

COMPUTER SIMULATION OF ADSORPTION OF C₆₀ FULLERENE MOLECULE ON RECONSTRUCTED Si(100) SURFACE

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The adsorption of the C₆₀ fullerene molecule has been studied in various configurations on a reconstructed Si(100) silicon surface. Among fullerenes, fullerene C₆₀ is of particular importance, since it has the most stable form and consists of 60 carbon atoms. Monocrystalline silicon has the diamond structure, the size of its crystal lattice is 5.43 Å. The MD-simulation calculations have been performed using the open source LAMMPS MD-simulator software package and the Nanotube Modeler computer program. The Tersoff interatomic potential has been used to determine the interactions between the Si-Si, C-C and Si-C atoms. The adsorption energy of the C₆₀ molecule on the reconstructed Si(100) surface, the bond lengths and the number of bonds formed depend on the adsorption geometry, i.e. at what point on the substrate the molecule is adsorbed and in what configuration.

Key words: Surface; Fullerene molecule; Adsorption; Silicon; Simulation; Brenner potential; Bond length; Atom; potential energy; Interaction

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INTRODUCTION

Fullerenes are of growing interest following the discovery of C₆₀ by Kroto H. W. et al. [1] and the success of Kratschmer W. et al. in obtaining pure C₆₀ and other members of the fullerene family [2]. Fullerenes are a promising material for creating electro-active elements in solar cells and active layers in thin-film organic transistors [3]. One of the current topics related to fullerenes is their adsorption on various substrates. Fullerenes adsorbed on substrates have great potential for practical application and the studies of fullerene and its compounds is of great fundamental importance [4,5]. The molecule adsorption of a number of substances, such as water, ammonia, ethylene and vinyl bromide, on the Si(100) surface has been studied experimentally [6-8]. The high density of π electrons of the C₆₀ molecules gives them the energy potential of a small organic molecule. The C₆₀ nanofullerene molecule is expected to provide high-performance electronics and optical functions, as well as exhibit interesting fabrication, high spherical symmetry, and ease of connectivity. Obviously, the use of C₆₀ adsorbed on an ideal Si(100) surface is very topical and actual in modern semiconductor technology [9, 10]. One of these promising applications is the use of endohedrally embedded fullerenes in quantum computers, for which the fullerene molecules are to be adsorbed on the surface silicon [11-13]. The appearance of superconducting properties in some alkali metals when they are coated with C₆₀ and C₇₀ fullerenes [14] and the treatment of the silicon surface with ions has intensified research in the field of HTSC materials science [15].

A number of theoretical and experimental studies of the interaction of C₆₀ and other representatives of the fullerene family with the Si(111) surface have been carried out. When designing and developing devices based on fullerenes in molecular electronics, information technology, and biomedical developments [16-18], C₆₀/Si(100) is of great importance [19-22]. In recent years, the adsorption of C₆₀ molecules on the Si(111) surface has been studied by density functional theory (DFT) [17,23,24]. The interaction between C₆₀ and the Si(111) surface was experimentally studied by scanning tunneling microscopy and spectroscopy (STM/STS) [22-26], as well as by other methods [18,27]. The experimental results on the temperature dependence of the adsorption of C₆₀ molecules on the Si(111) surface were published in [28].

To clarify the nature of the adsorption of C₆₀ molecules on the Si(100) surface, a great number of contradictory studies have been carried out. In some of these works, the researchers showed that the adsorption of C₆₀ is physisorption [29-31], while in some other studies this was denied and it was stated that the adsorption is chemisorption in its nature [32-37]. Among the theoretical calculations performed in this direction, ab initio theoretical calculations stand out [38-40], but the studies in this direction was carried out by predicting the structures formed when fullerene molecules are placed on the substrate surface, without taking into account any structural changes caused by the bonds between atoms on the silicon surface and C₆₀ atoms [21]. In the works of C. Hobbs et al. [41,42], the average Si-C bond length and adsorption energy for the adsorption of the C₆₀ molecule on the Si(100) surface were determined by ab initio DFT using Spanish Initiative for Electronic Simulations with Thousands of Atoms codes (SESTA). From the results of these works it is clear

that the bond length and the adsorption energy depend on configuration and number of bonds of the C₆₀ molecules adsorbed on the base surface. The work of K. Beardmore et al., using classical many-body potentials of the Brenner/Tersoff form [44-46], suggests that the bonds between the fullerene and the silicon surface are closer to Van der Waals bonds than to covalent ones. In this formalism, the silicon-carbon interactions are adapted to SiC bulk structures and C₆₀ molecules can be transferred incorrectly to the silicon surface.

