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Fullerenga doping qilingan kremniy klasterlarining o'zaro ta'sir jarayonlarini modellashtirish

Annotatsiya

Ushbu ish kremniy (Si_n) klasterlarining C60 fulleren molekulasiga doping qilinishi natijasida hosil bo'lgan yangi birikmaning fizik-kimyoviy xossalarini molekulyar dinamika (MD) usuli asosida o'rganishga bag'ishlangan. C-C, Si-Si, C-Si o'zaro ta'sirlarini ifodalashda Tersoff potensialidan foydalanilgan. LAMMPS ochiq paket dasturi yordamida modellashtirilgan va kremniy klasterlari doping qilingan fulleren C60 molekulasining struktura barqarorligi ushbu tizim potensial energiyasi yoki tizimdagi bitta atomga mos keluvchi o'rtacha potensial energiya qiymatlari orqali o'rganilgan.

Kalit so'zlar: fulleren molekulasi, kremniy klasterlari, modellashtirish, doping, Tersoff potensiali, atom, potensial energiya

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Моделирование процессов взаимодействия кремниевых кластеров, легированных в фуллерен

Аннотация

Данное исследование посвящено изучению физико-химических свойств нового соединения, образованного в результате допирования кластеров кремния (Si_n) в молекулу фуллерена C_{60}, с использованием метода молекулярной динамики (MD). Для моделирования межатомных взаимодействий C–C, Si–Si и C–Si применялся потенциал Терсоффа. Моделирование проводилось с помощью открытого программного пакета LAMMPS. Структурная стабильность молекулы фуллерена C_{60}, допированной

кластерами кремния, анализировалась на основе полной потенциальной энергии системы и средней потенциальной энергии, приходящейся на один атом.

Ключевые слова: Молекула фуллерена, кремниевые кластеры, моделирование, легирование, потенциал Терсоффа, атом, потенциальная энергия

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Modeling the interaction processes of silicon clusters doped into fullerene

Abstract

This study is devoted to the investigation of the physicochemical properties of a new compound formed by the doping of silicon (Si_n) clusters into a C_{60} fullerene molecule, using the molecular dynamics (MD) method. The Tersoff potential was employed to model the interatomic interactions between C–C, Si–Si, and C–Si atoms. The simulations were performed using the open-source LAMMPS package. The structural stability of the C_{60} fullerene molecule doped with silicon clusters was analyzed based on the system's total potential energy and the average potential energy per atom.

Key words: Fullerene molecule, silicon clusters, modeling, doping, Tersoff potential, atom, potential energy.

Kirish

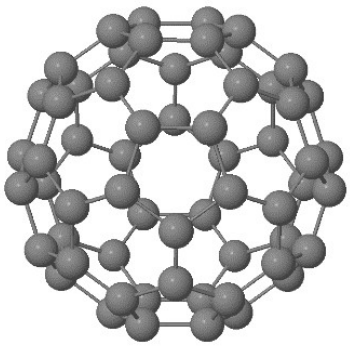
Bugungi kunda uglerod asosli nanomateriallar xususan, grafen, nanotrubkalar va fullerenlar nanoelektronika, optoelektronika hamda sensorli qurilmalarda keng qo‘llanilmoqda. Ayniqsa, fullerenga asoslangan tuzilmalar ustida olib borilayotgan ilmiy tadqiqotlar ularning fizik-kimyoviy xossalarini o‘zgartirish va boshqarish imkonini beruvchi doping usullarining rivojlanishiga sabab bo‘lmoqda. Zamonaviy materialshunoslikda yangi materiallar yaratish va mavjudlarini kerakli xossalarga ega qilib modifikatsiyalashda doping texnologiyasi alohida ahamiyatga ega [1]. Bu usul moddaning ichki tuzilmasiga chet atom yoki molekulalarni qo‘shish orqali uning elektron, optik, magnit va mexanik xossalarini tubdan o‘zgartirish imkonini beradi. Ayniqsa, nanoo‘lchamdagi karbon tuzilmalar**,** xususan fullerenlar**,** doping uchun juda qulay nanostrukturalar sirasiga kiradi [2-9]. Doping – material tarkibiga turli element atomlarini kiritish orqali ularning strukturaviy va funksional xossalarini maqsadli boshqarishga imkon beruvchi usul bo‘lib, nanomateriallar fizikasi va kimyosida keng qo‘llaniladi. Fullerenga Si, B, N, Ge kabi elementlarning kiritilishi (xususan, endohedral doping shaklida) natijasida uning elektron spektri, strukturaviy barqarorligi va kimyoviy faolligi sezilarli darajada o‘zgaradi [10-12]. $Si_n@C_{60}$ kabi endohedral tuzilmalar

