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RESEARCH ARTICLE

Defect induced magnetism on SiC monolayer

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Using spin-polarized density functional theory, magnetic induction by means of vacancy defect was studied on SiC monolayer. While pristine SiC monolayer is found to be a semiconductor with a direct band gap of 2.64eV, vacancy of both Si and C defect transforms it into metallic ferromagnetic material. Calculated magnetization density shows that Si vacancy results in a magnetic moment of while C vacancy results to a magnetic moment of . Observations reveals that magnetism mostly arises from the unpaired electrons that arise as a result of the removed Si/C atom and spin asymmetry arises mainly from the p-orbitals of Si/C as a result of vacancy. Our result shows that magnetism can be introduced in SiC monolayer effectively using vacancy defect and can further be altered depending on the type of defect.

Keywords : magnetism, monolayer, vacancy defect, spin-polarized DFT

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Introduction

Series of two dimensional nano-materials with distinctive physical and chemical properties have drawn much attention since graphene was successfully prepared in 2004.[1] These 2D materials exhibit intriguing and abundant physical properties, ranging from metallic conductor to semiconductor, which guarantee them promising wide applications in electronic and optoelectronic devices in nano-scale.[2,3] Many low dimensional materials having promising properties have already been studied for their extensive applications.[4-11] Furthermore, implantation of defects at the atomic site in low dimensional materials is also known to improve the optoelectronic properties and intense research works have been done through both theory and experiment,[12-14] opening a promising area for future nanodevices.

Among these monolayers, high spin states of the silicon vacancy defects in cubic silicon carbide (3C-SiC) have been predicted from first-principles calculation.[15] Also, local magnetic moments arising from vacancy of Si can be tuned by the charge states of the defects.[16] This opens a promising method towards transition-metal-free SiC magnetic semiconductors. As a result of its unique physical and promising electronic properties, SiC nanostructure have been studied in diverse form and synthesized using different approach.[17,18] Similar to the graphene layer, two-dimensional (2D) SiC monolayer has been proposed in the study of single-walled SiC nanotubes using theoretical study.[19, 20] Recent investigations have shown that SiC monolayer is quite stable and that the nanostructure itself is known to offer half-metallic magnetism.[21, 22]

In this study, we explore the vacancy effect on SiC

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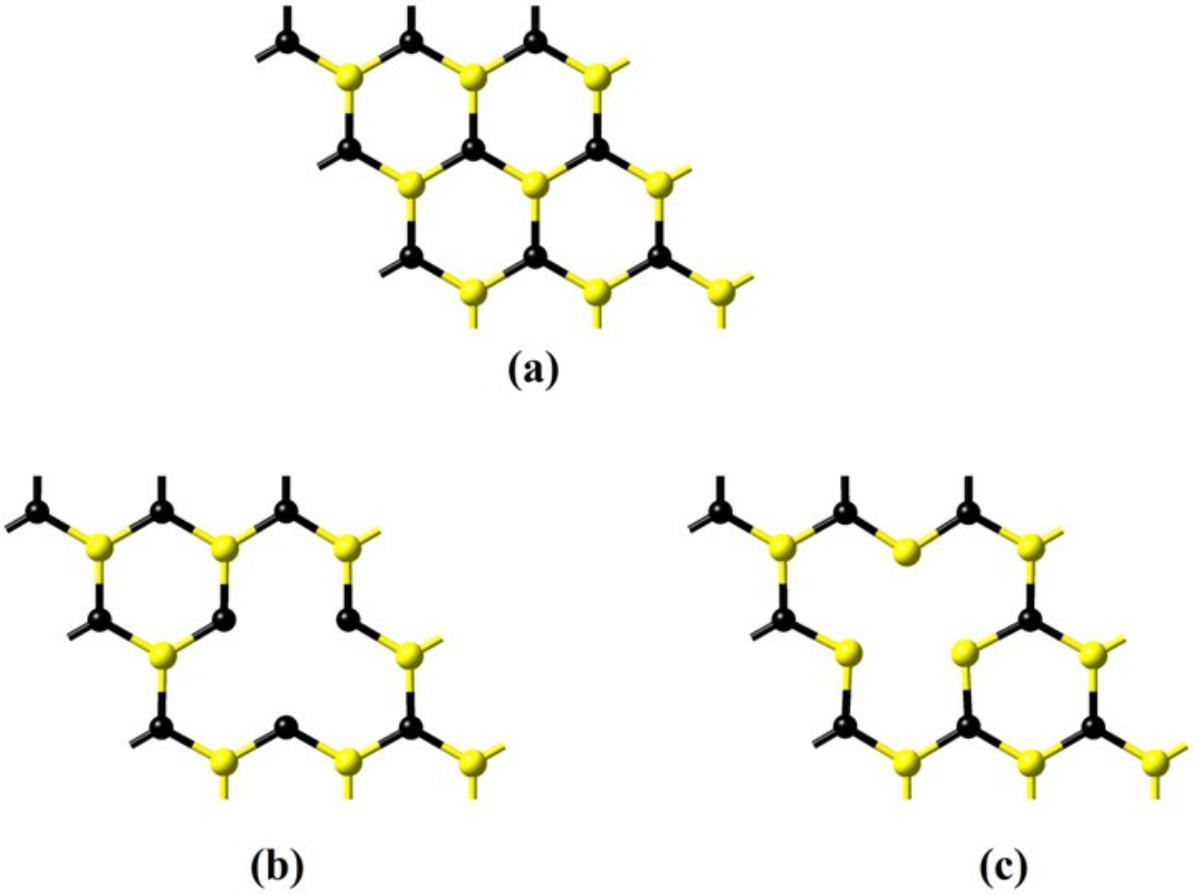

