

First Principle Calculation of a Negatively Charged Boron-Vacancy Center in Diamond for Highly-Sensitive Magnetic Sensor Applications

Aiko Kunisaki¹, Manoharan Muruganathan², Hiroshi Mizuta^{2,3} and Tetsuo Kodera¹

¹ Department of Electrical and Electronic Engineering, Tokyo Institute of Technology
2-12-1-NE-18 Ookayama Meguro-ku Tokyo, 152-8552, Japan
Phone: +81-3-5734-3421 E-mail: kunisaki.a.aa@m.titech.ac.jp

² Japan Advanced Institute of Science and Technology
1-1 Asahidai, Nomi, Ishikawa 923-1292, Japan

³ Univ. of Southampton
University Road, Southampton, SO17 1BJ, United Kingdom

Abstract

A negatively charged nitrogen-vacancy (NV) center has shown to be a promising candidate for highly-sensitive magnetic field sensors and other spin information devices. This paper aims to find a new candidate color center which is analogous to the NV center. We focus on a boron-vacancy (BV) center because B is used as a p-type dopant for diamond. Using first principle calculation, we study a negatively charged BV center. By analyzing the formation energy of the defect, the band structure and the defect energy levels, we reveal the BV^{-1} center has a spin-triplet ground state.

1. Introduction

The nitrogen-vacancy (NV) center in diamond, which consists of a carbon vacancy and an adjacent substitutional nitrogen impurity, has been well studied. Because the negatively charged NV center (NV^{-1}) have a spin-triplet ground state and an extremely long spin coherence time even at room temperature [1]. They can be optically initialized and read out at room temperature. With these excellent spintronic characteristics, the NV^{-1} center has been proven to be a promising candidate for various spin information device applications such as highly-sensitive magnetic sensors [2], quantum bits [3] and single photon sources [4]. Based on these favorable properties, other types of color centers in diamond and defects in other analogous materials have also been studied. J. R. Weber *et al.*, suggested a list of physical criteria for deep center defects and their host required for quantum bits [5]. Some kinds of defects such as the oxygen-vacancy (OV) center and the silicon-vacancy (SiV) center in diamond have been investigated for quantum bits [6] and single photon interfaces [7], respectively.

Searching for alternative defects similar to the NV^{-1} center, we employ the first principle calculation to elucidate their spintronic properties. In order to validate the accuracy of our simulation, we first simulated the OV center in diamond and confirmed a good agreement with the results reported by Y. G. Zhang *et al.* [6] After that we scrutinized the boron-vacancy (BV) center in diamond because B acts as p-type dopant for diamond. We calculated the formation energy to find out the statistic charge states of the defect, the band structure, the density of states, the defect energy levels.

2. Computational approach

In the present work we used the ‘SIESTA’ code [8] for the first principle calculation.

Our first-principle calculations are based on the spin-polarized density functional theory (DFT) within the generalized gradient approximation (GGA). Particular parametrization of the exchange-correlation functional is Perdew-Burke-Ernzerhof (PBE) version. We used the plane-wave basis sets with a mesh cutoff of 200Ry and pseudopotentials of the C and B atoms for geometry optimization. We adopted the structure of a single BV^{-1} center in the center of the $4 \times 4 \times 4$ diamond supercell. So we took a 63-atom-supercell with a single carbon vacancy in a cubic lattice into consideration. Calculations were conducted with $9 \times 9 \times 9$ Monkhorst-Pack k-point mesh for the Brillouin zone (BZ) integration. In the geometry optimization calculation, atomic coordinates were relaxed until the maximum atomic force got smaller than 0.01eV/Ang. With such coordinate calculations, the band structure, the density of states and the defect structure symmetry were revealed.

To identify the static charge state of the defect, the formation energy of the defect was evaluated by using the following equation for the individual charge states.

$$E^f[C : (B - V)^q] = E_{tot}[C : (B - V)^q] - E_{tot}[C : bulk] - \mu_B + 2\mu_C + q(\varepsilon_F + \varepsilon_{VBM}^{bulk} + \Delta V)$$

where $E^f[C : bulk]$ is the total energy of the bulk diamond supercell and $E^f[C : (B - V)^q]$ is the total energy of the diamond supercell containing the $(B - V)^q$ center in charge state q . μ_B and μ_C are chemical potentials of B and C atoms respectively. The chemical potentials were gained by using the total energies for bulk-diamond and boron-cluster divided by total number of atoms. ε_F is a Fermi level and ε_{VBM}^{bulk} is a valance band maximum (VBM) of the diamond bulk. ΔV is the effective potential alignment [9]. By plotting the formation energy as a function of ε_F , the statistic charge state q was obtained.

