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First-Principles Investigation of Charge Transfer Mechanism of B-Doped 3C-SiC Semiconductor Material

Abdullahi Alkali Dauda[1*], Muhammad Yusuf Onimisi[2], Adeyemi Joshua Owolabi[2], Hammed Adeniyi Lawal[1], Hassan Muhammad Gambo[2], Bashir Mohammed Aliyu[2], Surajo Bala[3], Muhammad Lamido Madugu[4], Muhammad Abdurrahman Nainna[1], Johnson Akinade Bamikole[5]

[1]Physics Department, Faculty of Science, Air Force Institute of Technology, Kaduna, Nigeria
[2]Physics Department, Faculty of Science, Nigeria Defence Academy, Kaduna, Nigeria
[3]Physics Department, Umaru Musa Yar'adua University, Batagarawa, Nigeria
[4]Physics Department, Faculty of Science, Gombe State University, Gombe, Nigeria
[5]Physics Department, Federal University of Lafia, Lafia, Nigeria
Email: *abdullahialkali95@gmail.com

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Abstract

This study delves into the charge transfer mechanism of boron (B)-doped 3C-SiC through first-principles investigations. We explore the effects of B doping on the electronic properties of 3C-SiC, focusing on a 12.5% impurity concentration. Our comprehensive analysis encompasses structural properties, electronic band structures, and charge density distributions. The optimized lattice constant and band gap energy of 3C-SiC were found to be 4.373 Å and 1.36 eV respectively, which is in agreement with previous research (Bui, 2012; Muchiri *et al.*, 2018). Our results show that B doping narrows the band gap, enhances electrical conductivity, and influences charge transfer interactions. The charge density analysis reveals substantial interactions between B dopants and surrounding carbon atoms. This work not only enhances our understanding of the material's electronic properties, but also highlights the importance of charge density analysis for characterizing charge transfer mechanisms and their implications in the 3C-SiC semiconductors.

Keywords

First-Principles Calculations, DFT, Boron (B)-Doped 3C-SiC, Charge Transfer

1. Introduction

Silicon carbide (SiC) is a wide-band gap semiconductor material that is widely used

in electronic and optoelectronic devices due to its unique physical and chemical properties [1]. It is a crystalline ceramic consisting of silicon and carbon atoms arranged in a repeating crystal lattice [2]. The bond between silicon and carbon is predominantly covalent, though it exhibits some degree of ionic character. The molar mass of SiC is 40.10 g/mol [3]. It is a simple chemical in which the silicon atom is joined to the carbon atom by a triple bond, leaving both atoms with a positive and negative charge. It is produced synthetically using the Acheson technique, which involves mixing pure silica sand (SiO_2) with finely ground coke (carbon) and heating the mixture to extremely high temperatures in an electric furnace. The separation between carbon atoms is 0.308 nm, and the space between them is 0.189 nm for silicon [4].

Silicon carbide (SiC) is an established yet increasingly important semiconductor, offering superior physical properties ideal for advanced power devices. SiC devices show great promise for high-temperature and radiation-resistant operation [4]. It also shows great promise as a platform for quantum technologies [5]. Specifically, numerous point defects have been both predicted and demonstrated to produce a solid-state material capable of quantum coherence, with individually addressable spin states [6].

The current research interests in this semiconductor material in electronics, it is due to its high thermal conductivity, high electric field breakdown strength, and high maximum current density, which makes it more promising than the common silicon for high-powered devices. It can also be used to design materials with proper band gaps [7]. Its elevated breakdown fields and reduced vulnerability to radiation and thermal influences offer substantial benefits in scenarios involving high temperatures or radiation exposure [8]. Silicon carbide finds application in various fields, notably in solar cells because of its exceptional stability. However, the inherent high band gap of pure SiC prompts exploration into non-stoichiometric silicon carbide variants to adjust the band gap for optimal absorption of solar radiation [9]. The cubic phase of SiC (3C-SiC) distinguishes itself by showcasing heightened thermal conductivity and breakdown field strengths when contrasted with other polytypes. This characteristic renders the cubic phase exceptionally suitable for advancing high-performance electronic devices [10]. It has also been utilized in constructing photonic cavities exhibiting remarkable quality factors, many researchers use the first-principles study to investigate the structural and electronic properties of 3C-SiC. It was reported that it has a wide band gap of about 2.502 eV, which indicates its semiconducting nature [11]. The interest in doped 3C-SiC has surged, opening up exciting possibilities for future electronic applications [8].

