KREMNIY SI(100)2×1 SIRTIDA ADSORBSIYALANGAN $C_{20}@C_N$ VA $C_{60}@C_N$ (N=1, 3) EKZOFULLERENLARINI FULLERENLAR ADSORBSIYASI MAVJUD BO'LMAGANDA VAQT PARAMETRLARI BO'YICHA BAHOLASH

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Annotatsiya. Ushbu tadqiqot ishida Si(100)2×1 sirtining dimer qatorida C_n (n=1, 3) uglerod klasterlari orqali adsorbsiyalangan $C_{20}@C_n$ va $C_{60}@C_n$ ekzofullerenlarining fullerenlar adsorbsiyasi mavjud bo'lmaganda C_{20} va C_{60} fulleren molekulalarining C_n uglerod klasterlarini fulleren molekulasiga ekzodrillovchi yakkalik C-C bog' bo'ylab o'tuchi o'q atrofidagi aylanma va tebranma (presetsion) harakat chastotalarini past temperaturalar sohasida ($T < 100$ K) temperaturaga bog'lanishi molekulyar dinamika usuli asosida ochiq manba simuliyatori LAMMPS paket dasturida modellashtirilgan holda o'rganildi.

Аннотация. В данной исследовательской работе изучено температурное (T < 100 K) поведение частот вращательных и колебательных (прецессионных) движений вокруг оси, проходящей вдоль одиночной экзодриллирующей C–C связи углеродных кластеров C_n (n = 1, 3), адсорбированных на димерном ряду поверхности Si(100)2×1 в составе экзофуллеренов $C_{20}@C_n$ и $C_{60}@C_n$, а также в отсутствие адсорбции фуллеренов. Исследование выполнено методом молекулярной динамики с использованием открытого симуляционного пакета LAMMPS.

Abstract. In this research work, the temperature dependence (T<100 K) of the rotational and oscillatory (precessional) motion frequencies around the axis passing through the single exo-drilling C–C bond of carbon clusters C_n (n = 1, 3), adsorbed on the dimer row of the Si(100)2×1 surface as part of the exofullerenes $C_{20}@C_n$ and $C_{60}@C_n$, as well as in the absence of fullerene adsorption, was studied. The study was carried out using the molecular dynamics method and modeled in the open-source simulator LAMMPS.

Kalit so'zlar: fulleren, kremniy, adsorbsiya, aylanma harakat, presetsiya, chastota, temperatura, energiya, bog', modellashtirish.

Ключевые слова: фуллерен, кремний, адсорбция, вращательное движение, прецессия, частота, температура, энергия, связь, моделирование.

Keywords: fullerene, silicon, adsorption, rotational motion, precision, frequency, temperature, energy, bond, modelling.

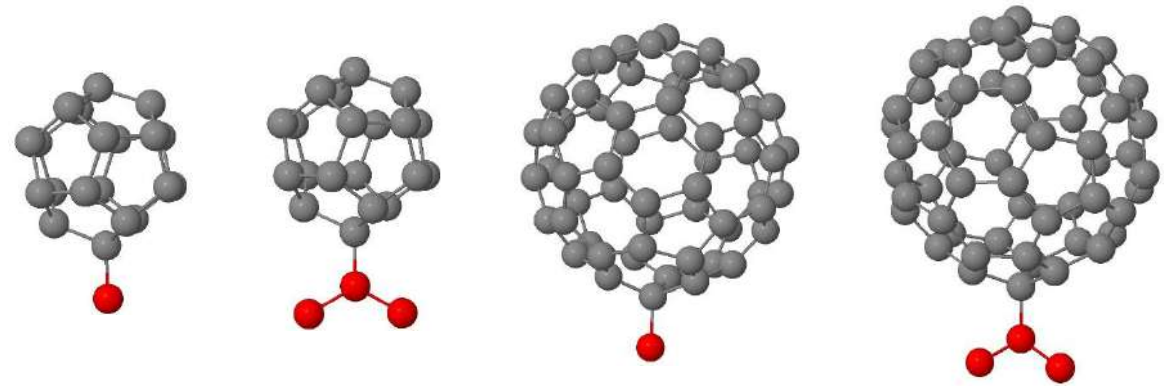
Fulleren molekulalari adsorbsiyalanishidan yuzaga keluvchi nanostrukturalar o'zining noyob fizik va kimyoviy xususiyatlari sababli bugungi kun ilmiy izlanishlarning muhim tadqiqot sohalaridan biri sifatida ilmiy izlanuvchilar e'tiborini jalb qilib kelayotgan yo'nalishlardan biri hisoblanadi. Jumladan, (100)2×1 rekonstruksiyali kremniy taglik sirtida C_{20} va C_{60} molekulalarining C_n uglerod klasterlari yordamida adsorbsiyalanishidan yuzaga keluvchi gibrid materiallar yarimo'tkazgichli qurilmalar o'rnini bosuvchi molekulyar qurilmalar ishlab chiqarishda ahamiyatli hisoblansa [1], organik quyosh elementlarining muhim tarkibiy qismi bo'lgan fulleren asosli gibrid materiallarda fulleren C_{60} molekulasining qatlam sirtida adsorbsiyalanishining mustahkam bo'lishligi katta ahamiyat kasb etadi [2] va $C_{20}@C_n$ va $C_{60}@C_n$ (n=1-5) ekzofullerenlari C_{20} va C_{60} fulleren molekulalariga nibatan kremniy Si(100) taglik sirtida qattiq yoki kovalent bog'lanishli Si-C bog'lar hosil qilgan holda adsorbsiyalanar ekan [3]. Mazkur omillarning mavjudligi o'laroq, kremniy tagliklar sirtida C_n uglerod klasterlari yordamida adsorbsiyalangan $C_{20}@C_n$ va $C_{60}@C_n$ ekzofullerenlarini fullerenlar adsorbsiyasi mavjud bo'lmaganda vaqt parametrlari bo'yicha baholash orqali tadqiq etish bugungi kun fulleren asosidagi qurilmalar (molekulyar tranzistorlar, sensorlar, kvant komponentlar) uchun molekulalarning sirtga nisbatan yo'nalishi va dinamik barqarorligi funksional xususiyatlarni belgilaydi.

