687	1.93 – 2.01
13	tC_{20}@C_2	-4.8900	1.95
14	tC_{20}@C_3	-4.6791	1.94 – 1.95
15	tC_{20}@C_3(1+2)	-7.9494	1.95
16	tC_{20}@C_3(2+1)	-6.4421	1.84 – 1.90
17	tC_{20}@C_4(1+1+2)	-5.6722	1.84 – 2.16
18	tC_{20}@C_4(1+2+1)	-4.2451	1.91 – 2.20
19	tC_{20}@C_4(2+2)	-4.3251	1.85 – 1.97
20	tC_{20}@C_5(2+1+2)	-7.6368	1.84 – 1.94
21	tC_{20}@C_5(2+2+1)	-4.5384	1.89 – 2.14

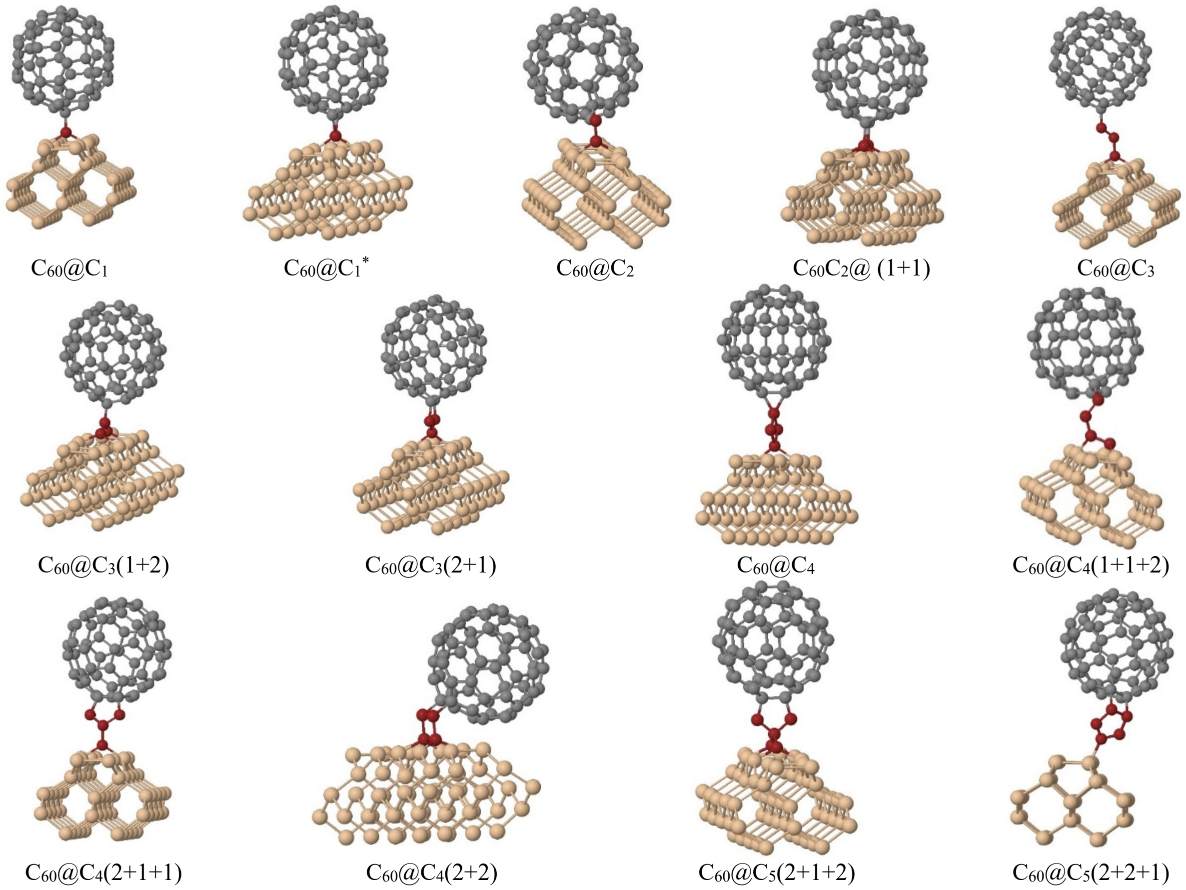
Table 2. Adsorption configurations, adsorption energies (eV) and Si-C bond length intervals (Å) of the C_{60}@C_n carbon clusters

