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Theoretical Study of the Electronic Features of Silicon-Carbon Crystal as a Semiconductor using Quantum Espresso

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Abstract: In this research, quantum simulations are applied to determine the electronic features of the Silicon-Carbon (SiC) crystal. The band structure (BS), the density of states (DOS), k-resolved DOS, and convergence calculations are conducted for the optimized SiC using the plane-wave (PW) method as implemented in the Quantum Espresso (QE) program. The calculated values of the band gap and Fermi energy show the values of 1.41 and 9.80 eV, respectively. Therefore, our scrutinized SiC crystal appears to be a notable semiconductor that can promise a new generation of solar cells.

Keywords: Quantum Espresso; band structure; semiconductor; DOS.

1. Introduction

The intrinsic optical and electronic properties of semiconductor materials play an important role in constructing an efficient solar cell. The critical property of a solar cell depends on whether the semiconductor absorbs the wide range of photons that are contained in solar radiation. The magnitude of such absorption deals with the active layer of an absorber, the wavelength of radiation, and the absorption coefficient. These parameters are directly related to the semiconductor's band gap energy (E_g) and band structure energy (E_b). Photons with higher energy than the absorber's E_g can be absorbed and can generate an electron-hole pair. The excess energy is converted into heat in the solar cell. Using a wide range of wavelengths results in low photocurrent of a solar cell with high efficiency and probability because that high fraction of photons is being converted into electricity and voltage. On the other hand, solar cells are usually made of semiconductors with narrow band gaps, which can absorb a smaller region of radiation but higher energy photons that lead to a lower photocurrent and voltage. Therefore, an absorber should have the optimum Eg to achieve the maximum conversion of energy and efficiency [1]. The other important concept is the band structure (BS), which can explain a crystal's optical and magnetic properties. The level of Fermi energy (E_F) determines the nature of the material. If the E_F is located in a band gap zone, the material is considered insulating (or semiconducting); otherwise, it is metallic [2]. In an insulator, the highest occupied band is called the valence band (VB), and the lowest unoccupied band is known as the conduction band (CB), at zero temperature (Figure 1).

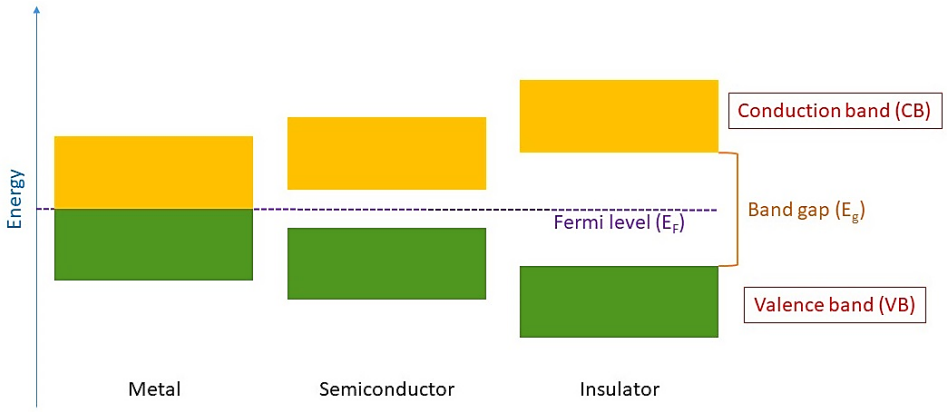

Figure 1. Illustration of metal, semiconductor, and insulator.

Conversely, the CB is occupied with electrons in a conductor, even at zero temperature [3]. Electrons can easily jump across the band gap toward the CB by applying an electrical field at any temperature above zero. The high energy of electrons can be obtained from thermal motion or agitation. The E_g of an insulator is usually 5 eV or above, which means the required energy for jumping electrons is less available, which leads to a weak electric current or lack of it in the presence of an external electric field. Most important semiconductors show Eg values ranging between 0.25 to 2.5 eV [4–6]. Silicons, which are widely used in electronics, solar cells, and biomedical and light-emitting devices, show the indirect band gap nature of the BS. The indirect band gap of silicon has been a chief obstacle until the last two decades. Various efforts have been devoted to studying and using nanoscale Si-based substances to discover and improve their optical properties in the last few years. Silicon nanocrystals display the visible photoluminescence that proves the partial overcoming of their indirect band gap. Nevertheless, many aspects remain to be discovered and disputed [7]. In this investigation, we conduct the BS, density of states (DOS), k-resolved DOS, and spin-orbit coupling (SOC) calculations for the optimized SiC nanocrystal, using the plane-wave (PW) method as implemented in Quantum Espresso (QE) program [8–10], based on the density functional theory (DFT) (Figure 2).

