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Molekulyar dinamika usullari yordamida C_{20} fullerenning rekonstruksiyalangan kremniy Si(001) sirti bilan o'zaro ta'sir jarayonlarini tahlil qilish

Annotatsiya

Ushbu ishda rekonstruksiyalangan kremniy Si(001) sirtida C_{20} fulleren molekulasining bir necha xil konfiguratsiyalar bilan sirtdagi dimer va trench qatorlarida adsobsiyalanish protsessi molekulyar dinamika usuli asosida LAMMPS ochiq paket dasturi yordamida semulatsiya qilingan holda o'rganilgan. Taglik va fulleren molekulasidagi atomlar orasidagi o'zaro ta'sirlashuvlar Tersoff atomlararo potensiali orqali ifoda qilingan holda, C_{20} ning kremniy taglikda adsorbsiya energiyalari aniqlangan. Olingan Si-C bog'lanish energiyalari va bog' uzunliklarini qiyosiy tahlili asosida barqaror bog'lanish holat va konfiguratsiyalari aniqlangan.

Kalit so'zlar: kremniy, fulleren molekulasi, modellashtirish, Tersoff potensiali, bog' uzunligi, atom, potensial energiya, adsorbsiya energiyasi, o'zaro ta'sir, sirt, dimer, trench, adsorbsiya.

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Анализ процессов взаимодействия фуллерена C_{20} с реконстуированной поверхностью кремния Si(001) методами молекулярной динамики

Аннотация

Приведены результаты моделирования процесса адсорбции молекул фуллерена C_{20} реконструированной поверхностью кремния Si(001), полученные методами молекулярной динамики (LAMMPS). Исследован процесс адсорбции молекулы фуллерена C20 реконструированной поверхностью кремния Si(001) в рядах димеров и траншей на поверхности. Взаимодействие между поверхностью и молекулами фуллеренов определелялись потенциалом Терсоффа. На основе сравнительного анализа полученных энергий и длин связей Si-C, определены стабильные состояния и конфигурации связей.

Ключевые слова: кремний, молекула фуллерена, моделирование, потенциал

Терсоффа, длина связи, атом, потенциальная энергия, энергия адсорбции, взаимодействие, поверхность, димер, канавка, адсорбция.

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Analysis of interaction processes of C_{20} fullerene with reconstructed silicon Si(001) surface using molecular dynamics methods

Abstract

In this work, the adsorption process of the C20 fullerene molecule with several different configurations on the reconstructed silicon Si(001) surface in dimer and trench rows on the surface was studied by simulation using the LAMMPS open package program based on the molecular dynamics method. The interactions between atoms in the substrate and the fullerene molecule are expressed by the Tersoff interatomic potential, and the adsorption energies of C20 on the silicon substrate were determined. Based on the comparative analysis of obtained Si-C bond energies and bond lengths, stable bond states and configurations were determined.

Key words: silicon, fullerene molecule, modeling, Tersoff potential, bond length, atom, potential energy, adsorption energy, interaction, surface, dimer, trench, adsorption.