yangi avlod nanoelektron qurilmalar va funksional nanomateriallar uchun istiqbolli platforma sifatida ko‘rilmoqda.[3-4]. Kremniy klasterlari doping qilingan fullerenlar yarimo‘tkazgich materiallar sirtida adsorbat ta’sirida yuzaga keluvchi hodisalarning mavjudligi bilan ilmiy-tadqiqotlarni talab qilmoqda [5-20].

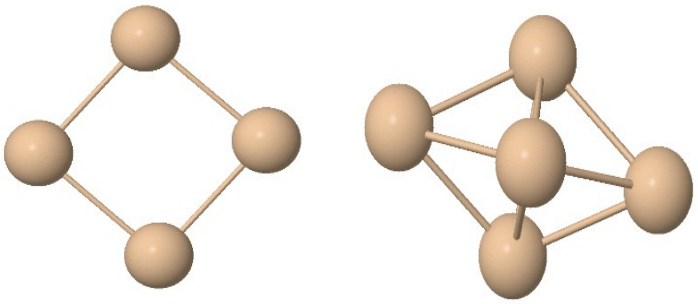
Aksariyat adabiyotlarda bu kabi tuzilmalar DFT (Density Functional Theory) usuli asosida o‘rganilgan. Ushbu usul yordamida qisqa vaqt davomida natija olinsada, lekin vaqt va haroratga bog‘liq jarayonlarni to‘liq ifodalab bera olmaydi [6-7]. Shu sababli, fullerenga kremniy kabi atomlarning doping qilinishi natijasida yuzaga keladigan strukturaviy o‘zgarishlar va barqarorlikni molekulyar dinamika (MD) usuli yordamida o‘rganish muhim ilmiy ahamiyat kasb etadi..

Metodologiya

Mazkur tadqiqot ishida kremniy klasterlari (Si_n) ning fulleren C_{60} molekulasiga doping qilinganda, fulleren qaysi maksimal atom sonigacha kremniy klasterlarini shikastlarsiz o‘z ichiga sig‘dira olish imkoniyati va hosil bo‘lgan tizimlarning minimum energiya holatidagi umumiy potensial energiyalari aniqlanib, molekulyar dinamika (MD) usuli yordamida o‘rganildi. Modellashtirish jarayonida atomlararo o‘zaro ta’sirlarni aniqlashda Tersoff potensiali qo‘llanildi[17]. Bu potensial karbon va kremniy atomlari orasidagi bog‘lanishlarni, bog‘lanish burchaklari va elektron zichligining ta’sirini hisobga olgan holda, ancha realistik natijalar beradi. Tersoff potensiali ayniqsa karbon asosidagi strukturalar (grafen, nanotrubka, fulleren) va ularning yarim o‘tkazgichlar bilan kombinatsiyasi uchun moslashtirilgan Barcha simulyatsiyalar ochiq manba kodiga ega bo‘lgan LAMMPS [18] dasturiy paketi yordamida amalga oshirildi va simulatsiya jarayoni JMOL [19] kompyuter dasturida vizualizatsiya qilindi. Fullerenga doping qilinadigan kremniy atomlarining koordinatalari JMOL kompyuter dasturi yordamida tayyorlandi.



1- rasm. C_{60} fulleren molekulasi

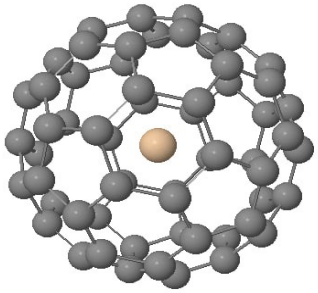


2- rasm. Si_4 va Si_5 kremniy klasterlarining ko‘rinishi

Natijalar tavsifi va tahlili

Hisoblashlar davomida C_{60} molekulasining o‘z strukturaviy yaxlitligini saqlab qolgan holda kremniy klasterlarini qabul qila olish chegarasi va bu holatdagi energetik barqarorlik baholandi. Dastlabki natijalar shuni ko‘rsatdiki, fulleren molekulasiga to‘qqiztagacha atomdan iborat kremniy klasterlari doping qilinganda, hosil bo‘lgan $Si_n@C_{60}$ birikmasi energiya jihatidan barqaror konfiguratsiyalarga ega bo‘ladi. Ushbu tizim uchun energiyani