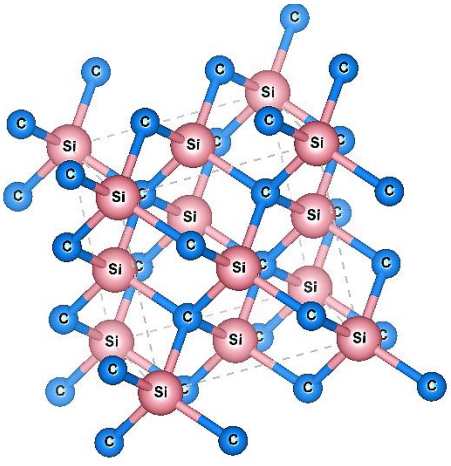

Figure 2. Molecular structure of SiC crystal.

2. Methods

All calculations are carried out using the first-principles pseudopotential method, based on the DFT and PW methods via the QE package. The figures and graphs are plotted using VESTA [11], GNUplot [12], Matplotlib [13], and Excel [14] programs. The structure of SiC

crystal is simulated by VESTA and then optimized using self-consistent field (SCF) calculation (see Supplementary Information). Pseudopotentials (PPs) are the proper replacement of the complex effects of the motion of the core electrons and nucleus with an operative potential. Since only the valence electrons are involved in this approximation, the DFT calculations become less computationally expensive. The projector augmented waves (PAWs) method was used to treat valence electron configuration [15]. The PAW method restores the pseudo-to-the-electron wavefunctions accurately. The cut-off kinetic energy (E_{cut}) and charge density are set at 60.00 and 244.00 Ry, respectively, with a mixing beta 0.70. The convergence of the SCF calculation is attained for the fully relaxed crystal.

3. Results and Discussion

3.1. Band structure (BS).

The electronic band structure describes the range of energies of electrons within the solid, which can explain the electrical resistivity and optical absorption properties. Band theory indicates that electrons of a solid can only possess energies of certain values that lead to the allowed (BS) and forbidden energy ranges (band gap). The electrons of a single atom occupy discrete energy levels during the atomic orbitals of a crystal lattice overlap with the nearby orbitals due to their proximity in space. Therefore, each distinct energy level splits into many levels with different energies. Nevertheless, the energy of adjacent levels is very close together, such as a continuum level. In our model, we calculate the BS of SiC using the exchange correlation of PBE (Figure 3). The gap that does not include any line and appears empty is known as the band gap, which separates the CB and VB zones. A dotted horizontal line that divides the graph into two parts, upper and lower, is called the E_F, which is equal to 9.80 eV and is located in the band gap zone. The upper and lower zones are considered the CB and VB, respectively. The band gap or minimum required energy for an electron to jump across from the VB to the CB is 1.41 eV, which introduces the SiC as a strong semiconductor.

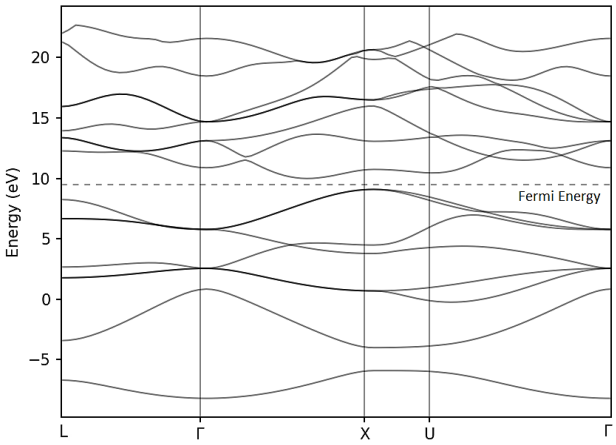

Figure 3. Electronic BS of SiC crystal.