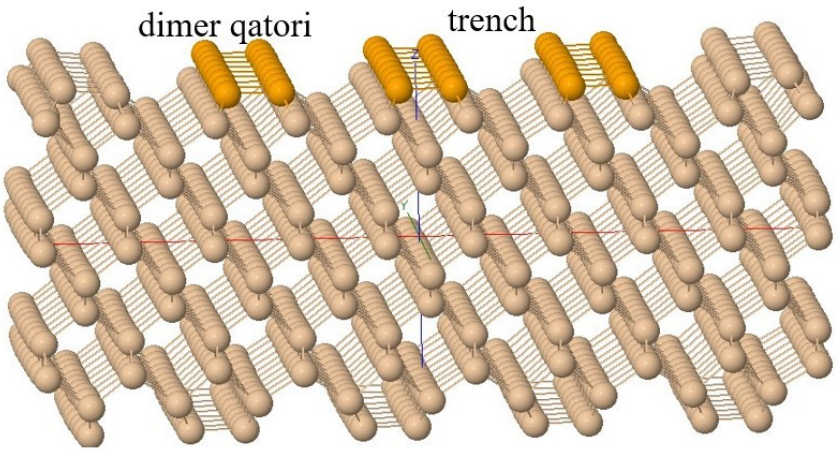
Kirish

Uglerodning allotropik shakl o’zgarishi bo’lgan fullerenlarning 1985 yilda kashf etilishi bilan uglerod nano-strukturalar davri boshlandi [1]. Fulleren molekulalarining turli o’lcham va shaklga egaligi sababli, ular yoqilg’i sanoati [2-4] va quyosh batareyalari [5,6], biyotibbiyot [7,8] va fullerenlar asosidagi mustahkamlanuvchi kompozitlar [9-11] sohalarida fullerenlargagina xos xususiyatlari bilan yorqin istiqbolga ega. C_{20} fulleren molekulasi fulleren oilasining eng kichik yoki eng kam sondagi uglerod atomlaridan tarkib topgan vakili bo’lib [12], u Eyler teoremasiga bo’ysungan holda 12 ta pentagondan iborat bo’ladi. C_{20} o’zining bir qator xususiyatlari bilan ko’pgina sohalarda amaliy istiqbolga ega, jumladan yuqori temperaturali o’ta o’tkazuvchanlik sohasida, bu boradagi nazariy izlanishlarni olib borgan olimlar Y. Miyamoto va M. Saito, I. Spagnolatti va boshqalar o’zlarining ishlarida buni ilgari surishgan [13-15]. Shuningdek, C_{20} molekulalarining kvant kompyuterlarda amaliy ahamiyati mavjud bo’lib, qattiq-holat kubitlari sifatida inkapsuliyatsiyalangan vodorod atomiga ega vodorodlangan C_{20} molekulasi ishlatilishi mumkin [16]. Ekspremental tarzda, neytral va kichik kinetik energiyaga ega fulleren (C_{20} – C_{32}) molekulalari yangi xususiyatlarga ega yupqa plyonka hosil qilish uchun har xil tagliklarga adsorbsiya qilingan [17]. C_{60} molekulasining kremniy taglikning (001) va (111) kesimli sirtlariga adsorbsiyasiga doir DFT (density functional theory) va MD (molekulyar dinamika) usullari asosidagi

nazariy ishlar [18-21] amalga oshirilganiga qaramasdan, C_{20} fulleren molekulasining kremniy Si(001) sirtda adsorbsiyalanishi bilan bog'liq nazariy ishlar kam uchraydi.
Ushbu tadqiqotning maqsadi – C_{20} fulleren molekulasining rekonstruksiyalangan kremniy Si(001) sirtida adsorbsiyalanish jarayonini molekulyar dinamika (MD) usuli asosida o'rganish, energiyani minimallashtirish usuli asosida fulleren molekulalarining adsorbsiyalanish energiyalari, adsorbsiyalanishda yuzaga keluvchi qo'shimcha Si-C bog'lar uzunligi va barqaror adsorbsiyalanish holatlari va ularga mos konfiguratsiyalarni aniqlashdan iborat.

Metodologiya

Tadqiqot davomida amalga oshirilgan barcha MD simulyatsiyalari ochiq manba MD simulyatori LAMMPS [22] paket dasturi va Nanotube Modeler [23] kompyuter dasturi orqali bajarildi. Taglik va C_{20} fulleren molekulalaridagi atomlar orasidagi Si-Si, Si-C va C-C o'zaro ta'sirlashuvlar ikkinchi tartibli Tersoff atomlararo potensiali yordamida ifodalandi [24]. C_{20} molekulasining kremniy taglikka adsorbsiyalanish jarayonlarida 1083 atomdan iborat, o'lchamlari $34 \times 34 \times 15.2$ Å ga teng kremniy monokristallidan foydalanildi. Simulatsiya jarayoni va adsorbsiyalanish holatlari JMOL [25] kompyuter dasturida vizualizatsiya qilinishi bilan bir qatorda, Si-C bog'lar uzunligi va zaruriy konfiguratsiya va holatlarga mos taglik va C_{20} fulleren molekulasiga tegishli atomlarning koordinatalari ham ushbu dastur yordamida olindi. Turli o'lcham va atom sonidagi tagliklar bilan qilingan natijalar solishtirilganda taglik o'lchami bilan bog'liq effektlar kuzatilmadi. Noze-Guver termostati [26] dan NVT ansambli uchun tanlangan haroratni doimiy ushlab turishda 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.