Also, in this research, we consider point defects as they play a crucial role in determining the concentration of charge carriers and influencing the electrical properties of semiconductor materials used in microelectronic devices [12]. In the case of SiC, p-type doping is achieved by introducing elements from the IA group of the periodic table. The p-type dopants commonly used are aluminum and boron. However, the introduction of dopant atoms such as boron and nitrogen

can alter the electrical properties of 3C-SiC, making it suitable for p-type semiconducting applications [13]. However, the effect of substitutional point defects of boron B on the electrical properties of 3C-SiC crystal has not been fully explored using first-principles methods.

The optimal arrangement of p-type dopants in SiC, as well as the material's stability under different doping conditions, has been investigated using first-principles analysis [14]. Further research has focused on understanding the conductivity mechanism of p-type dopants, specifically the significant role of boron in enhancing the material's conductivity [15].

We found that B substitutes the most favorably at a Si lattice site than at a C site, [14]. When the carbon atom is replaced by a boron atom in the 3C-SiC, the band gap of the B-SiC transforms from an indirect band gap to a direct band gap with band gap shrink as compared to other p-type. Petrenko in 2016, suggested that boron replacing carbon as impurity is a hyper-deep acceptor, which acts as the electron trap rather than increases the p-type conductivity.

To gain a comprehensive understanding of the electronic properties of 3C-SiC, it is essential to investigate the distribution of electrons within the crystal's atoms, as it directly impacts the charge transfer mechanism. Surprisingly, the reviewed literature has given less attention to this aspect, prompting the need for further exploration to improve our understanding of the electronic properties of 3C-SiC.

Also, the literature that discusses the electronic properties of the 3C-SiC focuses mostly on the band gap and density of state, without discussing the charge density that reveals information about the charge transfer mechanism in the material. This research attempts to systematically investigate the structural and electronic properties of B p-type doping in 3C-SiC, with a focus on an impurity concentration of 12.5%. Specifically, in addition to the properties mentioned, we will examine the bond length, bond angle, and charge density after the impurities are added to the crystal structure and investigate the effect of the impurities in the favorable lattice site on the electronic properties of the semiconductor material.

2. Materials and Methods

This research used the following material for analysis: Quantum Espresso V. 7.1 open source application packages, on the Linux Ubuntu operating system, to help implement the DFT and pseudopotential in practice for results analysis while Xcrysden was used to visualize the crystal structures.

To determine the defect properties in crystals, we performed the first-principles calculations. For this purpose, we used the density functional theory (DFT) implemented in Quantum ESPRESSO package qe. 7.1 [16]. The effective ionic potentials were approximated by the projector-augmented wave (PAW) method. The exchange-correlation energy of electrons was evaluated in the generalized gradient approach (GGA) within the perdew-burke-ezrope (PBE) scheme. The Brillouin-zone integrations were performed using special k-point sampling of the Monk-

horst-Pack scheme. In all calculations, we used a converged energy cut-off of 45 Ry and k-points 6 × 6 × 6 for the virgin and defective supercell.

We also performed geometry optimizations to determine the equilibrium crystal structure of the pure and defective supercell. The convergence criteria for the self-consistent field (SCF) cycle set to a maximum energy tolerance of 10^{-6} eV/atom, and the maximum force and stress tolerance of 10^{-3} eV/Å and 0.1 GPa, respectively. The analysis of the electronic properties was performed using the band structure and charge density calculations. Finally, the structural and electronic properties of the pure and defective supercell were compared to evaluate the effects of the doping impurities.