Figure 1: Optimized structure of (a) Pristine SiC monolayer, (b) Si-vacated SiC monolayer,

monolayer. Vacancy of both Si and C are considered independently and their respective role in the contribution in the induced magnetism is studied. Our investigation shows that Si vacancy offered higher magnetic moments than C vacancy which can be further analysed from the free electrons as a result of the missing atom. Contribution of the individual atoms surrounding the vacancy in inducing magnetism is also analysed. Using our result, we hope to provide essential information to the future synthesis and utilization of magnetic materials in nanoscience and nanotechnology without making use of the transition metals.

Computational details

A 3x3 supercell of SiC monolayer with 9 atoms each of Si and C is initially taken as the pristine structure. A vacuum of 15 Å is inserted along the z-direction to avoid the interactions between the monolayers during periodic calculations. Vacancy defect is then introduced by removing a single Si or C atom from the pristine structure. The defect structures are then optimized with a force tolerance of 0.01 eV/Å with energy convergence criteria of 10-5 eV.

All the computations are performed within the

Table 1: Bond length, formation energy, band gap and total magnetic moment of pristine, Si-vacated and C-vacated SiC monolayer

Structure	Si-C bond length (Å)	Formation energy (eV)	Band gap (eV)	Total magnetic moment (μ_B)
Pristine	1.77	-6.87	2.64	0
Si-vacated	1.76	-6.44	-	1.7
C-vacated	1.81	-6.50	-	0.9