1- rasm. Kremniy taglikdagi dimer va trench qatorlari

1- rasmda rekonstruksiyalanagan (001) sirtga ega va tadqiqot davomida taglik sifatida qo'llanilgan kremniy monokristali sirtidagi dimer va trench qatorlari tasvirlangan bo'lib, unda dimer qatoridagi Si-Si dimer bog'lar hosil qiluvchi kremniy atomlari to'q sariq rangda berilgan. Ikki dimer qatori orasidagi kanal (bo'shliq) – trench deb ataladi. C_{20} fulleren molekulasining adsorbsiyasi dimer qatori va trenchda kuzatilgan. Shuning uchun rn va tn qisqartmalardan foydalanilgan. n – adsorbsiyalanishda kuzatilgan bog'lar soni.

Adsorbsiya energiyasini hisoblash

Taglik sirtida adsorbsiyalangan molekula yoki klaster uchun adsorbsiya energiyasi E_{ads} taglik va unda adsorbsiyalangan molekula yoki klasterning muvozanat holatidagi to'liq energiyasi $E_{ads/¿¿}^{tot}$ dan taglik bilan molekula yoki klaster o'zaro ta'sirlashmagan vaqtdagi taglikning muvozanat holatidagi to'liq energiyasi $E_{¿}^{tot}$ va molekula yoki klasterning muvozanat holatidagi to'liq energiyasi E_{ads}^{tot} larning yig'indisini ayirmasiga teng [27-28]:

$$E_{ads} = E_{ads/¿}^{tot} - \left(E_{¿}^{tot} + E_{ads}^{tot}\right). ¿$$

C_{20} fulleren molekulasining kremniy taglikka adsorbsiyalanish energiyasi aniqlash uchun, dastlab, $0\,K$ temperaturada kremniy taglikning muvozanat holatidagi to'liq energiyasi $E_{¿}^{tot}$, keyin C_{20} fulleren molekulasining muvozant holatidagi to'liq energiyasi E_{ads}^{tot} hisoblab chiqildi. Bundan keyin esa, C_{20} fulleren molekulasining kremniy taglikka adsorbsiyalanish holatida taglik va C_{20} fulleren molekulasining muvozanatdagi to'liq energiyasi $E_{ads/¿¿}^{tot}$ ham $0\,K$ temperaturada aniqlandi va yuqoridagi formula asosida adsorbsiya energiyasi E_{ads} olindi. Barcha energiya qiymatlari LAMMPS ochiq paket dasturida energiyani minimaltirish usuli asosida hisoblandi.