No.	configurations	E_{ads} (eV)	λ (Å)
1	C_{60}@C_1	-4.8154	1.86
2	C_{60}@C_1^*	-4.4635	1.88
3	C_{60}@C_2	-2.5317	1.86
4	$C_{60}C_2$@ (1+1)	-5.638	1.94
5	C_{60}@C_3	-4.8035	1.86
6	C_{60}@C_3(1+2)	-8.5342	1.87
7	C_{60}@C_3(2+1)	-3.4031	1.91
8	C_{60}@C_4	-4.0955	1.89 – 1.90
9	C_{60}@C_4(1+1+2)	-10.8257	1.94 – 2.00
10	C_{60}@C_4(2+1+1)	-4.8039	1.86
11	C_{60}@C_4(2+2)	-3.1636	1.93 – 1.94
12	C_{60}@C_5(2+1+2)	-8.5874	1.87
13	C_{60}@C_5(2+2+1)	-2.9324	1.88
14	tC_{60}@C_1	-6.3041	1.95 – 2.14
15	tC_{60}@C_2	-1.5059	2.07
16	tC_{60}@C_2(1+1)	-1.1878	1.96
17	tC_{60}@C_2^*	-4.8662	1.95
18	tC_{60}@C_3	-1.1962	1.95
19	tC_{60}@C_3(1+2)	-7.9511	1.85 – 1.86
20	tC_{60}@C_3(2+1)	-4.9097	1.90
21	tC_{60}@C_4	-5.0921	1.90 – 2.09
22	tC_{60}@C_4(1+1+2)	-6.9512	1.83 – 1.90
23	tC_{60}@C_4(2+1+1)	-5.9131	1.87 – 2.02
24	tC_{60}@C_4(2+2)	-6.1636	1.86 – 1.90
25	tC_{60}@C_5(2+1+2)	-7.6248	1.90 – 2.10
26	tC_{60}@C_5(2+2+1)	-4.5442	1.89 – 2.14

**- These are cases where the C_1 and C_2 carbon atoms form double bonds with the C_{20} and C_{60} fullerene molecules, and such cases were observed with the C_{20}@C_1^*, C_{60}@C_1^*, and tC_{60}@C_2^* clusters.*

Side views of the adsorption of C_{20}@C_n and C_{60}@C_n carbon clusters on the silicon substrate in the dimer row and trench are shown in Figures 2, 4 and 3, 5, respectively. It can be seen from these figures that in the adsorption configurations of C_{20}@C_n and C_{60}@C_n carbon clusters in the dimer row, the cleavage of these bonds was observed in the dimer (Si-Si) bonds involved in the Si-C bond. This indicates that the interaction of C_n clusters with silicon atoms is stronger than the interaction between silicon atoms in the dimers. The opposite situation of the same aspect can be observed in the adsorption of $C_{20}@C_n$ and $C_{60}@C_n$ carbon clusters in the trench, i.e., the dimer bonds were not broken by the interaction of Si-C bonds formed with silicon atoms at the ends of the dimer bonds in the two dimer arrays. Also, under the influence of Si-C bonds formed between the silicon atoms in the second layer of the trench and the $C_{20}@C_n$ carbon clusters, the Si-Si bonds formed with the silicon atoms in this layer and the first layer (in dimer bonds) were broken.

Such new stable structures could enable high-temperature operation without the need for high-temperature cooling, for example when used as solid-state qubits in quantum computers. It is also known that replacing the carbon-coated silicon structures used in lithium-ion batteries with fullerene-coated silicon structures would increase the life cycle and performance of these devices [52].

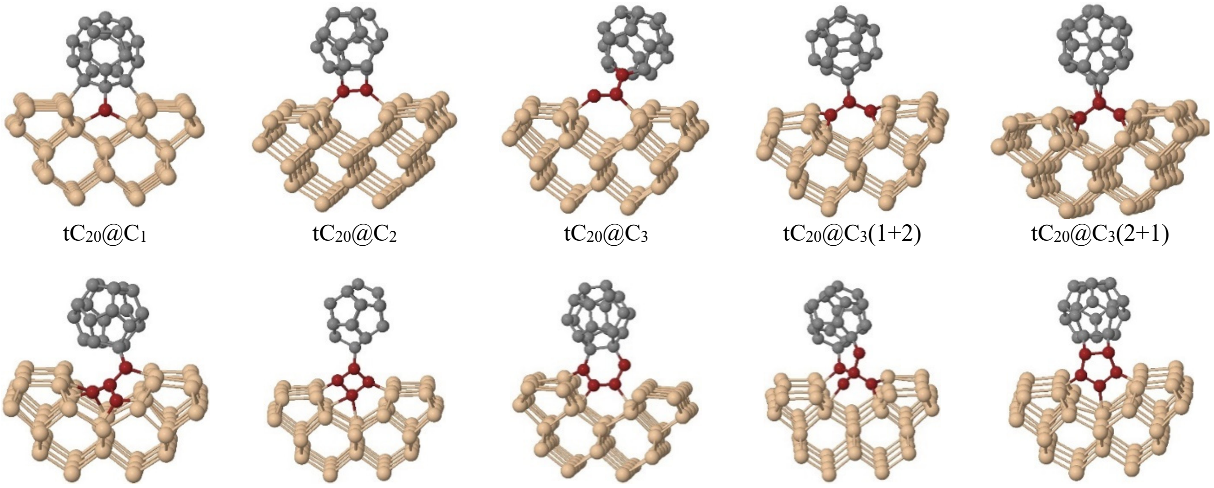


$C_{60}@C_1$ $C_{60}@C_1^*$ $C_{60}@C_2$ $C_{60}C_2@$ (1+1) $C_{60}@C_3$

$C_{60}@C_3$(1+2) $C_{60}@C_3$(2+1) $C_{60}@C_4$ $C_{60}@C_4$(1+1+2)

