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C_{60} fulleren molekulasining rekonstruksiyalanmagan kremniy Si(111) sirtida adsorbsiya jarayonlarini kompyuterda modellashtirish va tahlili.

Annotatsiya

Mazkur tadqiqot ishida C_{60} fulleren molekulasining rekonstruksiyalanmagan kremniy Si(111) sirti bilan o'zaro ta'sir jarayonlari molekulyar dinamika usuliga asoslangan ochiq paket LAMMPS dasturi yordamida simuliyatsiya qilindi. Fulleren molekulasining berilgan taglik sirtida adsorbsiya energiyasi energiyani minimaltirish orqali aniqlangan bo'lib, taglik va fulleren molekulasini tashkil etuvchi atomlar orasidagi o'zaro ta'sirlar Tersoff atomlararo potensiali yordamida ifodalangan. Shuningdek, o'zaro ta'sir vaqtida yuzaga keluvchi Si-C bog'lar uzunligi va ushbu bog'larning tabiati aniqlanib, erishilgan har bir konfiguratsiya uchun adsorbsiyaning kimyoviy yoki fizik xarakterda ekanligidan ularning barqarorligi haqida xulosalar qilingan.

Kalit so'zlar: fulleren, kremniy, adsorbsiya, konfiguratsiya, geksagon, pentagon, sirt, adsorbsiya energiyasi, bog', bog' uzunligi, potensial, kovalent bog'lar, atom.

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Компьютерное моделирование и анализ процессов адсорбции молекулы фуллерена C60 на нереконструированной поверхности кремния Si(111).

Аннотация

В данной исследовательской работе процессы взаимодействия молекулы фуллерена C_{60} с нереконструированной поверхностью кремния Si(111) моделировались с использованием пакета с открытым исходным кодом LAMMPS на основе метода молекулярной динамики. Энергия адсорбции молекулы фуллерена на заданной поверхности подложки определялась методом минимизации энергии, а взаимодействия между атомами, составляющими подложку, и молекулой фуллерена выражались с использованием межатомного потенциала Терсоффа. Также были определены длина связей Si-C, образующихся в ходе взаимодействия, и природа этих связей, а также сделаны выводы о стабильности адсорбции, будь то химическая или физическая природа, для каждой достигнутой конфигурации.

***Ключевые слова*:** фуллерен, кремний, адсорбция, конфигурация, шестиугольник, пятиугольник, поверхность, энергия адсорбции, связь, длина связи, потенциал, ковалентные связи, атом.

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Computer modeling and analysis of adsorption processes of C_{60} fullerene molecule on unreconstructed silicon Si(111) surface.

Abstract

In this study, the interaction processes of the C_{60} fullerene molecule with the unreconstructed silicon Si(111) surface were simulated using the open package LAMMPS program based on the molecular dynamics method. The adsorption energy of the fullerene molecule on a given substrate surface was determined by energy minimization, and the interactions between the atoms constituting the substrate and the fullerene molecule were expressed using the Tersoff interatomic potential. Also, the length of the Si-C bonds formed during the interaction and the nature of these bonds were determined, and conclusions were made about the stability of the adsorption for each configuration achieved, whether it was of a chemical or physical nature.

Key words: fullerene, silicon, adsorption, configuration, hexagon, pentagon, surface, adsorption energy, bond, bond length, potential, covalent bonds, atom.