3. Result and Discussion

A. Properties of defect-free 3C-SiC

The converged values of k-points and kinetic cut-off energy were used to further calculate variable relaxation to obtain the optimized value of the lattice constant of the 3C-SiC. The optimized value of the lattice constant was found to be 4.373 Å which is in agreement with the result 4.381 Å presented in the literature [16].

The primary parameters used in this project are listed in **Table 1**. However, to gain more confidence in using these data on the calculations, several different material properties such as the bond length, bond angle, and bulk modulus of bulk 3C-SiC were also studied. The results of the bond length, bond angle, and bulk modulus are shown in **Table 2**. The calculated result was compared with data from other simulation works as listed in **Table 2**.

The value of the charge density cutoff energy in **Table 1** was used as 8 times the value of the wave function cutoff energy for any calculations that used the plain argumentative wave (PAW) pseudo potentials [17].

Table 1. The optimized primary parameters for calculating the ground state properties of 3C-SiC.

SiC system	Wave function cutoff energy (Ry)	Charge density cutoff energy (Ry)	k-point	Lattice constant (Angstrom Å)
8 atoms/cell	50	360	6 × 6 × 6	4.3733

Table 2. The lattice parameter and bond length in angstrom, bond angle in degrees, bulk modulus in GPa and band gap in eV.

Reference	Present work	Muchiri *et al.* (2018)	Bui (2012)
Lattice parameter (Angstrom Å)	4.3733	4.3574	4.3815
Bond length9 (Angstrom Å)	1.983	1.901	-----
Bond angle (Degrees °)	109.472	109.471	-----
Bulk modulus (GPa)	191.8	198.2	210
Band gap (eV)	1.3689	1.34	1.40

The electronic band structure of 3C-SiC was also investigated at high symmetry points of the zinc-blende Brillouin zone. The computed electronic band gap energy was found to be 1.36 eV, which is comparable to other theoretical data that used a similar computational approach as shown in **Table 2**. The band structure of the pure 3C-SiC as illustrated in **Figure 1**, revealed the semiconducting nature of the material. The band gap was measured from the top of the valence band at the zone center to the bottom of the conduction band at the X-axis. An indirect band gap from the Γ-point to the X-point was observed, which is in agreement with theoretical data. The Fermi level was normalized by subtracting the energy from the Fermi energy value to make it a reference energy level. The band gap energy calculated for 3C-SiC was lower than the experimental data, which could be attributed to the tendency of density functional theory to underestimate the electron-electron interactions and suffer from a self-interaction error. This result implies that the parameters used for bulk SiC calculations were reliable. Various band gap correction methods such as hybrid functionals B3LYP and HSE06 can be used to improve the performance of DFT calculations in determining the band gap energy of materials [18].

In 3C-SiC, silicon (Si) and carbon (C) atoms form a repeating lattice structure. The charge density calculation allows us to visualize and understand how electrons are distributed around the atomic nuclei. Studying the charge density will give more insights into the charge transfer mechanisms, bonding nature, and electronic properties of 3C-SiC. It helps in understanding the behavior of the semiconductor material and its potential applications in various fields, such as electronics, optoelectronics, and power devices.