The aim of this work is to determine adsorption energies and bond lengths for various adsorption configurations of C₆₀ fullerene molecules on the reconstructed Si(100) silicon surface, as well as to determine the dependence of these parameters on all possible adsorption configurations that can be realized on the Si(100) surface.

In connection with the above, in this work, the results of studying the interaction of the C₆₀ molecule with the reconstructed Si(100) surface have been highlighted, and the interaction process has been considered by molecular dynamics (MD) simulation.

DESCRIPTION OF THE OBJECT AND RESEARCH METHODS

Fullerenes are large carbon-framework molecules that are considered to be three-dimensional analogues of benzene. Among fullerenes, Buckminster fullerene (C₆₀) is of particular importance, since it has the most stable form and consists of 60 carbon atoms. The molecule shape resembles a truncated icosahedron, that is, a soccer ball consisting of 12 pentagons and 20 hexagons [2]. One of the important properties of C₆₀ is its high symmetry having 120 symmetry operations in which the molecule can return to itself, like rotation around an axis and reflection in a plane. This makes C₆₀ the most symmetrical molecule [47]. C₆₀ has two types of bonds: a C₅-C₅ single bond in a pentagon (the bond length 1.45±0.015 Å) and a C₅-C₆ double bond in a hexagon (the bond length 1.40±0.015 Å). Each carbon atom in the molecule forms a bond with three side atoms through sp²-hybridization [48,49]. The diameter of the C₆₀ molecule is about 7 Å. Chemically, the fullerene molecule is quite stable; it decomposes at a temperature of 1000°C, and when heated to a temperature of 1500°C in the absence of air, it takes the form of graphite [50].

Silicon is a chemical element with atomic number 14, chemical symbol Si, and atomic weight 28.085. Monocrystalline silicon has the structure of diamond, the size of its crystal lattice is 5.43 Å. The closest distance between atoms in the lattice is 2.35 Å [51].

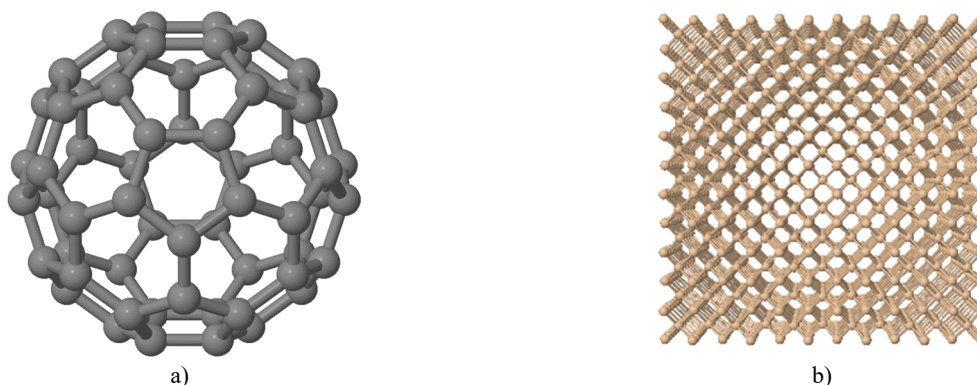


Figure 1. Geometric structures of fullerene C₆₀ (a) and silicon (b) used in this work

All MD-simulation calculations in our work were performed using the open source LAMMPS MD-simulator software package [52] and the Nanotube Modeler computer program [53]. The Tersoff interatomic potential was used to determine the interactions between Si-Si, C-C and Si-C atoms. In all cases, a reconstructed silicon single crystal measuring 34 × 34 × 15.2 Å with 1083 atoms (Fig. 1b) and a fullerene molecule with 60 atoms (Fig. 1a) with periodic boundary conditions were used. The generated C₆₀ molecule, the reconstructed silicon single crystal and the interaction processes between them were visualized in the JMOL computer program [54]. When comparing the results obtained for reconstructed single crystals with the number of atoms 1963 and 17670, no size effects were found. To maintain a constant selected temperature of the NVT ensemble, a Nose-Hoover thermostat was used [55]. The Wehrl speed synchronization circuit was integrated with a time step of 1.0 fs. The system's center of mass was fixed to avoid any forward motion during the simulation. Each simulation lasted from 10 to 40 ns until equilibrium was reached.