Kirish

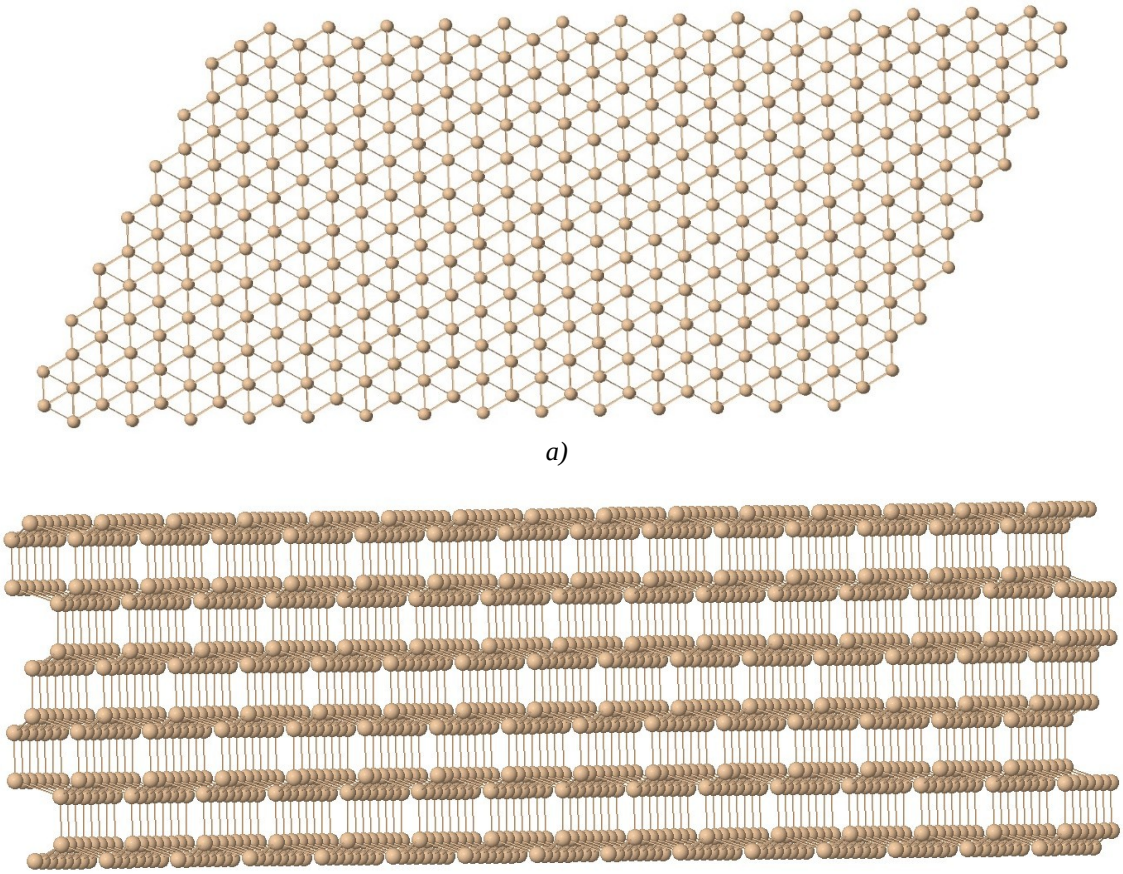
Uch o'lchamli yirik organik molekulalarning turli yarimo'tkazgich qattiq sirtlarda adsorbsiyasi istiqbolli texnologik yechimlarni taklif etayotganligi sababidan intensiv o'sib borayotgan yo'nalishlardan biri hisoblanadi. Shu singari potensial istiqbolga ega tadbiqlardan biri kremniy taglik sirtida adsorbsiyalangan fulleren molekulalarining kelajak hisoblash mashinalari bo'lmish kvant kompyuterlarida qattiq-holat kubitlarida foydalanish mumkin ekanligidir [1-4]. Fulleren molekulalarining o'ziga xos xilma-xil o'lcham va shakllarga ega ekanligidan, ulardan yoqilg'i sanoati [5-7], kompozit materiallar [8-10] va quyosh batareyalari, biotibbiyot [11-14] bilan bog'liq sohalarda qo'llanilishi faqatgina fullerenlargagina xos xususiyatlari bilan amaliy ahamiyatga ega hisoblanadi. C_{60} fulleren molekulasining metall va yarimo'tkazgich materiallar sirti bilan ta'sirlashuv jarayoni STM, XPS va boshqa bir qator qurilmalar yordamida eksperimental tarzda o'rganilgan [15,16]. Rekonstruksiyalangan kremniy Si(001) 2×1 va Si(111) 7×7 sirtida C_{60} fulleren molekulasining adsorbsiyasi zichlik funksional nazariyasi (DFT) va molekulyar dinamika (MD) usulida tadqiq qilingan [17-20]. Shunga qaramasdan, C_{60} fulleren molekulasining rekonstruksiyalanmagan kremniy Si(111) sirtida adsorbsiya jarayonini nazariy jihatdan kam tadqiq qilingan. rekonstruksiylanmagan kremniy Si(111) sirti birinchi va ikkinchi qatlamdagi atomlar joylashuvi, ularning to'yinish darajasining boshqa kesimlardan farq qilishi fulleren C_{60} molekulasining ushbu sirtda adsorbsiyasi (100) va (110) sirtlarida kuzatilgan adsorbsiyalardan keskin farq qiladi. Ushbu keskinlikni natijalar tahlilida bayon qilinadi. Shuningdek, kremniy Si(111) sirtidagi atomlar joylashuv struksturasi fulleren molekulasining