The analysis of the charge density, as depicted in **Figure 2**, provides valuable insights into the charge transfer mechanism in 3C-SiC and determines the regions of high and low electron density within the crystal. Specifically, it reveals that a significant portion of the valence electrons tends to accumulate near the

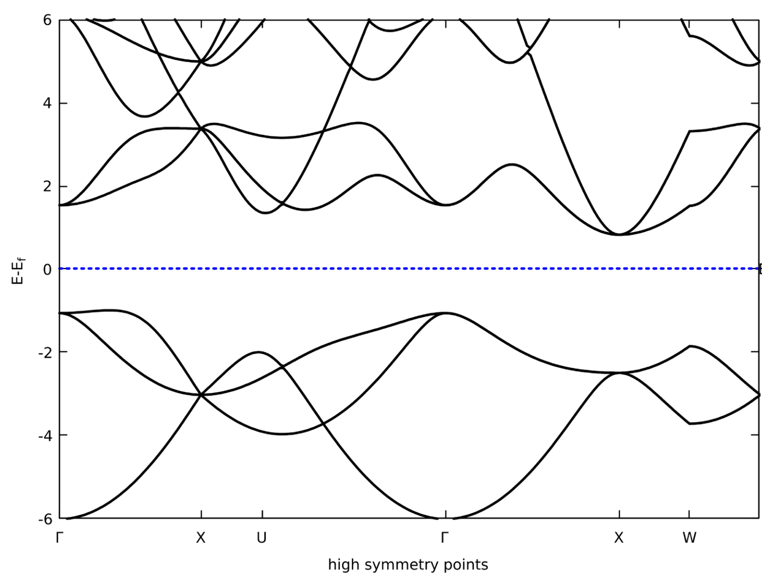

Figure 1. Band structure of pure 3C-SiC.

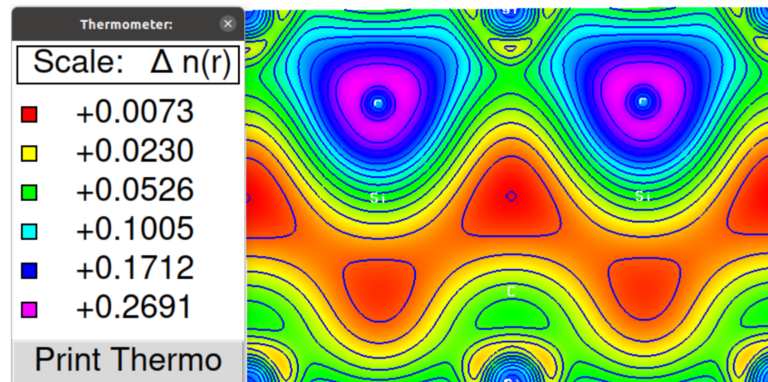

Figure 2. Charge density of defect free 3C-SiC.

carbon atom. This is because carbon lacks p states in the core, which means no constraints are preventing the valence p states from accumulating near the carbon nuclei. In other words, electro-negativity which is the tendency of an atom to attract an electron to its nucleus, for C is much higher than that of Si (2.55 and 1.90 respectively). Consequently, electrons can easily flow from silicon to carbon, resulting in a higher electron density near carbon atoms. This observation aligns with the conclusions drawn by other researchers [19].

B. Structural properties of B-doped 3C-SiC

To prevent the defect-defect interaction we modeled the 3C-SiC unit cell to a $2 \times 2 \times 2$ supercell for all defect calculations. After B was doped in the 3C-SiC crystal structure we ran variable cell relaxation calculations to allow the atoms to relax to the most stable equilibrium state in their various lattice position and enable getting optimized geometry of the 3C-SiC structure. We observed that the lattice constant was 4.2492 Å after doping B, less than the initially observed from the pure 3C-SiC. Also, the new bond length and bond angle were observed to be 1.5875 Å and 109.471 Degrees respectively. The value of the bond length was found to correlate with the lattice constant as expected. This is because the Si has an atomic radius of 1.554 while the B is 1.274, which is smaller than the former.

The geometric deformation of the 3C-SiC structure when B substitutes Si resulted in to decrease in the supercell volume. When B is doped into the 3C-SiC crystal structure, it results in a decrease in the lattice constant, indicating a stronger bond formation. This suggests that B atoms can effectively substitute Si atoms in the crystal lattice without causing significant structural changes.