$C_{60}@C_4$(2+1+1) $C_{60}@C_4$(2+2) $C_{60}@C_5$(2+1+2) $C_{60}@C_5$(2+2+1)

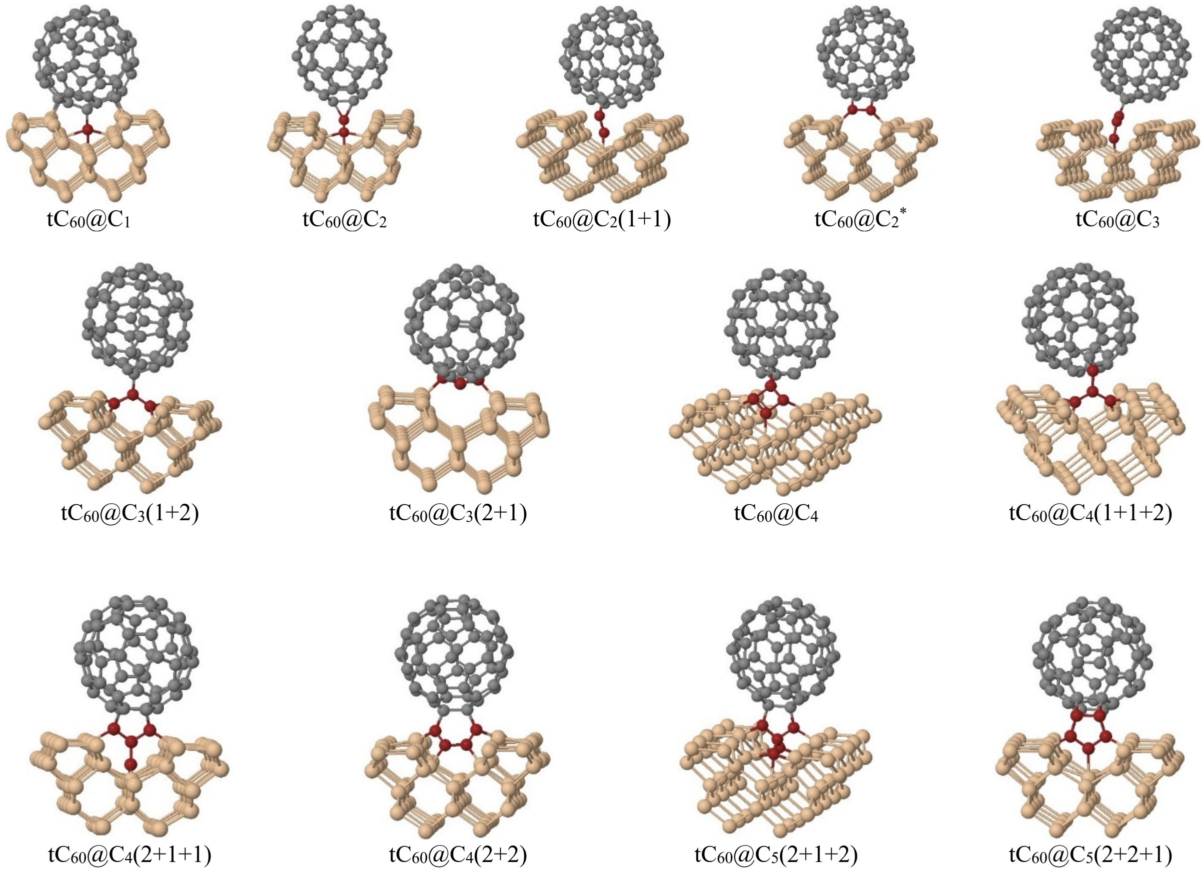
Figure 3. Adsorption states of $C_{60}@C_n$ carbon clusters in dimer arrays on the surface of a silicon substrate



$tC_{20}@C_1$ $tC_{20}@C_2$ $tC_{20}@C_3$ $tC_{20}@C_3$(1+2) $tC_{20}@C_3$(2+1)

$tC_{20}@C_4$(1+1+2) $tC_{20}@C_4$(1+2+1) $tC_{20}@C_4$(2+2) $tC_{20}@C_5$(2+1+2) $tC_{20}@C_5$(2+2+1)

Figure 4. Adsorption states of $C_{20}@C_n$ carbon clusters along the trench (dimer row spacing).