Mazkur tadqiqot ishining maqsadi – rekonstruksiyalanmagan kremniy Si(111) sirtida C_{60} fulleren molekulalarining adsorbsiya jarayonlarini o'rganish bilan birgalikda, adsorbsiyalanish konfiguratsiyalari va ular orasidan barqaror adsorbsiya holatlarini aniqlash, shuningdek ushbu jarayonda yuzaga keluvchi Si-C bog'lanishlarning uzunligi va ularning tabiatini tadqiq qilishdan, shuningdek, chiqarilgan xulosalar asosida ba'zi tadqiqot yoki tadqiqot natijalari tadbiq etiladigan amaliy ishlarga tavsiyalar berishdan iborat.

Metodologiya

Ushbu ishda ko'rib chiqilgan barcha o'zaro ta'sir jarayonlari MD usuliga asoslangan ochiq manba LAMMPS [21] paket dasturidan foydalingan holda modellashtirilgan bo'lib, C_{20} fulleren molekularining koordinatalari Nanotube Modeller [22] dasturi yordamida olingan. O'zaro ta'sir jarayonlari, ya'ni kuzatilgan adsorbsiya jarayonlari JMOL [23] visualizatsiya dasturi yordamida namoyish qilingan. Taglik sifatida olingan kremniy monokristali o'lchamlari 54×27×16 Å bo'lgan rombik parallelepipeddan bo'lib, u 1432 ta kremniy atomidan iborat. Kremniy taglik va C_{60} fulleren molekulasi atomlari orasidagi o'zaro ta'sir ikkinchi tartibli Tersoff [24] atomlararo potensiali yordamida ifoda qilingan. JMOL dasturi yordamida oldindan C_{60} molekulasining adsorbsiyasi kuzatilgan konfiguratsiyalari vizualizatisiya qilindi va shu bilan birgalikda, kremniy monokristalining rekonstruksiyalanmagan (111) kesimli sirti ham ushbu dastur yordamida hosil qilindi. Olingan natijalarga o'lcham effektining ta'sir mavjud emasligi, boshqa o'lchamli tagliklar yordamida tekshirib ko'rilib, mazkur effektning ushbu jarayonda hech qanday ahamiyatga ega emasligi aniqlandi. Tanlangan haroratni o'zgarmas saqlab turish uchun Noze-Guver termostati [25] dan foydalanildi. Verle tezlik-vaqt sxemasi 1.0 fs vaqt qadami bilan integratsiyalandi. Simuliyatsiya vaqtida sodir bo'lishi mumkin

bo’lgan ilgarilanma harakatlarni hisobga olmaslik maqsadida sistema massa markazi qo’zg’almas qilib tanlandi. Barcha simuliyatsiyalar muvozanatli holatni egallagunlaricha 100 ns dan 200 ns gacha vaqt oralig’ida amalga oshirildi. Bundan tashqari, har bir konfiguratsiyaga mos adsorbsiya jarayoniga tegishli kattaliklar molekulaning taglikka nisbatan turli balandlik holatlarida tekshirilib, ularning eng minimal qiymatlari natija sifatida olindi.



a)

b)

1-rasm. kremniy taglikning yuqoridan va yondan ko’rinishi.