C. Electronic properties

1) Band structure

Compared to those of pure 3C-SiC, the band structures of B-doped 3C-SiC exhibit more complicated energy levels. According to the valence band maximum and the conduction minimum level, some impurity bands are moving a little bit closer to the Fermi level. At the gamma point of the band, the structure is both the top of the valance band and the bottom of the conduction band. It is a direct band structure as illustrated in **Figure 3**, which is similar to what has been observed in the reviewed literature.

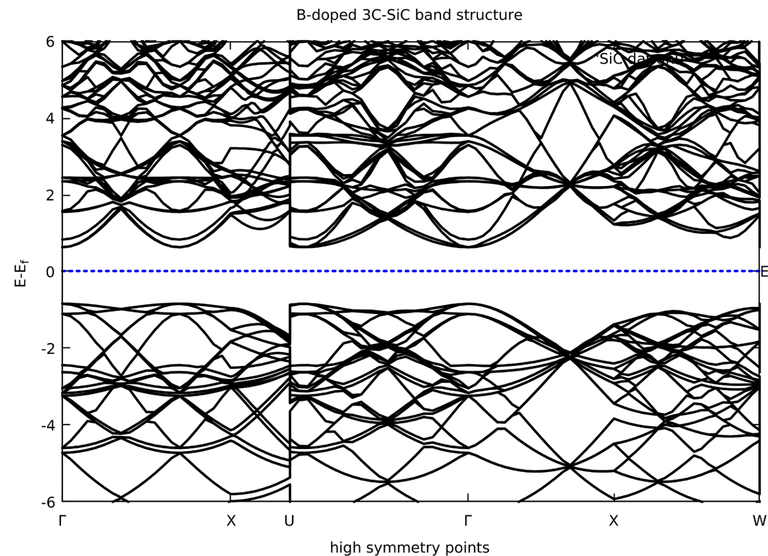

Figure 3. Band structure of boron-doped 3C-SiC.

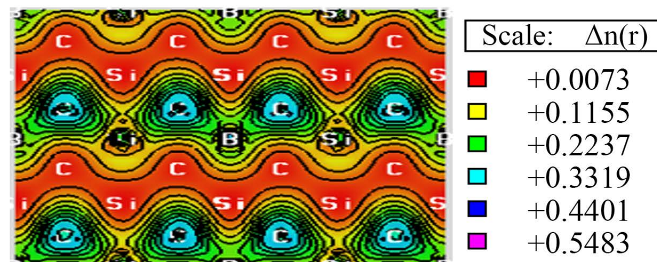

Figure 4. Charge density of B-doped 3C-SiC.

The introduction of this dopant in 3C-SiC leads to a reduction in the energy separation between the conduction band minimum and valence band maximum. As a result, new energy states emerge within the band gap of 3C-SiC. These additional energy states facilitate the movement of electrons from the valence band to the conduction band, ultimately resulting in enhanced electrical conductivity [20].

The enhanced conductivity makes it attractive for power electronics, field-effect transistors (FETs), and high-frequency devices operating at high temperatures. B-doped 3C-SiC can potentially outperform silicon-based devices in these applications due to its superior thermal and electrical properties.

2) Charge density

In **Figure 2**, an inhomogeneous charge distribution within the Si-C bond along the (110) plane is depicted. This observation confirms the previously reported bonding characteristics between Si and C atoms in 3C-SiC, as anticipated [16]. Furthermore, **Figure 4** illustrates minimal interaction between the C and Si atoms situated between the layers, represented by the red separation. The charge density along the (110) plane was established for the defect 3C-SiC system. The calculations were done with B-point defects and showed a significant interaction between the dopant and the surrounding C atoms as observed in **Figure 4**, compared to the defect-free crystal as observed in **Figure 2**.