C_{20} va C_{60} fulleren molekulalarining C-C bog' bo'ylab o'tuvchi o'q atrofidagi aylanma va ma'lum yo'nalishdagi soda tebranma (presetsion) harakatlariga o'xshash harakatlar ochiq zanjirli alkanlar (C_nH_{2n+2}) guruhining barchasida fulleren molekulalaridagi singari σ bog'lanishli markaziy C-C bog' atrofida kuzatiladi [4-9]. Alkanlarda CH_3 guruhlarning ichki aylanma harakatiga potensial to'siqlar mavjud, masalan, etan uchun ushbu qiymat ≈ 12 kJ/mol ni tashkil qiladi va u maksimal va minimal konformatsiyalar orasidagi energiya farqlari hisobidan yuzaga kelib, ushbu potensial energiya burilish (dihedral) burchagining funksiyasi bo'lib, uto'liq 360° aylanish doirasida uchta ekvivalent minima (qadamli) va uchta maksima (tutilgan) ni ko'rsatadi [5]. Steric/repulsion modeliga ko'ra, eclipsed holatda bitta CH_3 dagi vodorodlar ikkinchi CH_3 dagi vodorodlarga yaqinlashadi, bu esa H–H itarilishga olib kelgan holda ta'sirlashuv energiyasini oshiradi [10].

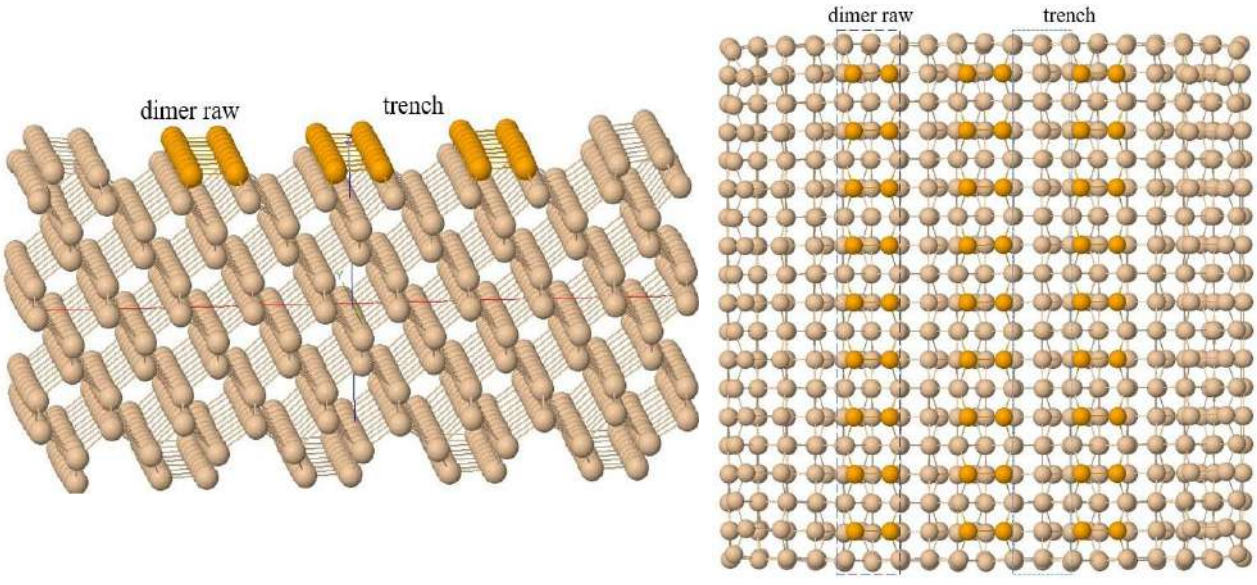
Mazkur tadqiqot ishida Si(100)2×1 sirtning dimer qatorlarida C_n (n=1, 3) uglerod klasterlari orqali adsorbsiyalangan $C_{20}@C_n$ va $C_{60}@C_n$ ekzofullerenlarining C_{20} va C_{60} fulleren molekulalarining bevosita Si(100)2×1 sirtda adsorbsiyasi kuzatilmagan hollarda ushbu fullerenlarning C-C bog' bo'ylab o'tuvchi o'q atrofidagi aylanma va shu o'qga nisbatan tebranma harakatlari molekulyar dinamika (MD) usulida modellashtirish orqali bu ikki harakatning

