FIRST-PRINCIPLES STUDY OF LITHIUM ADSORPTION ON SiC

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We present a study of electronic and magnetic properties of two-dimensional (2*D*), monolayer of silicon carbide SiC in honeycomb structure. In order to investigate the Li-adsorbed graphene supercells with single vacancies, we have used spin-polarized density functional theory (*DFT*). The effect of adsorption on 2*D* SiC monolayer magnetic properties is also investigated. The existence of adsorbents on SiC has an effect on its physical properties.

Keywords: SiC, Li adsorbed SiC, *DFT*, local spin density approximation
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INTRODUCTION

Lately, the extensive research has been initiated toward the development of promising novel materials, which leads to successful syntheses of SiC [1,2]. Silicon (Si) and carbon (C) belong to group IV of the periodic table, and both of them have four valence electrons. It is possible to form layered structure by mixing C and Si owing to Si shows properties quite similar to that of C. Despite many intriguing properties, one of the biggest difficulties for graphene to be used as an electronic material is its lack of an energy bandgap in the electronic spectra. In experiment, it has been [3, 4] shown that a finite energy bandgap can be induced due to the role of SiC substrate which is an intrinsic property of epitaxial graphene.

Silicon carbide (SiC) crystallizes in either a cubic or a hexagonal form and exbihits interesting polytypism. Have [5] been performed the first successful exfoliation of true 2*D* SiC from bulk SiC. The 2*D* form of SiC will naturally benefit from these overall SiC properties. Furthermore, as a result of reduced dimensionality and quantum confinement, 2*D* SiC is predicted to exhibit exotic optical and electronic properties, that are very useful for various applications [6–8].

In this paper is developed by the first-principles calculations to explore the feature-rich properties of the Li-adsorbed on SiC. The effects of SiC adsorbed by Li on electronic structure are investigated. We also presented the results of calculations adsorption energy and magnetic moment.

COMPUTATIONAL METHODS

The electronic and magnetic properties of adsorption of lithium adatom on face centered cubic structure of 2×1 SiC and hexagonal structure of 3×1 SiC are studied theoretically. These investigations are performed by DFT using local spin density approximation (LSDA) method by employing the ATK program package. In addition, the band structure and density of states are investigated for the SiC. First-principles calculations of SiC properties were carried out on the based on the spin-polarized density functional theory. The local spin density approximation in the Perdew–Zunger (*PZ*) parameterization was employed for the exchange–correlation functional. The kinetic cut-off energy was 150*Ry*. The primitive cell of SiC was relaxed and optimized with force and stress tolerances of 0.01$eV/Å$ and 0.01eV/Å^3, respectively. A *2x2x2k* point was used for geometry optimization and total energy calculations.

DISCUSSION

The calculated energy characteristics and magnetic moments of Li adsorbed on face centered cubic and hexagonal structure of SiC. The lattice constant for face centered cubic structure is $a=9.22456Å$ and Si–C bond length is 1.883$Å$, which are in good agreement with previous results [9]. In face centered cubic Si_8-C_9 bond length is 1.883$Å$, Si_8 – Li 1.545$Å$, Li-C_9 1.265$Å$ respectively. The lattice parameter of hexagonal SiC is determined such as $a=b=9.285Å$. In hexagonal structure for SiC structure Si_{23}-C_{13} bond length is $1.896Å$, Si_{11} –C_{13} 1.895$Å$, Li-C_{13} 2.189$Å$, Si_{23}–Li 1.346$Å$, respectively. Comparison between our calculated results of values of the total magnetic moments (μB) for Li adsorbed on different structures of SiC are given Table 1.

The Li adsorbed on different atomic structures of SiC are represented in fig.1.

The total magnetic moments were investigated for Li adsorbed on cubic SiC monolayer. In addition, adsorption is another promising way to modulate electronic and magnetic properties of 2*D* materials. The different values of magnetic moment Li adsorbed on SiC depend on the space groups of structure. The total magnetic moment of Li adsorbed on face centered cubic structure Si_9C_9 is 0.71μ_B, hexagonal structure $Si_{18}C_{18}$ is 0.88μ_B, respectively. The optical spectrum of cubic monolayer structure SiC have presented in fig.2. We can determine the static dielectric constant, $Re[\epsilon(\omega=0)] =10$. Theoretical studies have also found that 2*D* SiC has very rich optical properties, such as strong photoluminescence, non-linear optical properties, and excitonic effects as a result of quantum confinement effects [14-16].

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Table 1.

The value of magnetic moment for in Li atom adsorbed on SiC

Li adsorbed SiC	E_{ad} (eV)		d_{LiC} (Å)		magnetic moments
Li adsorbed on 3×1 SiC (hexagonal)	7.2	6.67[10]	1.896(Si_{23}-C_{13}) 2.189(Li-C_{13}) 1.346(Si_{23} –Li)	1.758 (Si–C) [11], 2.27[7]	0.88μ_B 0.99 μ_B [13]
Li adsorbed on 2×1 SiC (face centered cubic)	-	-	1.545 (Si_8-Li) 1.883(Si_8-C_9) 1.265(Li-C_9)	1.89 (C-Si)[12]	0.71μ_B

