Charge-induced Magnetism in Si with Bi-carbon Clusters

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1. Introduction

Dilute magnetic semiconductor (DMS) has attracted great interest according to its potential as a fundamental material in the applications of spintronic devices (SD) and non-volatile magnetic memory (NMM). In practical and massive production prospects, the applications have to meet to low cost, room temperature operation and reliable mature fabrication technology. Looking at today's development, the modern advanced silicon technology is the best choice to satisfy these requirements. Consequently, the exploring of a Si-based ferromagnetic material for constructing Si-based SD and NMM devices is a vital important subject. Although many dilute magnetic semiconductors, such as Co/GaAs [1,2], Mn/GaAs [3], Si vacancies in SiC [4] and C-doped ZnO [5], have been proposed and widely studied in the last decades, none of them is physically and chemically compatible with Si. In this paper, we report theoretical study of bi-carbon cluster in bulk Si (BCCS) using the density functional theory (DFT). The calculated band structures and spin density of states (SDOS) reveal a charge-induced magnetism in the BCCS system. This property allows us to realize a field-controlled magnetism that is useful in the applications of Si-base SD and NMM.

2. Model and Theoretical Settings

In this work, the DFT as implemented in the CASTEP code is applied to study the band structures and magnetic properties of BCCS. The interaction between core and valence electrons is included by an effective (norm-conserving) pseudo-potential. The generalized gradient approximation of Perdew and Wang [6] is used for the exchange-correlation functional. The screened-exchange local density approximation (sX-LDA) [7] is used to correct the underestimated band-gap in wide-gap semiconductor using DFT. The k-mesh point is $1 \times 1 \times 1$ for 64-atom supercell, and the cutoff energy for the bases functions is 600 eV.

Before the calculations of band structures and SDOS the structure with one substitutional bi-carbon cluster for 64-atom supercell is fully relaxed as shown in Fig. 1(a). The bi-carbon cluster in Si crystal, that has O_h ($Fd\bar{3}m$) symmetry, forms a Rhombohedral structure with D_{3d} ($R\bar{3}m$) symmetry. Both of them are nonmagnetic with neutral charge in the structures.
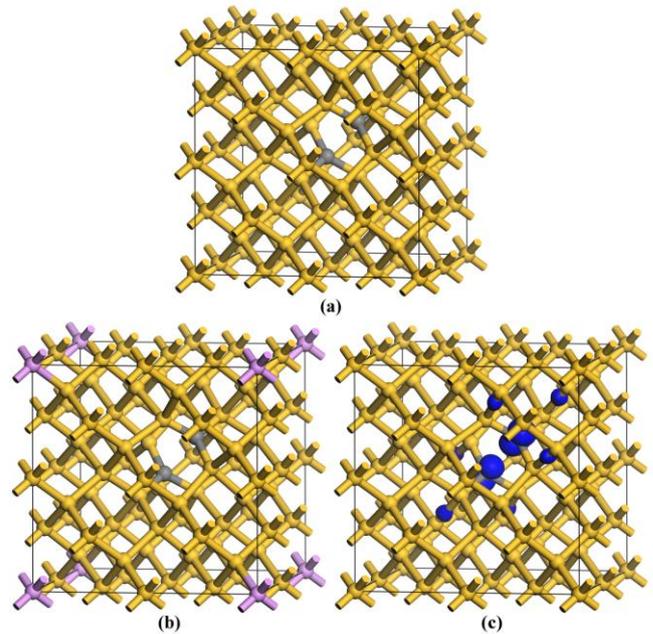

Fig. 1 (a) The structure of a 64-atom supercell with a substitutional bi-carbon cluster, (b) P-doped structure and (c) the net spin-density distribution of q = -1.

3. Results and Discussions

The calculated band structure and SDOS for zero (q = 0) and one (q = -1) extra electron charge in the system are given in Figs. 2 and 3, respectively. The structure with extra charge is equivalent to phosphorous-doped one, as shown in Fig. 1(b), where the separation between P atom and C cluster is set to as far as possible. The dopant P has one more electron than Si, and thus provides extra electrons to the host.

The calculated results show two main features: (i) the C-C bond lengths for different charging conditions are 3.345 Å (q = 0) and 3.433 Å (q = -1). (ii) Both band structure and net spin density indicate that the system of q = 0 is nonmagnetic, but that of q = -1 is ferromagnetic. The high electro-negativity of carbon atom attracts the electron from its neighbor Si to the carbons, as shown in Table-I the electron population at C, 1st nearest neighbor Si (1NN-Si) and 2nd nearest neighbor Si (2NN-Si) sites. The increased electron charge at C sites increases the Coulomb repulsive force between the C atoms. This is the main reason to C-C bond-length elongation. The stretched length weakens the

interaction between the C atoms, provides a small energy splitting between bonding and anti-bonding C-molecule states, and thus forms two impurity states in the energy gap. This is much different from the structure with two separated C atoms, which has only one impurity state in the gap (the results are not shown in this article).