Natijalar tavsifi va tahlili

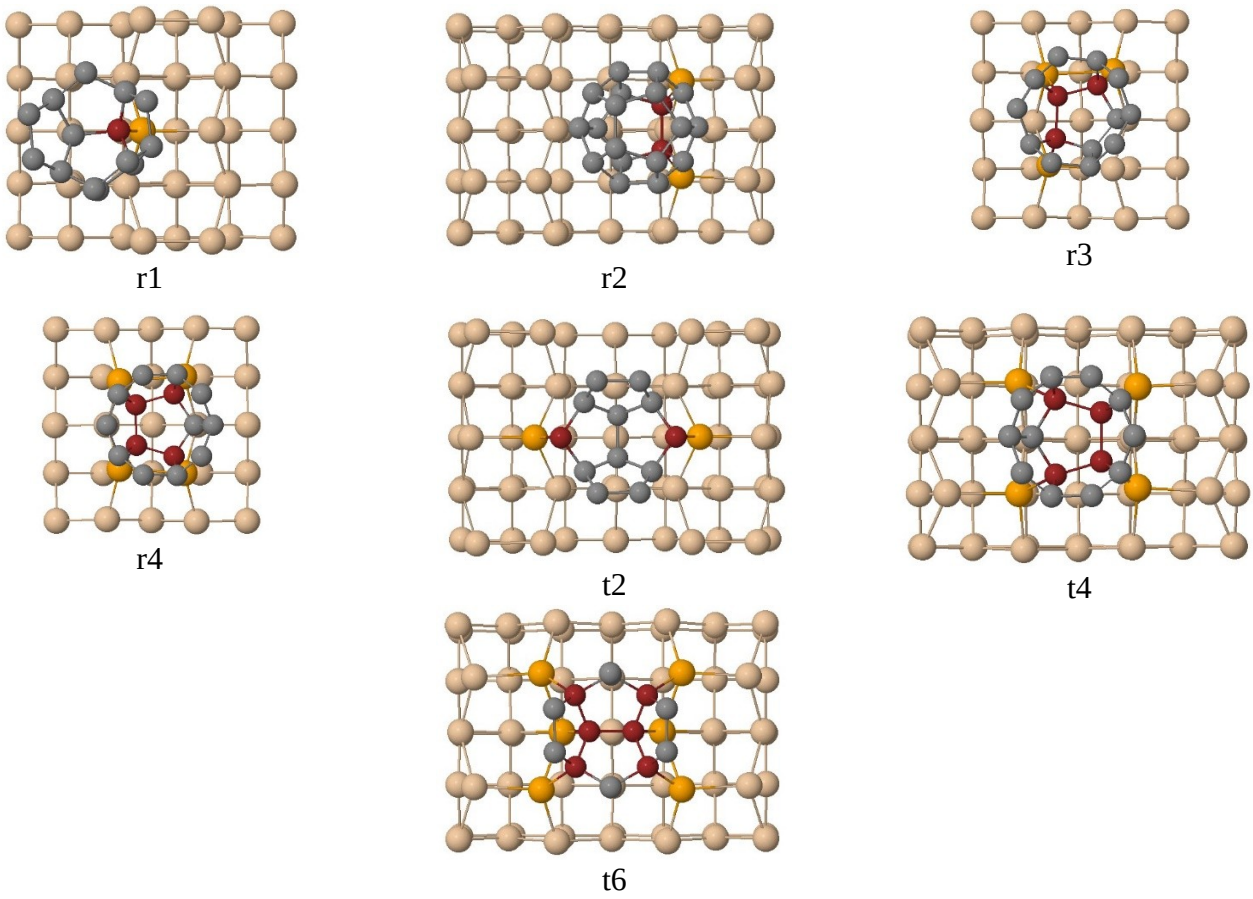
Tadqiqot ishi davomida C_{20} fulleren molekulasining rekonstruksiyalangan kremniy Si(001) sirtida dimer qatori va trench ustida 7 xil konfiguratsiya bilan adsorbsiyalanishi aniqlandi va ayni konfiguratsiyalar uchun adsorbsiya energiyasi, adsorbsiyalanishda yuzaga keluvchi Si-C bog'lar uzunligi yuqorida ta'kidlangandek tartibda hisoblab chiqildi. Ushbu natijalar quyidagi 1- jadvalda bayon qilingan.

1-jadval. C_{20} fulleren molekulasining kremniy Si(001) sirtda adsorbsiyalanish holat va konfiguratsiyalariga mos adsorbsiya enrgiya va yuzaga keluvchi Si-C bog'larning uzunliklari.