3. Results and Discussion

First of all, we performed the geometry optimization of the BV center and found out the structure of the defect possesses a C_{3v} symmetry, which is the same as the NV center

and the OV center [3, 6]. (Fig. 1. (a)) Then, the formation energy E^f was calculated with changing the excess charge $q = -2, -1, 0, +1, +2$ as a parameter. (Fig. 1. (b))

At the same time, the band structures and the density of states were obtained for the individual charge states as shown in Figs. 2 (a) and (b). Among these results, we chose the charge state $q = -1$ because it is stable when $\varepsilon_F = 0.7 \sim 1.4$ eV and the BV^{-1} center possesses the spin-triplet ground state. On the other hand, the BV^0 center is stable when $\varepsilon_F = 0 \sim 0.7$ eV, but it does not possess the spin-triplet ground state. We therefore focused on the properties of the BV^{-1} center.

The spin-down and spin-up bands are clearly separated. From the band structures, we defined the defect energy level at the Γ point. (Fig. 3) With the Pauli exclusion principle and Hund's rules, the occupied electron configuration is $a_{1(1)}^2 e_x e_y$ in the ground state. We plotted the wave functions for each energy levels. (Fig. 4) From this, we revealed the $a_{1(2)}^{\uparrow}$ level and the $e_{x,y}^{\uparrow}$ levels originate from the boron impurity and the first-neighbor carbon atoms, respectively.

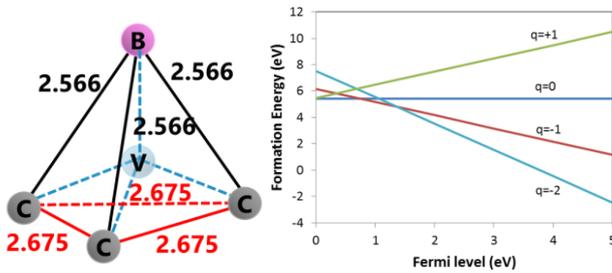


Fig. 1. (a) Structure of BV center. (b) Formation energy for each charge q .

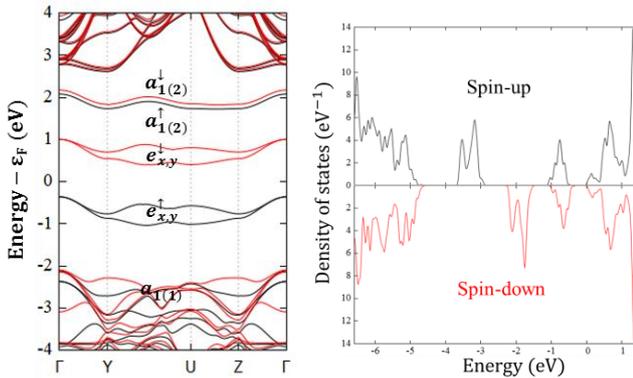


Fig. 2. (a) Band structure. (b) Density of states.

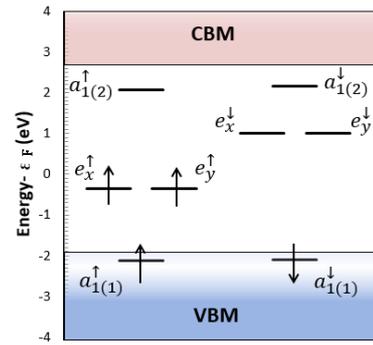


Fig. 3. Defect energy level.

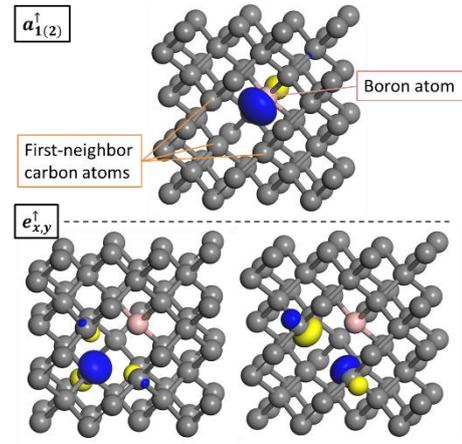


Fig. 4. Wave functions of each levels.

4. Conclusions

We concluded that the BV^{-1} center can be an alternative candidate for spin information devices such as highly-sensitive magnetic sensors. We revealed the BV^{-1} center is stable for ε_F ranging from 0.7 to 1.4 eV and it possesses the spin-triplet ground states. As boron is used as a p-type dopant for diamond, it may be easier to introduce the BV center into future diamond devices to visualize magnetic field distributions in the device.

References

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