The charge density analysis demonstrates that B doping exhibits a more pronounced interaction between the dopant and surrounding C atoms. This suggests that B atoms have a stronger influence on the charge transfer mechanism and bonding nature within the crystal structure.

4. Conclusions

The convergence tests led to optimized parameters for accurate calculations. The properties of pure 3C-SiC were successfully determined, aligning with previous studies. The band structure calculations revealed a direct band gap of 1.36 eV, indicating that 3C-SiC is a semiconductor. The density of states analysis confirmed the band gap and provided information about the available electronic states. The charge density analysis showed the distribution of electrons around the atomic nuclei and indicated the charge transfer mechanism in 3C-SiC.

B doping leads to a reduction in the band gap, enhanced electrical conductivity, stronger charge transfer interactions, and a significant contribution from B orbitals in the conduction band. Tailored B doping can create materials with specific light absorption or emission properties, potentially enabling light-emitting diodes (LEDs) or solar cells based on 3C-SiC. By manipulating the band gap through doping, 3C-SiC could be engineered for efficient light emission or absorption in desired wavelengths.

The examination of charge density in addition to what other researchers have done on 3C-SiC provided valuable insights into the spatial distribution of electric charge within the material and its implications for charge transfer, bonding, and electronic properties. This contributes to the understanding of the behavior of electrons in the crystal lattice of 3C-SiC and its relevance to various applications. Additionally, exploring the impact of different doping concentrations, combinations of impurities, and other impurities on the properties of 3C-SiC would provide further insights into the material's behavior.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

References

[1] Xi, J.Q. (2017) First-Principles Study of Point Defect Behavior at Interfaces and In-Plane Strain Fields. Ph.D. Thesis, University of Tennessee, Knoxville. https://trace.tennessee.edu/utk_graddiss/4718

[2] Abderrazak, H. and Bel Hadj Hmida, E.S. (2011) Silicon Carbide: Synthesis and Properties. In: Gerhardt, R., Ed., *Properties and Applications of Silicon Carbide*, IntechOpen Limited, London, 361-388. https://doi.org/10.5772/15736

[3] Zhao, X., Chen, D.L., Ru, H., Zhang, N. and Liang, B. (2011) Oxidation Behavior of Nano-Sized SiC Particulate Reinforced Alon Composites. *Journal of the European Ceramic Society*, **31**, 2255-2265. https://doi.org/10.1016/j.jeurceramsoc.2011.05.049

[4] Lambrechts, W. and Sinha, S. (2017) A Review on Si, SiGe, GaN, SiC, InP, and GaAs as Enabling Technologies in EW and Space. In: Lambrechts, W. and Sinha, S., Eds.,

SiGe-Based Re-Engineering of Electronic Warfare Subsystems, Springer, Cham, 301-329. https://doi.org/10.1007/978-3-319-47403-8_10

[5] Zhu, Y., Yu, V.W.-Z., and Galli, G. (2023) First-Principles Investigation of Near-Surface Divacancies in Silicon Carbide. *Nano Letters*, **23**, 11453-11460. https://doi.org/10.1021/acs.nanolett.3c02880

[6] Anderson, C.P., Bourassa, A., Miao, K.C., Wolfowicz, G., Mintun, P.J., Crook, A.L., Awschalom, D.D., *et al*. (2019) Electrical and Optical Control of Single Spins Integrated in Scalable Semiconductor Devices. *Science*, **366**, 1225-1230. https://doi.org/10.1126/science.aax9406

[7] Silungwe, D. (2016) Computational Modeling of the Electronic and Structural Properties of Chalcopyrite-Type Semiconductors and Platinum Group Metal Chalcogenides. Ph.D. Thesis, University of Zambia, Lusaka.