№	Konfigurtasiya	E_{ads} (eV)	λ (Å)
1	r1	-2.362	1.91
2	r2	-3.295	1.96
3	r3	-3.910	1.97-2.00
4	r4	-4.891	1.97-2.01
5	t2	-1.352	2.02-2.03
6	t4	-4.295	2.05-2.06
7	t6	-7.292	1.96-2.07

1- jadvalda C_{20} fulleren molekulasining kremniy Si(001) sirtda kuzatilgan adsorbsiyalanish konfiguratsiyalariga mos adsorbsiya energiyasi E_{ads} va Si-C bog'larning uzunliklari λ qiymatlari berilgan. Olingan natijalarning solishtirma tahlili shuni ko'rsatdiki, C_{20} fulleren molekulasining trench sohasida r4, t4 va t6 konfiguratsiyalar barqaror adsorbsiya deb, hisoblash mumkin. Bunga sabab, ushbu konfiguratsiylarga mos adsorbsiya energiya qiymatlarining nisbatan yuqori va bog' uzunliklarining qisqa ekanligidir. Barqaror adsorbsiya holatlarining aynan trench sohasida ko'proq kuzatilishining sababi ushbu sohalarda C_{20} fulleren molekulasidagi uglerod atomlari taglik yaqinroq holatlarni egallash imkonining mavjudligi natijasida bog'lar sonining ortishi bilan kovalent bog'lar hosil bo'lish ehtimolining ortishi natijasida ko'proq sondagi kovalent bog'larning yuzaga kelishidir. Buni

Si-C bog’lar uzunliklarini adabiyotlarda berilgan qiymati bilan solishtirish orqali ham amin bo’lish mumkin. Adabiyotlardagi Si-C bog’lar uzunligi 1.93-1.94 Å qiymatga teng bo’lib [30], barqaror adsorbsiyalanish holatlariga mos Si-C bog’ uzunliklari ichida ushbu qiymatdan kichik va unga yaqin qiymatlar mavjudligini ko’rish mumkin. Nobarqaror holatlarda adsorbsiya enrgiyasi kichik va ushbu holatlardagi bog’ uzunliklarining aksariyati adabiyotdagi qiymatdan katta ekanligi, ularning kuchsiz nokovalent bog’lar ekanligidan dalolat beradi.



2- rasm. C_{20} fulleren molekulasining kremniy Si(001) sirtda dimer qatorlari va trenchda adsorbsiyalanish holatlarining yuqoridan ko’rinishi

C_{20} fulleren molekulasining tadqiqot ishida aniqlangan adsorbsiyalanish holatlari va konfiguratsiyalariga mos simulatsiya tasvirlari 1- rasmda taqdim qilingan bo’lib, unda sariq rangdagi atomlar kremniy, to’q kulranglilari esa C_{20} fulleren molekulasidagi uglerod atomlari hisoblanadi. Si-C bog’lanish hosil qilgan kremniy va uglerod atomlari mos ravishda to’q sariq va malla ranglarda berilgan.

Xulosa

Fulleren C_{20} molekulasining rekonstruksiyalangan kremniy Si(001) sirtida adsorbsiya-siga doir tadqiqotda erishilgan natijalar tahlili natijasida quyidagicha xulosalarga kelindi: molekulaning kremniy taglik sirtida adsorbsiyalanish energiyasi va ushbu jarayonda hosil bo’luvchi kremniy va uglerod atomlari orasidagi bog’lanishlar uzunligi molekula dimer yoki trenchda adsorbsiyalanishiga bog’liq va adsorbsiyalanish konfiguratsiyasiga qarab o’zgarib boradi; ayni bir adsorbsiyalanish holatidagi bog’lar uzunligi turlicha va ular ham kovalent, ham nokovalent bog’lanishlarga mos keladi; molekulaning trench qatorida adsorbsiya

holatlari qolgan holatlarga nisbatan barqarorligi bilan ajralib turadi, shuningdek barqaror adsorbsiyalanish holatlarida kovalent bog'lar soni bog'lanish konfiguratsiyasiga bog'liq ravishda bir va undan ortiq sonda bo'lishi mumkin; adsorbsiya vaqtida Si-C bog'lanishda qatnashuvchi atomlarni o'z ichiga oluvchi Si-Si va C-C bog'lar uzunligi ortadi.

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