CALCULATION OF ADSORPTION ENERGY

The adsorption energy E_{ads} for a molecule or atom adsorbed on the substrate surface is the total potential energy of the substrate and the adsorbed molecule $E_{ads/sub}^{tot}$, the potential energy of the substrate in the state when they do not interact $E_{sub/tot}$ and the potential energy of the adsorbed molecule $E_{ads/tot}$ is equal to the subtraction of the sum [56,57]:

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

Initially, the potential energy $E_{sub/tot}$ of interaction of the atoms composing a silicon single crystal at a temperature of 0 K was determined, and in the same test the potential energy $E_{sub/tot}$ of interaction of the C₆₀ molecule atoms was

obtained. At the next stage, the potential energy of the entire system $E_{ads/sub}^{tot}$ was determined for the case when a C_{60} molecule is adsorbed on a silicon substrate. All the calculations were performed in the LAMMPS package program.

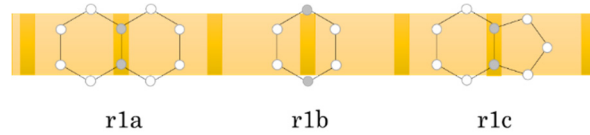


Fig. 2. Bonds of the C_{60} molecule in a dimer series with one dimer

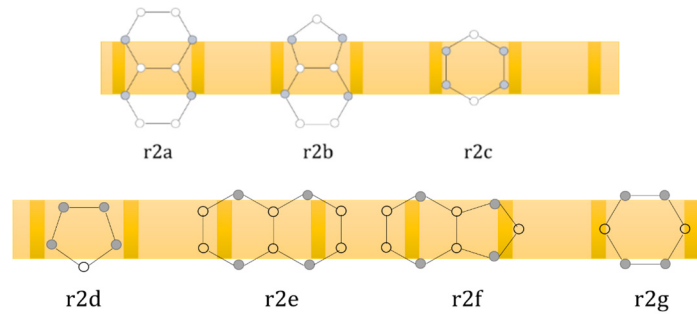


Fig. 3. Bonds of the C_{60} molecule with two dimers on rows of dimers

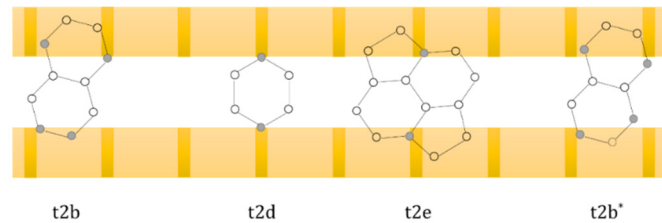


Fig. 4. Bonds of the C_{60} molecule on a trench with two dimers

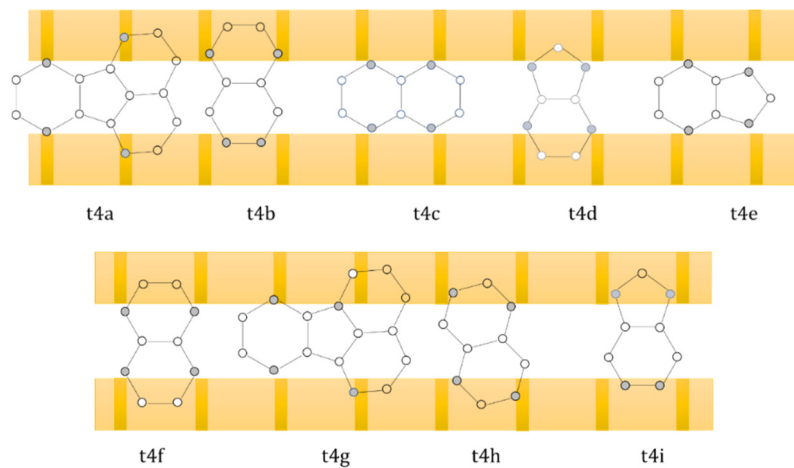


Fig. 5. Bonds of the C_{60} molecule on the trench with four dimers

DESCRIPTION AND ANALYSIS OF RESULTS

The results obtained are very convenient to analyze, classifying them into different configurations. A similar classification was made in [21,41-43]. A recent work by C. Hobbs et al. [42] studied the adsorption of C_{60} in 26 different configurations on a Si(100) surface; in this work, most of the above configurations and two new adsorption configuration states were classified as follows: trench is the space between two rows of dimers; adsorption on trench between four dimers (t4); adsorption on trench between two dimers (t2); adsorption with two dimers in a series of dimers (r2); adsorption with one dimer in a series of dimers (r1).