minimallashtirish orqali hisoblangan atomlar soniga mos keluvchi potensial energiyalari mos ravishda n=1,2,3,4,5,6,7,8,9 va E_1 = –6.80 eV, E_2 = –6.74 eV, E_3 = –6.68 eV, E_4 = –6.56 eV, E_5 = –6.40 eV, E_6 = –6.29 eV, E_7= –6.07 eV, E_8 = –5.86 eV, E_1 = –5.68 eV ga teng bo‘ldi. Kremniy klasteridagi atomlar soni oshirilganda, tizimdagi bitta atomga to‘g‘ri keluvchi potensial energiya qiymati kamayganligi aniqlandi. Bu esa, klasterning atomlar soni ortib borishi bilan fulleren molekulasi strukturasi ichidagi deformatsiya va atomlararo o‘zaro ta’sir kuchlarining o‘zgarishiga olib kelishini ko‘rsatadi. Si_n klasteridagi kremniy atomlarining ko‘payishi fullerendagi barqarorlik kamayishiga sabab bo‘ladi, bu esa C_{60} karkasining elastik chegarasiga yaqinlashishiga olib kelishi mumkin.Olingan hisoblash natijalari ilgari olib borilgan nazariy tadqiqotlar [4-16] va ba’zi eksperimental kuzatuvlar [5-17] bilan yaxshi mos tushadi. Shuningdek, Si_n klasterlarining C_{60} molekulasi ichida barqaror holatda joylashishi uchun klaster hajmi kritik chegaraga ega ekani, bu chegaradan oshirilganda esa fulleren strukturasi deformatsiyalanishi yoki shikastlanishi ehtimoli ortishi o‘rganilgan. 4-rasmda, kremniy klasterlari C_{60} fulleren molekulasiga doping qilinganda olingan natijalar bo‘yicha grafik chizildi, bunda atomlar soniga mos keluvchi energiyani kamayib borishi ko‘rsatilgan.



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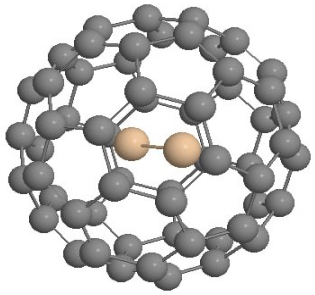

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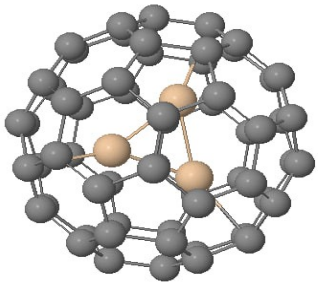

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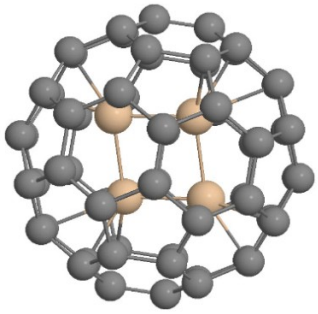

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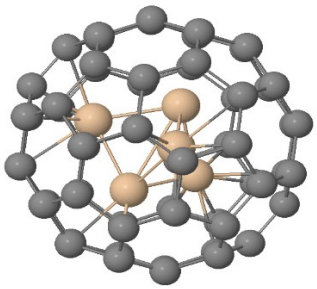

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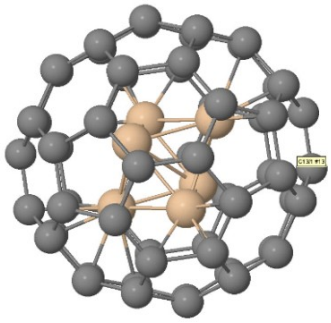

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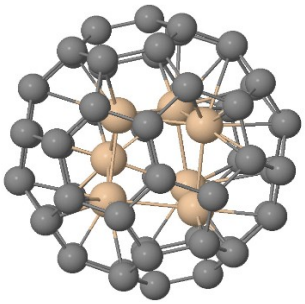