chastotalarini past temperaturalar sohasida ($T < 100$ K) temperaturani 10 K qadam bilan oshirib borish orqali temperturaga bog'lanishi tadqiq etilgan.

Yuqorida aytib o'tilgan modellashtirish ishlari LAMMPS ochiq paket dasturi [11] yordamida amalga oshirilgan. Olingan natijalarni vizualizatsiya qilish va ko'rib chiqalayotgan har bir harakat parametrlarini aniqlash uchun JMOL [12] kompyuter dasturidan foydalanilgan. C_{20} va C_{60} fulleren molekulalarining geometrik modellarining koordinatalari Nanotube Modeler [13] kompyuter dasturining ma'lumotlar bazasidan olingan. C_1 va C_3 uglerod klasterlarining C_{20} va C_{60} fulleren molekulalariga ekzodrillanishi, $C_{20}@C_1$, $C_{60}@C_1$ va $C_{20}@C_3$, $C_{60}@C_3$ (2-rasm) ekzofullerenlarining C_1 va C_3 uglerod klasterlari yordami Si(100)2×1 sirtda adsorbsiyasi LAMMPS paket dasturida MD usulida simuliyatsiya qilindi. $34 \times 34 \times 15.2$ Å o'lchamli va 1083 atomdan iborat Si(100) taglik (1-rasm) dastlab LAMMPS paket dasturida yordamchi dastur yozish orqali olindi va undagi 2×1 rekonstruksiya adabiyotlarda [14] ta'kidlangan singari JMOL kompyuter dasturida olindi. Simuliyatsiya qilinayotgan tizim temperaturasi, uning hajmi va undagi atomlar soni NVT ansambli yordamida boshqarildi.