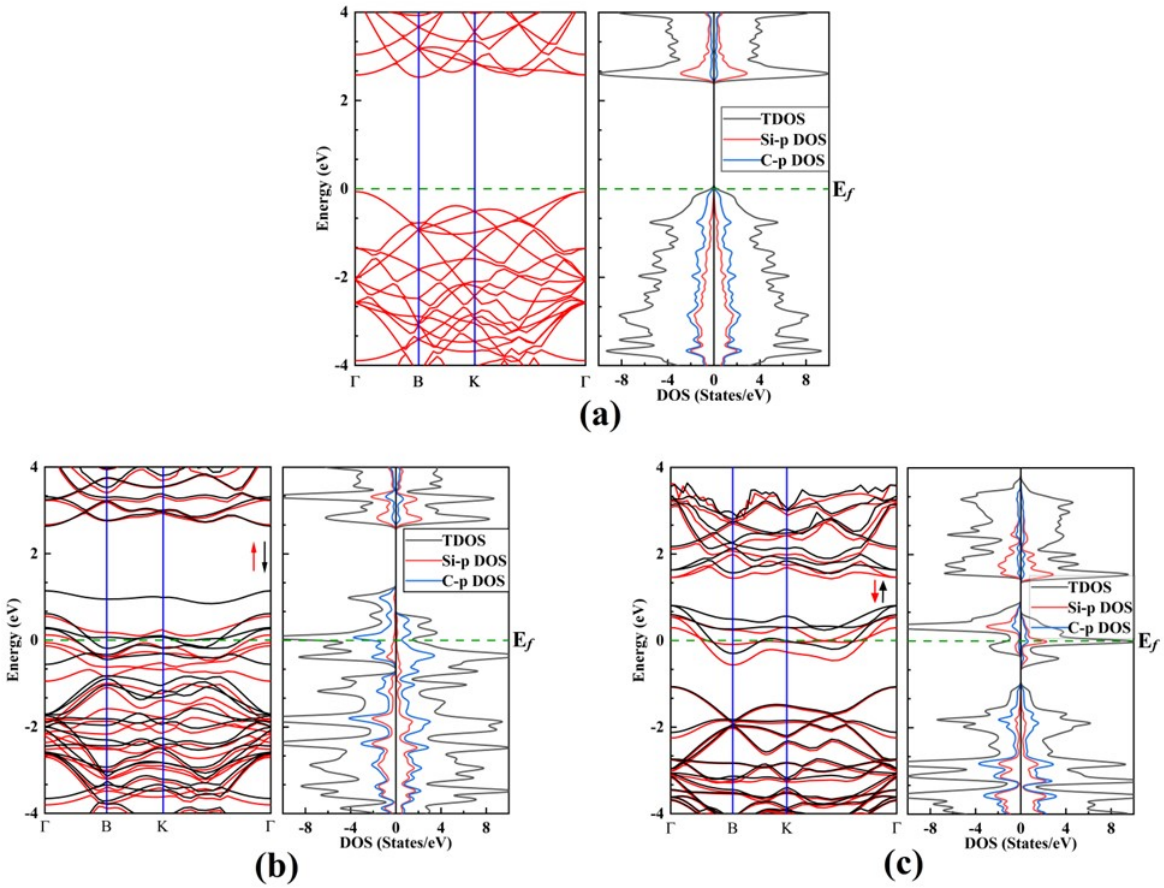

Figure 2: Band structure and projected density of states (PDOS) of (a) Pristine SiC monolayer, (b) Si-vacated SiC monolayer,(c) C-vacated SiC monolayer

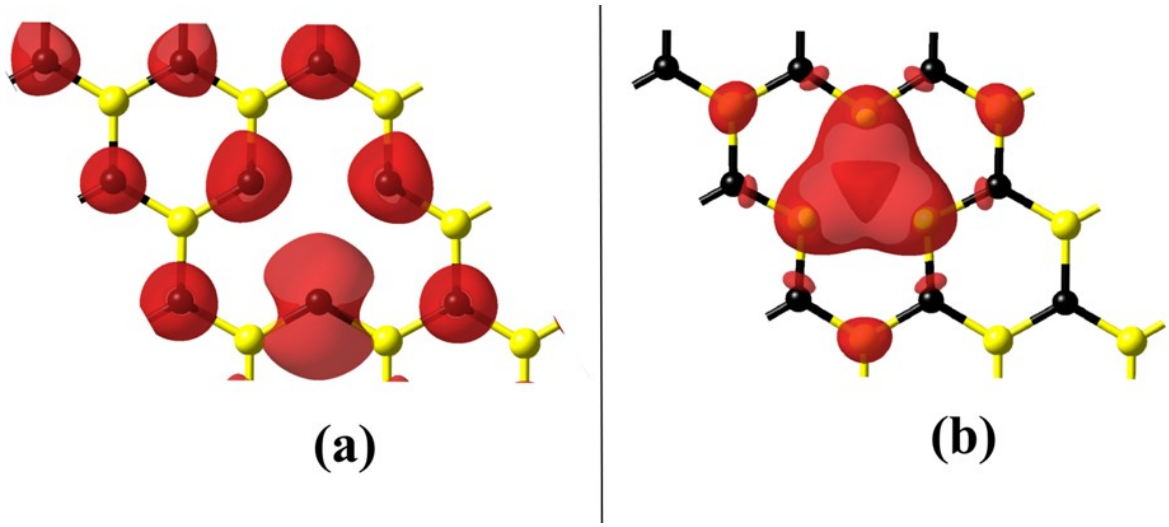

Figure 3: Magnetization density of (a) Si vacated and (b) C-vacated SiC monolayer