1-rasmda C_{60} fulleren molekulasining adsorbsiyasi kuzatilgan rekonstruksiyalan-magan kremniy Si(111) kesimi (*a*) va ushbu monokristallning yondan ko’rinishi (*b*) tasvirlangan.

Adsorbsiya energiyasini hisoblash

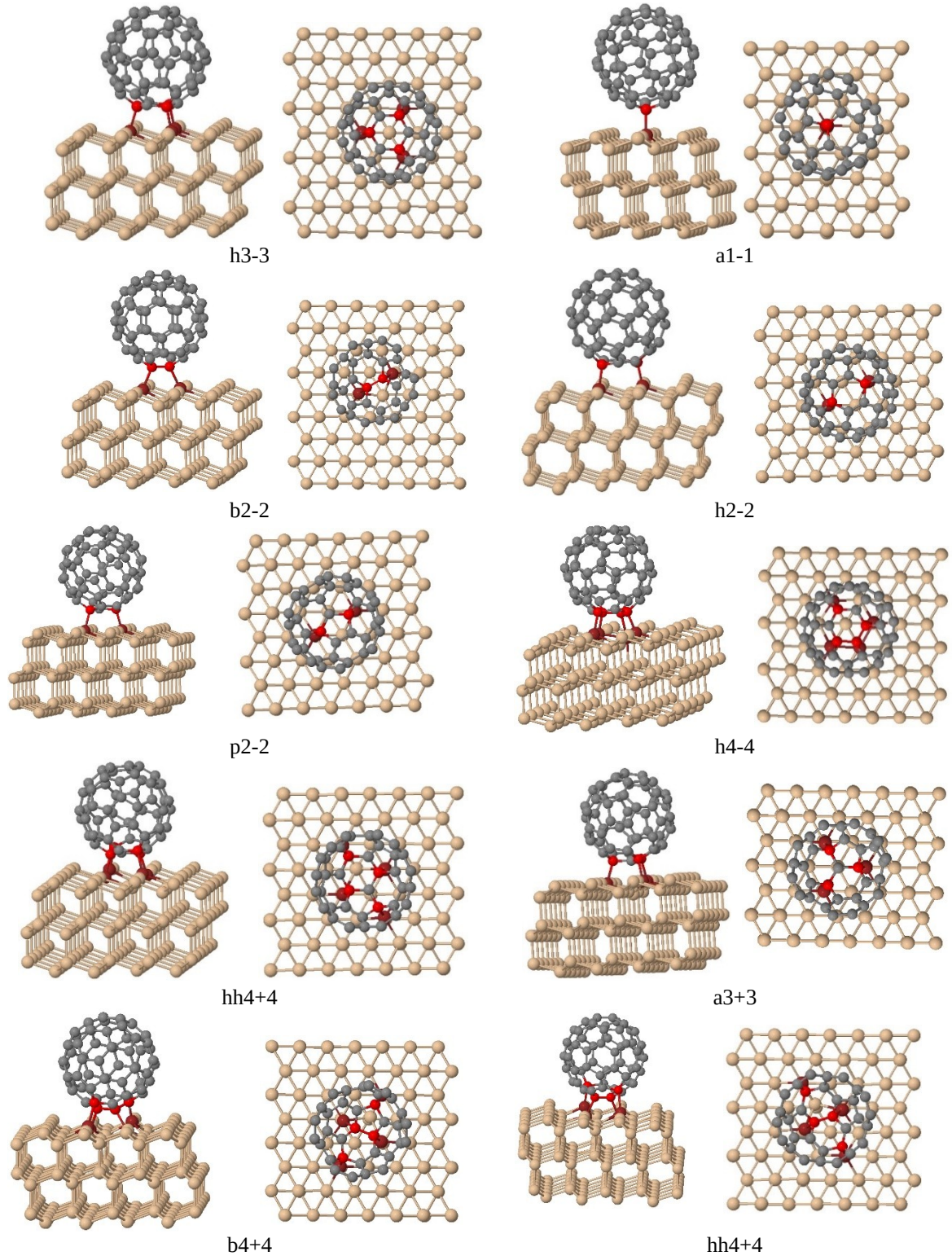
Metall yoki yarimo’tkazgichli tagliklar sirtida adsorbsiyalangan klaster, molekula yoki atomlarning sirt bilan bog’lanish energiyalari ko’pgina MD yoki DFT usuliga asoslangan nazariy ishlarda [26-29] molekula taglikka adsorbsiyalangan holatdagi butun sistema potensial energiyasidan taglik va molekula o’zaro ta’sir holatida bo’lmagandagi yig’indi potensial energiyalarining ayirmasiga teng bo’ladi, ya’ni