$C_{20}@C_1$ $C_{20}@C_3$ $C_{60}@C_1$ $C_{60}@C_3$

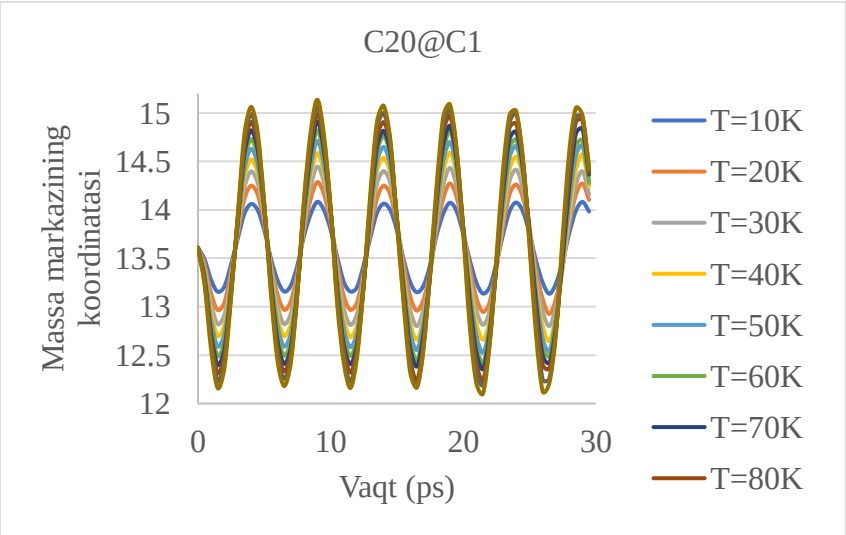


a) *b)*

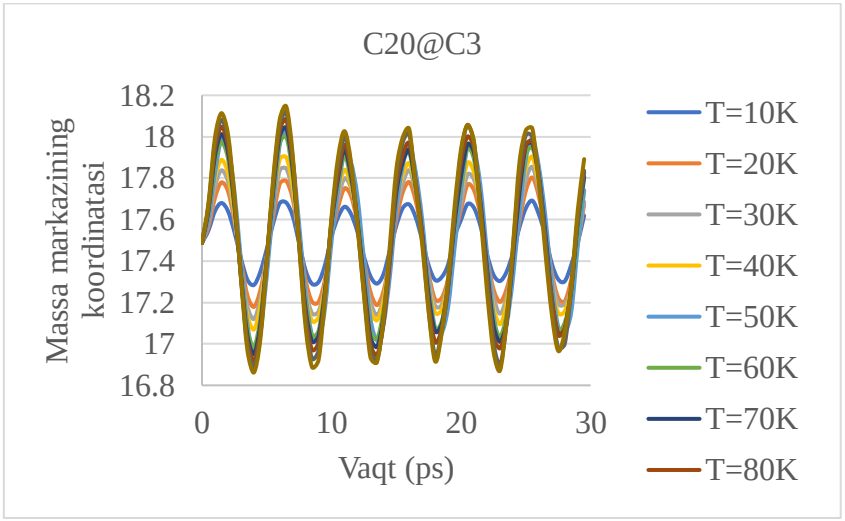
1- rasm. Si(100)2×1 taglikning yondan (*a*) va yuqoridan (*b*) ko'rinishi

Si(100)2×1 sirtining dimer qatorida $C_{20}@C_n$ va $C_{60}@C_n$ ekzofullerenlar C_n uglerod klasterlari bilan adsorbsiyalanib, C_n uglerod klasteridagi uglerod atomlari soni n=1, 3 va C_n klasterining C_{20} va C_{60} fulleren molekulalari bilan ekzodrillanishi yagona C-C bog' orqali kuzatilganda fulleren molekulalari Si(100)2×1 sirtda adsorbsiyalanmasdan, klasterning ekzodrillanishiga sabab bo'lgan C-C bog' bo'ylab o'tuvchi o'q atrofida aylanma va tebranma (presetsion) harakatlarni amalga oshiradi. Agar C_n uglerod klasteri undagi atomlar soni n=1, 3 bo'lib, fulleren molekulalariga ikki va undan tadan ortiq sondagi C-C bog'lar yordamida ekzodrillansa, fulleren molekulalarining aylanma harakati kuzatilmasdan, yagona tebranma harakati kuzatildi. Bunga sabab, fulleren molekulalarining aylanma harakatiga to'sqinlik qiluvchi potensial to'siq yakka bog'lanishli holatdagidan keskin ortib ketishidir. Agar uglerod klasterdagi atomlar soni n=2-5 va uning shakli chiziqli bo'lsa, fulleren molekulalari kremniy taglik sirtiga yiqilib, fullerenli adsorbsiya kuzatilishi natijasida tadqiqotda o'rganilgan harakatlar kuzatilmadi. Shuningdek, C_n uglerod klasteridagi atomlar soni n=4, 5 bo'lib, klasterning shakli n=1, 3 bo'lgandagi kabi fulleren molekulasiga yakkalik C-C bog' yordamida ekzodrillanishga imkon bergan hollarda, fulleren molekulalari taglik sirtiga yiqilib, sirtda fullerenli adsorbsiyalanish ikkala harakatning ham sodir bo'lishiga imkon bermas ekan.

Tizim temperaturasi 10 K qadam bilan oshirib borilganda fulleren molekulalarining C-C bog' bo'ylab o'tuvchi AB o'q atrofidagi aylanma harakati jadallashib, ya'ni ushbu harakatning chastotasi ortib borishligi aniqlandi. Shuningdek, fulleren molekulalarining presetsion harakat chastotasining ham tizim temperaturasiga bog'liqligi tizim temperaturasini 10 K qadam bilan oshirib borish orqali tadqiq qilinganda temperaturaning qaralayotgan sohasida ushbu harakat chastotasining o'zgarishsiz qolishi aniqlandi (2- va 3- rasmlar).