The adsorption of fullerenes on all the configuration classifications is schematically presented in Figures 2-5. New configurations are marked with an asterisk (*). In the Figures, the rows of dimers are shown in golden color, and individual dimers are shown in dark golden color. The colorless space between the dimers represents trenches; the carbon atoms that formed the Si-C bond upon adsorption are shown as black circles, and those that did not participate in the bond are shown as white circles. These atoms belong to hexagons and pentagons that participate in adsorption.

The adsorption energy values calculated in this work are given in Table. 1 in comparison with the results obtained in GGA (generalized gradient approximation) and LDA (local-density approximation) [41,42] and [21]. All the energy values are in eV. The Si-C bond lengths are calculated for all configurations in Table 2 and given in Å, as compared to adsorption energies.

Table 1. Adsorption energies calculated in the LAMMPS program, as compared to the GGA, LDA methods and values calculated in [21].

№	Configuration	LAMMPS	GGA (SIESTA)	LDA (SIESTA)	[21]
1	r1a	-1.984	-1.72	-2.72	-3.53
2	r1b	-1.434	-1.50	-2.53	-3.28
3	r1c	-2.061	-0.93	-1.87	-2.90
4	r2a	-3.538	-2.58	-3.93	-4.83
5	r2b	-3.860	-2.49	-3.74	-4.33
6	r2c	-3.594	-2.00	-3.27	-4.15
7	r2d	-2.602	-0.87	-2.08	-2.69
8	r2e	-2.493	-1.69	-3.01	-3.94
9	r2f	-2.990	-2.19	-3.40	-4.10
10	r2g	-1.988	-1.1	-2.38	-3.13
11	t2a	-	-	-	-4.78
12	t2b	-4.744	-	-	-4.40
13	t2b*	-4.953	-	-	-
14	t2c	-	-0.07	-1.56	-3.08
15	t2d	-	-1.61	-2.83	-
16	t2d*	-5.752	-	-	-
17	t2e	-3.168	-1.57	-2.72	-
18	t4a	-3.438	-2.16	-3.94	-5.71
19	t4b	-4.743	-2.53	-4.00	-5.31
20	t4c	-5.755	-2.63	-4.1	-4.96
21	t4d	-5.167	-1.96	-3.42	-4.85
22	t4e	-5.433	-1.90	-3.38	-
23	t4f	-4.799	-2.17	-3.59	-
24	t4g	-5.058	-2.53	-4.02	-
25	t4h	-4.882	-1.94	-3.59	-
26	t4i	-4.571	-1.83	-3.41	-
27	t4j	-	-1.98	-3.55	-