$$E_{ads} = E_{tag/mol} - \left(E_{tag} + E_{mol} \right).$$

Bunda E_{ads} – C_{60} fulleren molekulasining kremniy taglik sirtida adsorbsiyalanish energiyasi, $E_{tag/mol}$ – kremniy taglik va fulleren molekulasining o’zaro ta’sirlashuv vaqtidagi to’liq potensial energiyasi, E_{tag} va E_{mol} mos ravishda taglik va fulleren molekulasining o’zaro ta’sirlashmagan vaqtdagi, ya’ni yakkalangan holatdagi potensial energiyalari hisoblanadi. Ushbu energiya qiymatlari $0\,K$ haroratda taglik va fulleren molekulalarining muvozanatli holatida, energiyalarning aniqlanish shartiga mos ravishda, ular o’zaro ta’sirlashgan va yakkalangan holatlarida LAMMPS ochiq paket dasturida energiyani minimallashtirish orqali aniqlandi.

Natijalar tavsifi va tahlili

Mazkur tadqiqot ishida C_{60} fulleren molekulasining rekonstruksiyalanmagan kremniy Si(111) sirtida 10 xil konfiguratsiya bilan adsorbsiyalanishi va har bir konfiguratsiyaga mos adsorbsiya energiyalari, o’zaro ta’sir jarayonida yuzaga keluvchi har bir Si-C bog’ uzunligi va ushbu bog’larning kovalent yoki nokovalent bog’lanish tabiatiga ega ekanligiga ko’ra kimyoviy yoki fizik bog’lanish xarakteriga ega ekanligi aniqlandi. Tadqiqot ishida aniqlangan miqdoriy natijalar quyidagi 1- jadvalda o’z aksini topgan.



2-rasm. C_{60} fulleren molekulasining rekonstruksiyalanmagan kremniy Si(111) sirtida kuzatilgan adsorbsiyalarining yondan va yuqoridan ko’rinishi. Bunda Si-C bog’lanishlarni yuzaga keltirgan kremniy va uglerod atomlari mos ravishda jigarrang va qizil ranglarda ifodalangan.

1- jadvalning birinchi ustunida fulleren molekulasining adsorbsiyalanish konfiguratsiyalari berilgan bo’lib, ushbu klassifikatsiya – fulleren molekulasidagi pentagon, geksagon, bridj va tugundagi atomlarning bog’lanishda ishtirok etuvchi soni bilan belgilashga asoslangan. Masalan, C_{60} fulleren molekulasi geksagoni (hexagon) dagi 3 ta

atom kremniy taglik sirtidagi uchta kremniy atomi bilan Si-C bog'lanish hosil qilgan bo'lsa, ushbu konfiguratsiya h3-3 kabi belgilandi.

1- jadval. C_{60} fulleren molekulasining taglik sirtida adsorbsiyalanish konfiguratsiyalari va ularga mos adsorbsiya energiyalari va bog' uzunliklari.