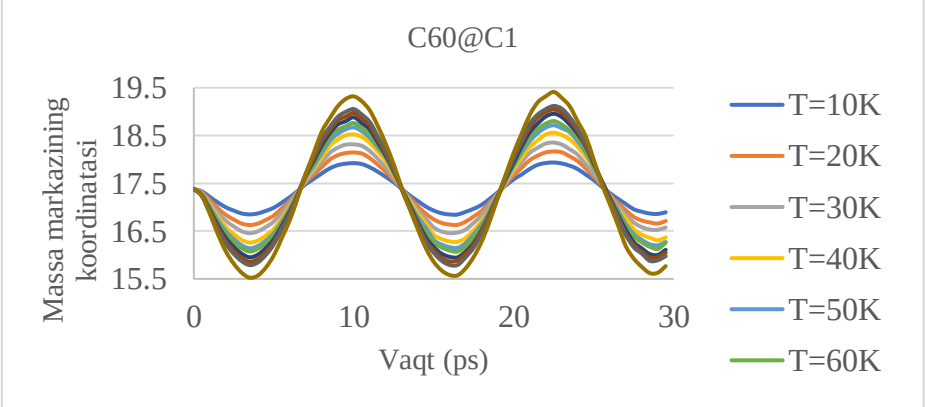


a)

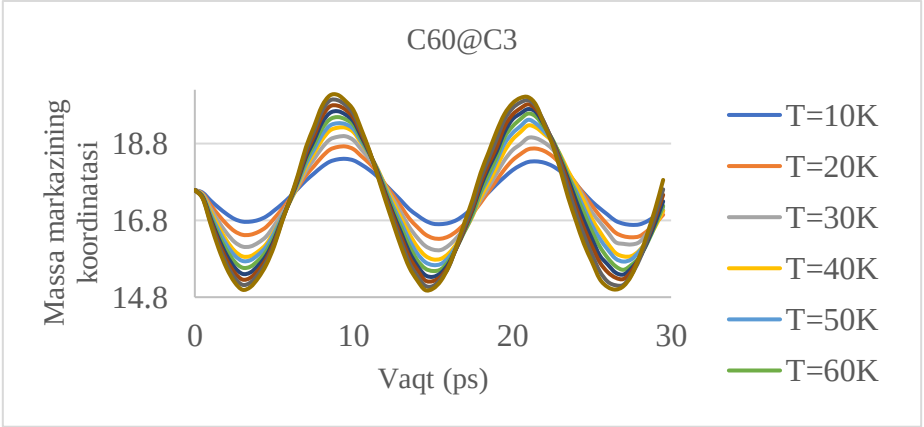


b)

2- rasm. $C_{20}@C_1$ va $C_{20}@C_3$ ekzofullerenlarining presetsion harakatadi C_{20} fulleren molekulasi massa markazi koordinatasining (x yoki y) vaqtga bog'lanishi.



a)



b)

3-rasm. $C_{60}@C_1$ va $C_{60}@C_3$ ekzofullerenlarining presetsion harakatadi C_{60} fulleren molekulasi massa markazi koordinatasining (x yoki y) vaqtga bog'lanishi.

2- va 3- rasmlardagi grafiklardan ko'rinib turibdiki, temperaturaning 10 K qadam bilan ortib borishi davomida $C_{20}@C_n$ va $C_{60}@C_n$ ekzofullerenlarining presetsion harakat chastotasi o'zgarishsiz

qolmoqda, faqat C_{20} fulleren molekulasi massa markazining tizim 0 K temperatura yaqinida bo'lganda egallaydigan holatdan og'ish masofasi (amplitudasi) ortib bormoqda. Mazkur og'ishlarning o'zgarish qiymatlari boshlang'ich temperatura o'zgarishlarida katta qiymatli va qaralayotgan temperatura intervalining oxiriga qarab esa kichik qiymatli bo'lib bormoqda. Bunga sabab sifatida fulleren molekulasining presetsion harakat kinetik energiyasining qaralayotgan og'ish qiymatlarining kvadratiga ($E \sim \Delta x^2$) proporsional ekanligini ko'rsatish mumkin.

Xulosa

Si(100) 2×1 sirtning dimer qatorida C_n uglerod klasterlari bilan adsorbsiyalangan $C_{20}@C_n$, $C_{60}@C_n$ ekzofullerenlarining n=1, 3 bo'lgan hollarda fullerenlar adsorbsiyasi mavjud bo'lmaganda C_{20} va C_{60} fulleren molekulalarining C_n uglerod klasterlarini fulleren molekulalariga ekzodrillovchi yakkalik C-C bog' bo'ylab o'tuvchi o'q atrofidagi aylanma harakat chastotasi past temperaturalar sohasida (T<100 K) temperatura ortishi bilan ortib boradi, ammo ularning presetsion harakat chastotasi temperaturaga bog'liq emasligi kuzatildi.

Adabiyotlar

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