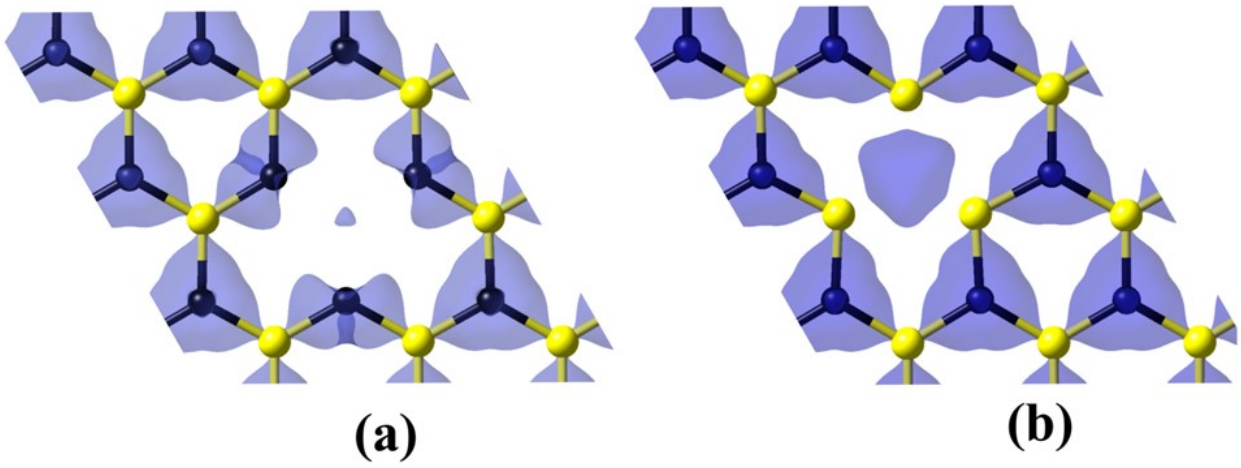

Figure 4: Total charge density of (a) Si vacated and (b) C-vacated SiC monolayer

framework of spin-polarized plane-wave density functional theory (DFT) as implemented in the Vienna Ab initio Simulation Package (VASP).[23] The ionic potentials are represented by Projector Augmented Wave Potentials (PAW)[24] with electron exchange correlation represented by Generalized Gradient Approximation (GGA) as implemented by Perdew, Burke and Ernzerhof (PBE).[25] An energy cut-off of 400 eV is used for the plane-wave expansion of the electronic wave function and the Brillouin zone integration is performed using 8 x 8 x 1 k-point mesh within the Monkhorst-Pack scheme.[26] For electronic properties calculation, the Brillouin zone is sampled by 12 x 12 x 1 k-point mesh. The partial occupancies were treated using the tetrahedron method with Blöchl corrections.[27]

Results and Discussion

In order to understand the impact of vacancy defect, the structural and electronic properties of pristine SiC are first calculated. Relaxed SiC monolayer structure after optimization is shown in Fig 1(a). Optimized honeycomb SiC monolayer shows an average bond length of 1.77 Å and lattice parameter of 3.07 Å. Unlike graphene, which possess zero band-gap, SiC monolayer is found to possess direct band gap of 2.64 eV at Γ-point, showing p-type semiconductor property as shown in Fig 2(a). These findings are consistent with other earlier reports.[22,28] To confirm its stability, formation energy is also calculated and given in Table 1. For defect structure, vacancy is then introduced by removing a single Si or C atom from the pristine structure as shown in Fig 1(b) and 1(c). With Si-defect, as shown in Fig, 1(b), the bond length of the nearest SiC monolayer changes to 1.76 Å offering almost no changes as compared to the pristine structure. On the other hand, Fig. 1(c) shows that C-defect results in an increased bond length of 1.81 Å. Nonetheless, calculated formation energies of all the structures reveal stability in their respective structure.

In the case of electronic properties, induction of both the vacancies results in semiconductor-to-metallic transition. This metallic character mainly arises from the p-orbitals of Si and C atom as observed from the PDOS plot in Figure 2. In the case of Si-vacancy, shifting of the valence band maxima (VBM) is observed, crossing the Fermi level for both the spin states and resulting in metallic property. In the case of C-vacancy, VBM shifts away from the Fermi level but new states are observed in the Fermi region from the p-orbitals of both Si and C atom, which again results in full metallic character of the structure.

In order to gain further insight on the magnetism, magnetisation density plot of the vacancy defect structures are given in Figure 3. In Si vacancy, magnetism mainly arises from the C-atom nearest to the vacancy defect with magnetic moment of 0.3 μB. Other C-atoms neighbouring the vacancy also contributes ~0.05 μB each as shown in Fig. 3(a). Meanwhile in the case of C vacancy, magnetism mainly comes from the net magnetic moment of the vacancy surrounding Si-atoms, with an individual magnetic moment of ~0.7 μB. The observed magnetic moment clearly shows that the differences in the charge transfer or the imbalance of charge transfer; caused by the vacancy, result in the formation of unpaired electrons among atoms surrounding the vacancy and in the subsequent neighbouring atoms. This is confirmed from the total charge density plotted in Figure 4.

Conclusion

From our study of SiC monolayer using spin-

polarized Density Functional Theory (DFT), we have found that SiC monolayer can be transformed into a magnetic material using vacancy defect and that the intensity of magnetism can be varied depending on the type of defect introduced, i.e., Si/C vacancy. While pristine SiC monolayer is found to be a semiconductor with a direct band gap of 2.64 eV, Si vacancy results in a magnetic moment of 1.7 μB while C vacancy results to a magnetic moment of 0.9 μB. Our study shows that magnetism mostly arises from the unpaired electrons that arise as a result of the removed Si/C atom and spin asymmetry arises mainly from the p-orbitals of Si/C as a result of vacancy. Further study with larger supercell will be able to provide whether the intensity of magnetism can be controlled using the number of vacancy defect introduced. Nonetheless, our calculations provide possibility of transforming semiconductor into metallic material without the presence of transition metals, hopefully providing information for understanding of magnetism in monolayer system.

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