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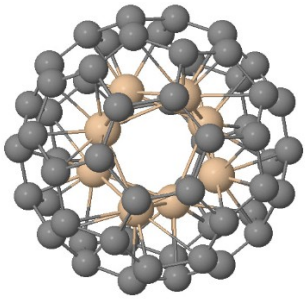
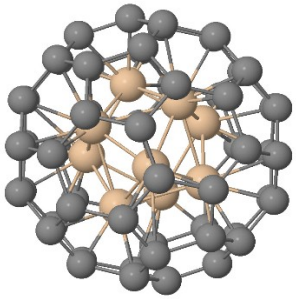
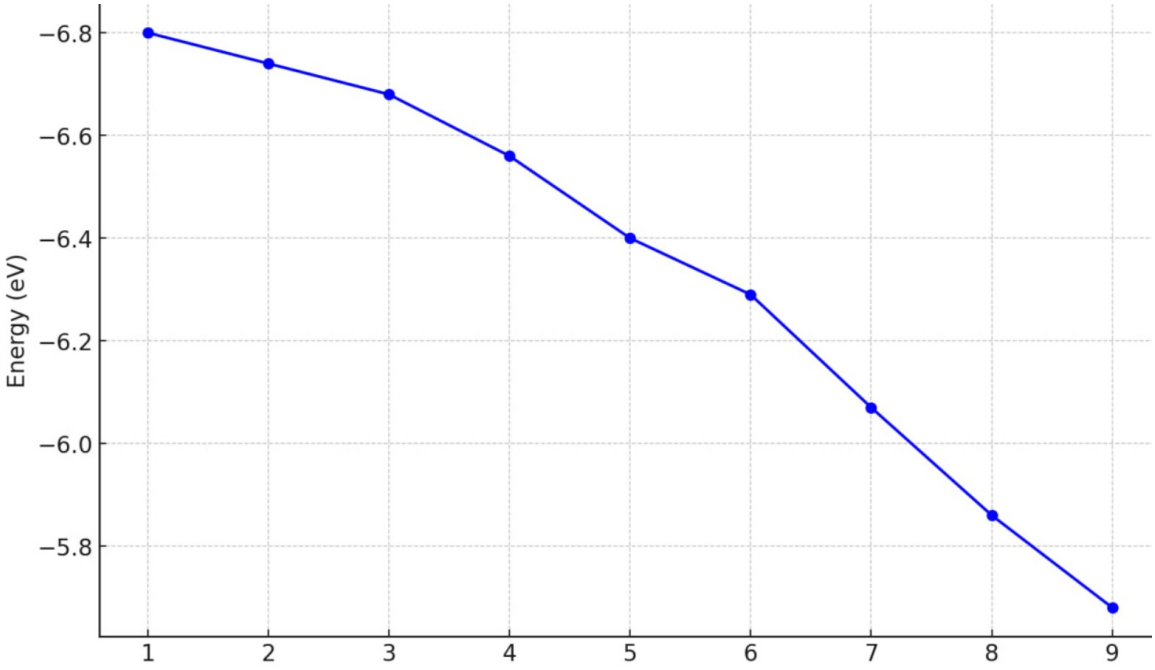


n=8



n=9

3- rasm. C_{60} fulleren molekulasiga kremniy Si (kremniy) klasterlari doping qilingandan keyingi holatlarining ko’rinishi



4- rasm. Energiyaning atomlar soniga bog‘liqlik grafigi

Xulosa

Tadqiqot davomida olingan hisoblash natijalari shuni ko‘rsatdiki, $Si_n@C_{60}$ doping qilingan fulleren tizimida dopant atomlar soni n ortib borishi bilan, tizimdagi har bir atomga to‘g‘ri keluvchi o‘rtacha potensial energiyaning absolyut qiymati ham izchil kamayadi**.** Bunday holat, bir tomondan, tizimda to‘plangan potensial energiyaning umumiy miqdoriga bog‘liq bo‘lsa, boshqa tomondan, fullerena qobig‘ining dopantlar bilan o‘zaro ta’sir kuchi va deformatsiyalanish darajasiga ham bog‘liq. Shuningdek, dopant atomlar sonining maksimal chegarasi mavjud bo‘lib**,** bu qiymatdan oshirilganda fullerena strukturasida barqarorlik buzilishi, ya’ni molekulaning geometriyaviy shikastlanishi ehtimoli ortadi. Ushbu chegaraviy qiymat C60 molekulasining endohedral dopantlarga nisbatan sig‘dirish qobiliyati bilan aniqlanadi.

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