$tC_{60}@C_1$ $tC_{60}@C_2$ $tC_{60}@C_2(1+1)$ $tC_{60}@C_2^*$ $tC_{60}@C_3$

$tC_{60}@C_3(1+2)$ $tC_{60}@C_3(2+1)$ $tC_{60}@C_4$ $tC_{60}@C_4(1+1+2)$

$tC_{60}@C_4(2+1+1)$ $tC_{60}@C_4(2+2)$ $tC_{60}@C_5(2+1+2)$ $tC_{60}@C_5(2+2+1)$

Figure 5. Adsorption states of $C_{60}@C_n$ carbon clusters along the trench

CONCLUSIONS

According to the results obtained, the following conclusions were drawn: a) the adsorption of C_n (n=1-5) carbon clusters exodrilled fullerene C_{20} and C_{60} molecules on the reconstructed silicon Si(001) surface differs from the adsorption of pure C_{20} and C_{60} fullerene molecules on this substrate surface by a sharp stability [19]; b) the adsorption of $C_{20}@C_n$ and $C_{60}@C_n$ carbon clusters in the dimer series is more stable than the adsorption in the trench and, depending on the length of the Si-C bonds, they consist of covalent bonds; c) the adsorption energy does not depend on the number of bonds formed during the interaction, since physical bonds also exist within these bonds. The highly stable adsorption of $C_{20}@C_n$ and $C_{60}@C_n$ carbon clusters on the reconstructed silicon Si(001) surface leads to potential applications in electronics, optoelectronics, catalysis, and materials science. This is because the strength and stability of the fullerene-silicon bonds enable long-term operation, increased reliability, and reduced temperature sensitivity.

Acknowledgements

The authors are grateful for fruitful collaborations with Dr. Farid Umarov. This work was assisted by the fundamental research program of the Academy Science of Uzbekistan.

ORCID

Ishmumin D Yadgarov, https://orcid.org/0000-0002-4808-2258

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КОМП'ЮТЕРНЕ МОДЕЛЮВАННЯ ДОСЛІДЖЕННЯ ПРОЦЕСІВ АДСОРБЦІЇ ВУГЛЕЦЕВИХ КЛАСТЕРІВ C20@Cn ТА C60@Cn (n=1-5) НА РЕКОНСТРУЙОВАНІЙ ПОВЕРХНІ КРЕМНІЮ Si(001)

Ікром З. Уролов[a,b], Фарід Ф. Умаров[c], Ішмумін Д. Ядгаров[a], Ганібой Т. Рахманов[b], Хайтмурод І. Джабборов[d,e]
[a]Інститут іонно-плазмових та лазерних технологій ім. У.А. Аріфова Академії наук Республіки Узбекистан,
100125, Ташкент, вул. Дурмон Юлі, 33
[b]Національний університет Узбекистану імені Мірзо Улугбека, Республіка Узбекистан,
100174, Ташкент, вул. Університетська, 4
[c]Казахстансько-британський технічний університет, Алмати, вул. Толе бі 59, Казахстан
[d]Ташкентський державний технічний університет імені Ісламa Карімова, Ташкент, Узбекистан
[e]Ташкентський університет інформаційних технологій імені Мухаммада аль-Хорезмі, Ташкент, Узбекистан

У сучасній галузі нанотехнологій однією з вимог сучасного напрямку є здатність вуглецевих наноструктур мати міцний зв'язок з поверхнею підкладки серед матеріалів, утворених внаслідок взаємодії різних підкладок з поверхнею різних підкладок. Вивчення та ідентифікація нових структур з подібними властивостями є однією з проблем, що стоять перед сучасними теоретичними дослідженнями. Поточна дослідницька робота була проведена як одне з рішень вищезазначених проблем, в якій адсорбція молекул фулерену на кремнієвих підкладках за допомогою методу молекулярної динаміки (МД) є продовженням нашої роботи з адсорбції молекул фулерену C20 та C60 на поверхні кремнію Si(001), реконструйованого вуглецевими кластерами Cn (n=1-5), була змодельована за допомогою пакета з відкритим кодом LAMMPS на основі методу молекулярної динаміки. Використовуючи міжатомний потенціал Терсоффа, було виражено взаємодії між атомами субстрату, кластером Cn та молекулами фулерену, а також визначено енергії адсорбції вуглецевих кластерів C20@Cn та C60@Cn, довжину та природу зв'язків Si-C, а також стабільні стани адсорбції в траншеях та рядах димерів.

Ключові слова: *молекула фулерену; основа; кластер; траншея; масив димерів; моделювання; потенціал; зв'язок; симуляція; адсорбція*