№	Konfigurtasiya	E_{ads} (eV)	λ (Å)
1	h3-3	4.22	1.95-1.96
2	a1-1	1.63	1.94
3	b2-2	1.75	2.02
4	h2-2	2.80	1.94-1.95
5	p2-2	2.87	1.95
6	h4-4	1.92	2.09-2.12
7	hh4+4	2.59	1.92-2.23
8	a3+3	4.71	1.9-2.05
9	b4+4	2.78	1.91-2.07
10	hh4+4	2.13	1.97-2.11

1- jadvaldagi natijalarga e'tibor berilsa, h3-3 va a3-3 konfiguratsiyali adsorbsiyalarda bog'lanish energiyalari tadqiqot ishida kuzatilgan eng kichik adsorbsiya energiyasidan deyarli uch marta katta qiymatga ega ekanligini ko'rish mumkin. Bunday keskinlikni ushbu holatlarning har birida kuzatilgan ikkita kovalent bog'lar sababli deyish mumkin, shuningdek ushbu holatlarda C_{60} fulleren molekulasining pentagonal konturidagi C¿C juft bog'lar uzulib, kremniy atomi bilan Si−¿C kovalent bog'lar hosil qiladi. Buni adsorbsiyadan oldin 1.48 Å uzunlikdagi C¿C juft bog'larning adsorbsiyadan keyin 1.54 Å uzunlikdagi C−¿C yakkalik bog'ga aylanishida ko'rishimiz mumkin. Kuzatilgan b2-2 konfiguratsiyali adsorbsiyada bog'lanish energiyasi 1.75 eV ni tashkil qilib, bu holatda ikkita 2.02 Å uzunlikdagi fizik bog' (Van der Vaals bog'lari) hosil bo'lgan bo'lib, bunday deyishmizga sabab, har bir bog'ga to'g'ri keluvchi o'rtacha bog'lanish energiyasi 1 eV dan kichik va shuningdek, adabiyotlarda keltirilgan uzunligi 1.93 – 1.94 Å atrofida [30] bo'ladigan S−¿C kovalent bog' uzunligidan katta. Bu kabi tahlilga tayanadigan bo'lsak, ushbu tadqiqotda olingan quyidagi konfiguratsiyadagi adsorbsiyalarni kimyoviy adsorbsiya sifatida tasdiqlash mumkin: h3-3, a1-1, h2-2, p2-2, hh4+4, a3+3 va b4+4.

Xulosa

Olingan natijalarni o'zaro solishtirma tahlil qilish va turli kesimli kremniy tagliklar sirtida fulleren C_{60} molekulasining adsorbsiyasini MD usulida modellashtirish orqali olingan natijalar bilan taqqoslab quyidagiga xulosalarga kelindi: fulleren C_{60} molekulasi rekonstruksiyalanmagan kremniy Si(111) taglikning faqat birinchi qatlamidagi kremniy atomlari bilan Si-C bog'lanishlarni hosil qiladi; fulleren C_{60} molekulasidagi C=C juft bog'lar uzilib, kremniy atomi bilan Si-C kovalent bog' hosil qiladi va ushbu bog'lar hisobiga C_{60} molekulasining sirtdagi adsirbsiyasi barqaror bog'lanish kasb etadi; adsorbsiya energiyasi ta'sirlashuvda yuzaga keluvchi Si-C bog'lar soniga bog'liq bo'ladi; fulleren C_{60} molekulasi rekosntruksiyalanmagan kremniy Si(111) kesimli taglikda adsorbsiyasi kimyoviy va fizik (Van der Vaals) bog'lari yuzaga keladi; fulleren molekulasi ta'sirida Si-C bog'lanishda ishtirok etuvchi kremniy atomlariga ega Si-Si bog'lanishlarda kichik o'zgarishlar bo'lib, buning natijasida ushbu bog'lar uzunligi ortadi va o'zaro ta'sir potensial energiyasining absolyut qiymati kamayadi. Shuningdek, fulleren C_{60} molekulasining kremniy Si(100) [31] va nuqsonli Si(100) [32] sirtdagi adsorbsiyalarida kuzatilgan adsorbsiya energiyalariga nisbatan ko'rib o'tilgan kesimli sirtdagi adsorbsiya energiyalari kichikroq qiymatlarni qabul qilar ekan.

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