Table 2. Si-C bond lengths (in Å) for all configurations

№	Configuration	LAMMPS	GGA (SIESTA)	LDA (SIESTA)	[21]
1	r1a	1.99-2.00	2.02-2.03	1.98-1.99	1.99-1.99
2	r1b	2.02-2.02	2.01-2.02	1.97-1.97	1.98-1.98
3	r1c	1.99-2.02	2.02-2.03	1.97-2.01	1.99-2.00
4	r2a	1.99-2.00	1.98-1.99	1.94-1.97	1.96-1.98
5	r2b	1.96-1.98	1.99-2.07	1.93-2.05	1.97-2.02
6	r2c	1.99-2.00	2.05-2.09	2.02-2.05	2.01-2.07
7	r2d	2.00-2.06	2.03-2.06	2.00-2.02	2.00-2.02
8	r2e	2.02-2.02	2.01-2.05	1.98-2.01	1.99-1.99
9	r2f	1.99-2.01	2.01-2.07	1.96-2.04	1.97-2.04
10	r2g	2.02-2.07	2.05-2.10	2.02-2.05	2.03-2.07
11	t2a	-	-	-	2.02-2.11
12	t2b	1.95-1.99	-	-	1.92-2.47
13	t2b*	1.93-2.00	-	-	-
14	t2c	-	2.08-2.10	2.04-2.06	2.03-2.03
15	t2d	-	1.99-2.03	1.95-1.99	-
16	t2d*	1.96-1.97	-	-	-
17	t2e	1.93-1.94	2.00-2.04	1.95-1.99	-
18	t4a	1.96-2.01	2.00-2.03	1.96-1.98	1.93-1.98
19	t4b	1.95-1.99	1.97-2.03	1.95-2.01	1.95-1.98
20	t4c	1.97-1.97	2.02-2.20	1.98-1.99	1.96-1.98
21	t4d	1.98-1.99	2.02-2.19	1.98-2.12	1.97-2.19
22	t4e	1.96-1.99	2.03-2.09	1.98-2.06	-
23	t4f	1.98	2.01-2.03	1.97-1.98	-
24	t4g	1.93-1.99	2.00-2.04	1.97-1.99	-
25	t4h	1.93-1.99	2.02-2.06	1.98-2.03	-
26	t4i	1.95-2.01	2.04-2.10	2.00-2.05	-
27	t4j	-	1.95-2.07	1.93-2.02	-

Table 1 shows that by comparing the adsorption energies of the C₆₀ molecule obtained in LAMMPS calculations, one can see that the bond energies of the t4 type have significantly higher values than the bond energies of other types (r2 or t2). The bond lengths shown in Table. 2 have slightly larger values in the bond configurations r1 and r2 than in the bond configurations t2 and t4. It can be seen that the adsorption energies of the C₆₀ molecule are closer to the results given in [21], and the obtained bond lengths do not differ sharply from the results of GGA, LDA and [21] given in Table 2.

CONCLUSION

As a result of the study, the following conclusions can be made: a) the adsorption energies of the C₆₀ molecule on the reconstructed Si(100) surface, the bond lengths and the number of formed bonds depend on adsorption geometry, i.e. at what point on the substrate the molecule is adsorbed and in what configuration; b) comparison of the obtained adsorption energies shows that the adsorption states on the rows of dimers (on the trench) become stable; c) adsorption energy depends on the number of bonds, and an increase in the number of bonds leads to an increase in adsorption energy; d) bonds with high adsorption energy have a shorter length.

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**КОМП'ЮТЕРНЕ МОДЕЛЮВАННЯ АДСОРБЦІЇ МОЛЕКУЛИ ФУЛЕРЕНУ C60
НА РЕКОНСТРУКЦІЙНІЙ ПОВЕРХНІ Si(100).**

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Досліджено адсорбцію молекули фулерену C60 у різних конфігураціях на реконструйованій поверхні Si(100) кремнію. Серед фулеренів особливе значення має фулерен C60, який має найбільш стабільну форму і складається з 60 атомів вуглецю. Монокристалічний кремній має структуру алмазу, розмір його кристалічної решітки 5,43 Å. Розрахунки MD-симуляції були виконані з використанням пакета програмного забезпечення LAMMPS MD-simulator з відкритим кодом та комп'ютерної програми Nanotube Modeler. Міжатомний потенціал Терсоффа використовувався для визначення взаємодії між атомами Si-Si, C-C і Si-C. Енергія адсорбції молекули C60 на реконструйованій поверхні Si(100), довжини зв'язків і кількість утворених зв'язків залежать від геометрії адсорбції, тобто в якій точці на підкладці молекула адсорбується та в якій конфігурації.

Ключові слова: *поверхня; молекула фулерену; адсорбція; кремній; моделювання; потенціал Бреннера; довжина зв'язку; атом; потенційна енергія; взаємодія*