For q = 0, as shown in Fig. 2(b), the band structure in comparison with bulk Si (see Fig. 2(a)) clearly shows two impurity bands that are above the valence-band maximum. These impurity states are originated from p-p σ interaction of C-C molecule to form a bonding and anti-bonding states. The bonding state is fully occupied, and the anti-bonding one is empty. Since all of the bands are spin degenerate, no net spin presents in the structure and implies a nonmagnetic property.

Once an extra electron charge is added in the structure, the spin polarization occurs (see Figs. 2(c) and 2(d) for q = -1 and doped P, respectively). A nonzero net spin is populated at the anti-bonding state as shown in Fig. 1(c) the net-spin density distribution, and forms a local magnetic moment of 1.0 μ_B. The energy of the spin polarized state is lower than that of spin-unpolarized state by ~ 0.45 eV, implying that the local magnetic moment may be stable even at room temperature.

To study the magnetic coupling between the local moments, a double size of supercell by placing two 64-atom units side by side is used. This supercell contains two bi-carbon clusters. In self-consistent calculations, different initial-spin configurations give two stable magnetic structures: one is ferromagnetic (FM) and another is anti-ferromagnetic (AFM). The energy difference between AFM and FM ($\Delta E = E_{AFM} - E_{FM}$) allows us to estimate the magnetic interaction J_0 using the equation $\Delta E = 4 \times J_0 \times S^2$ based on the Heisenberg model [4,8], where S is the net spin in a C cluster. The calculated results of ΔE and J_0, that both of them are 176.26 meV, show that the FM coupling is preferable for the charged and P-doped BCCSs.

Table-I Electron Population Distribution

q	C site	1NN-Si site	2NN-Si site
0	4.65	3.5844	3.9786
-1	4.9606	3.5715	3.9865

4. Conclusions

Our first-principles calculations show that the charged state and spin-polarization in BCCS are controllable by gate-induced extra charge or doped P atoms in Si host. This configuration may be achieved by the ultra-shallow ion-implantation and pulsed-laser annealing techniques, which have been widely used to fabricate nanometer scale devices. After C-ion irradiation with ultra-high dose and ultra-low energy, a high-energy pulsed laser is applied to recover crystallization within an ultra-short time (a few milliseconds), so that the C atoms do not have enough time to diffuse away from each other and thus form bi-carbon clusters. The controlled magnetism can be achieved by a

metal-oxide-semiconductor field-effect structure. This property is useful in the SD and NMM applications.
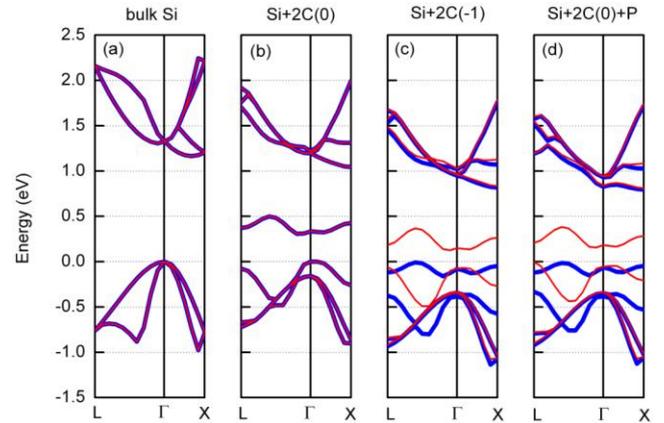

Fig. 2 The band structures for (a) bulk Si, (b) q=0, (c) q=-1, (d) doped P and (d) bulk Si. The blue lines indicate the up spin and the red lines the down spin.

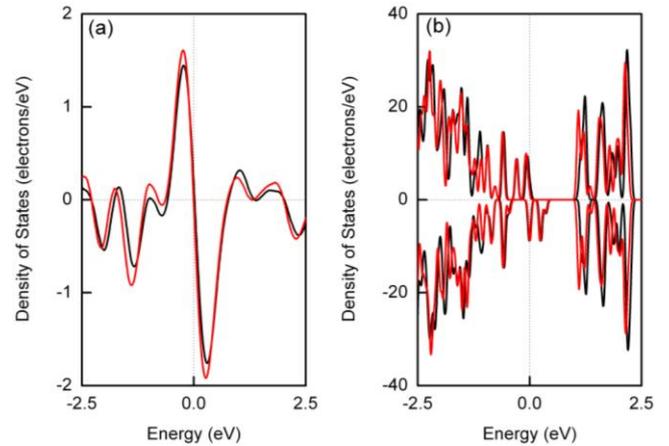Fig. 3 (a) net SDOS and (b) SDOS for q = -1 (red lines) and p-doped (black lines) structures.

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