[8] Schultz, P.A., Van Ginhoven, R.M. and Edwards, A.H. (2021) Theoretical Study of Intrinsic Defects in Cubic Silicon Carbide 3*C*-SiC. *Physical Review B*, **103**, Article ID: 195202. https://doi.org/10.1103/PhysRevB.103.195202

[9] Alkhaldi, N.D., Barman, S.K. and Huda, M.N. (2019) Crystal Structures and the Electronic Properties of Silicon-Rich Silicon Carbide Materials by First Principle Calculations. *Heliyon*, **5**, E02908. https://doi.org/10.1016/j.heliyon.2019.e02908

[10] Zirkelbach, F., Stritzker, B., Nordlund, K., Lindner, J.K.N., Schmidt, W.G. and Rauls, E. (2011) Combined *Ab Initio* and Classical Potential Simulation Study on Silicon Carbide Precipitation in silicon. *Physical Review B*, **84**, Article ID: 064126. https://doi.org/10.1103/PhysRevB.84.064126

[11] Kaur, T. and Sinha, M.M. (2020) First Principle Study of Structural, Electronic, and Vibrational Properties of 3C-SiC. *AIP Conference Proceedings*, **2265**, Article ID: 030384. https://doi.org/10.1063/5.0017269

[12] Ganchenkova, M.G., Супрядкина, И.А., Абгарян, К.К., Бажанов, Д.И., Мутигуллин, И.В. and Бородин, В.А. (2015) Influence of the *Ab Initio* Calculation Parameters on Prediction of Energy of Point Defects in Silicon. *Izvestiâ Vysših Učebnyh Zavedenij*, **18**, 23-30. https://doi.org/10.17073/1609-3577-2015-1-23-30

[13] Granadeiro Costa, A.R. (2018) Lattice Location of Impurities in Silicon Carbide. Ph.D. Thesis, Instituto Superior Técnico, Lisbon.

[14] Rurali, R., Godignon, P., Rebollo, J., Hernández, E. and Ordejon, P. (2003) First-Principles Study of *n*-Type Dopants and Their Clustering in SiC. *Applied Physics Letters*, **82**, 4298-4300. https://doi.org/10.1063/1.1583870

[15] Sheng, B., Niu, M. and Shao, X. (2011) Conductivity and Magnetic Properties Study on Doped Semiconductor Material of 3*C*-SiC: A First-Principle Investigation. 2011 *International Conference on Electric Information and Control Engineering*, Wuhan, 15-17 April 2011, 5758-5761. https://doi.org/10.1109/ICEICE.2011.5777405

[16] Bui, T. (2012) Structural and Electronic Properties of Cs-Doped SiC: A First-Principles Investigation. Ph.D. Thesis, Boise State University, Boise.

[17] Romero, J., Phillips, E., Ruetsch, G., Fatica, M., Spiga, F. and Giannozzi, P. (2018) A Performance Study of Quantum ESPRESSO's PWscf Code on Multi-Core and GPU Systems. In: Jarvis, S., Wright, S. and Hammond, S., Eds., *High-Performance Computing Systems. Performance Modeling, Benchmarking, and Simulation*, Vol. 10724, Springer, Cham, 67-87. https://doi.org/10.1007/978-3-319-72971-8_4

[18] Gao, Y., Zhang, F.C. and Zhang, W.H. (2014) The Electronic and Structural Properties of 3*C*-SiC: A First-Principles Study. *Advanced Materials Research*, **971-973**, 208-212. https://doi.org/10.4028/www.scientific.net/AMR.971-973.208

[19] Zhao, G.L. and Bagayoko, D. (2000) Electronic Structure and Charge Transfer in 3C-

and 4H-SiC. *New Journal of Physics*, **2**, Article 16.
https://doi.org/10.1088/1367-2630/2/1/316

[20] Ding, R., Yang, Y., Ren, X., Xi, X. and Zhang, B. (2009) First-Principles Study of Boron Doping-Induced Band Gap Narrowing in 3C-SiC. 2009 16*th IEEE International Symposium on the Physical and Failure Analysis of Integrated Circuits*, Suzhou, 6-10 July 2009, 563-566.