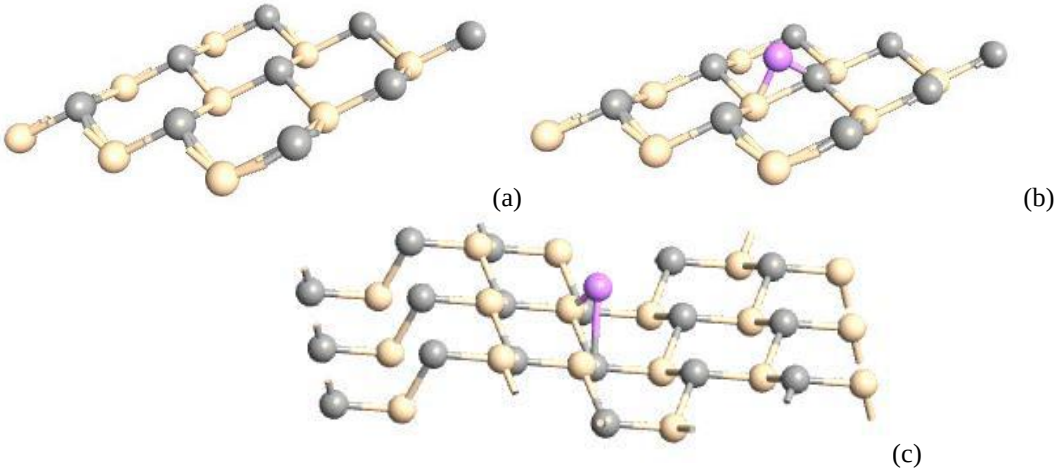

Fig.1. Atomic structure of (a) pristine cubic 2×1 SiC, (b) Li adsorbed on face centered cubic 2×1 SiC, (c) Li adsorbed on hexagonal 3×1 SiC.

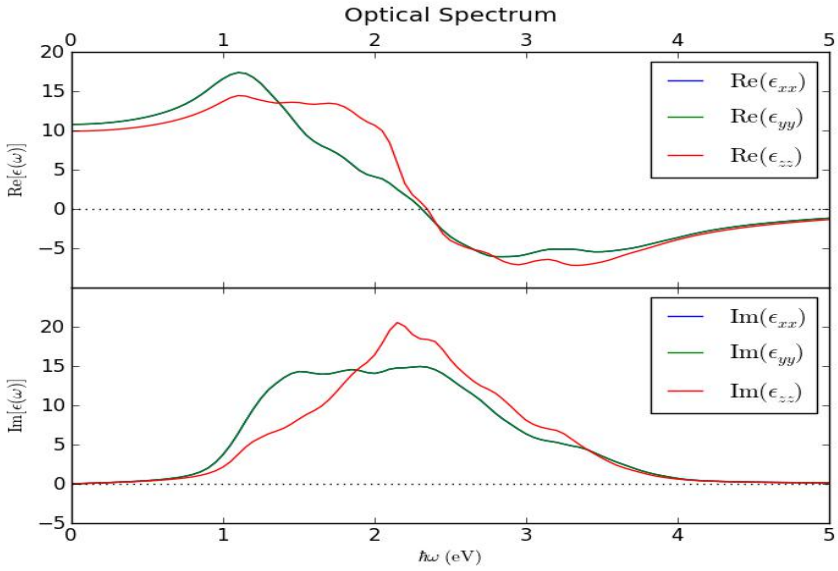

Fig. 2. Optical spectrum of SiC

CONCLUSION

The use of spin-polarized *DFT* calculations of the properties of cubic and hexagonal SiC shows that the properties change due to edge states in the SiC structure. The magnetic properties of face centered cubic and hexagonal crystal structure of SiC were studied. In particular, the magnetic moments for different symmetric group of SiC differ from each other. First principle calculation of total spin polarization shows that Li adsorbed on cubic (0.71μ_B) and hexagonal (0.88μ_B) SiC structure magnetic moment raises with altering of geometric ordering atoms. The atomic radius of face centered cubic SiC between Si and Li is 1.346*Å*, and between Si and Li is 1.545*Å*. In another structure, in hexagonal SiC the atomic radius between Li and C is 2.189*Å* and between Si and C is 1.895*Å* (Table 1).

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Li ATOMUNUN SiC SUPERQƏFƏSİ ÜZƏRİNDƏ ADSORBSİYASININ TƏMƏL PRİNSİPLƏRDƏN ÖYRƏNİLMƏSİ

İkiölçülü Silikon karbid (SiC) strukturunun elektron və maqnit xassələrinin təməl prinsiplərdən tədqiqini təqdim etmişik. Li atomu ilə adsorbsiya edilmiş SiC strukturunu araşdırmaq üçün spin-polyarizasiya olunmuş sıxlıq funksional nəzəriyyəsindən (DFT) istifadə edilib. Adsorbsiyanın ikiölçülü SiC monolayında yarana bilən maqnit xassələri və ona təsiri araşdırılıb. SiC-də adsorbentlərin olması onun fiziki xassələrinə təsir göstərir.

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ИЗУЧЕНИЕ ИЗ ПЕРВЫХ ПРИНЦИПОВ АДСОРБЦИИ ЛИТИЯ НА SiC

Мы представляем исследование электронных и магнитных свойства двухмерного (2D) монослоя карбида кремния SiC в сотовой структуре. Чтобы исследовать Li-адсорбированные SiC суперячейки мы использовали спин-поляризованную теорию функционала плотности (DFT). Исследовано также влияние адсорбции на магнитных свойств монослоя двухмерной SiC. Наличие адсорбентов на SiC влияет на его физические свойства.