3.2. Density of states (DOS) and k-resolved DOS.

One of the most significant benchmarks in examining the nature of semiconductors is the DOS. The DOS of a crystal describes the proportion of occupied and unoccupied states as a function of energy. In doing the DOS calculations, first, we perform the SCF calculation followed by the non-SCF calculation with denser k-points. The green-colored region (VB) of the calculated DOS diagram of SiC crystal indicates a higher probability of the presence of

electrons under 9.25 eV energy (Figure 4). On the other extreme, the unoccupied levels lay above 10 eV energy. A higher DOS at a particular energy level indicates that many states are available for occupation. The E_g is 1.41 eV, which validates the results obtained from the BS calculations.

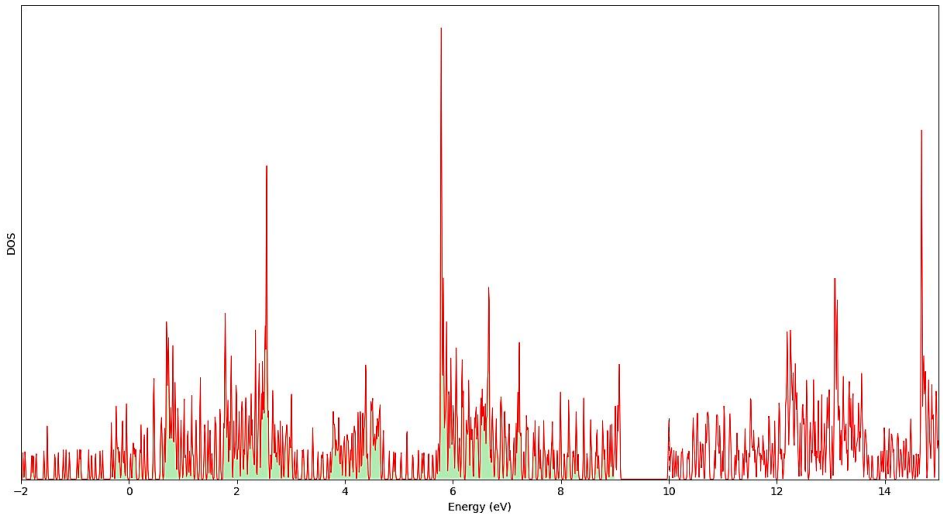

Figure 4. The DOS plot of SiC crystal.

In the following, we calculate the k-resolved DOS plot for spin-up and spin-down bands of Si atoms (Figure 5). The k-resolved DOS is useful when the overlap of states is high and shows the contribution of states of a specific atom concerning total BS. The color scale is normalized compared to the maximum weight of an atomic state across the k-points. The E_g of Si atom is under the Fermi energy of SiC crystal, which means the heterostructure of SiC crystal compensates for the indirect bandgap of the Si atom.

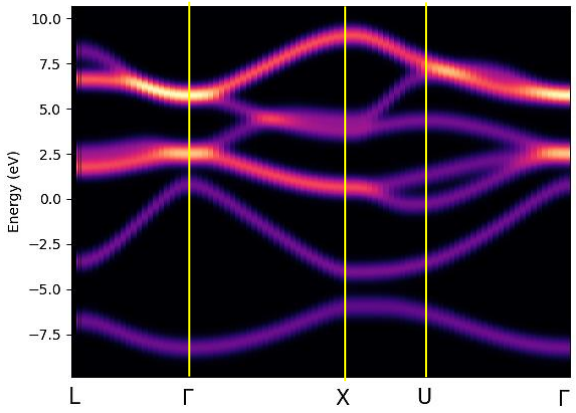

Figure 5. The k-resolved DOS plot of SiC crystal (spin up and spin down bands for Si atoms).

3.3. Convergence graph.

The kinetic energy cut-off (ecutwfc or E_{cut}) optimization is usually done to confine the number of plane waves with energy lower than E_{cut} and reach the optimum E_{cut}. This kind of convergence is required for efficiency while maintaining the accuracy of calculations. We conduct the SCF calculation for SiC and plot the total energy (E_{tot}) against the E_{cut} in Ry (Figure 6). The optimum E_{cut} turns out as 60 Ry for E_{tot} of -64.71 Ry.

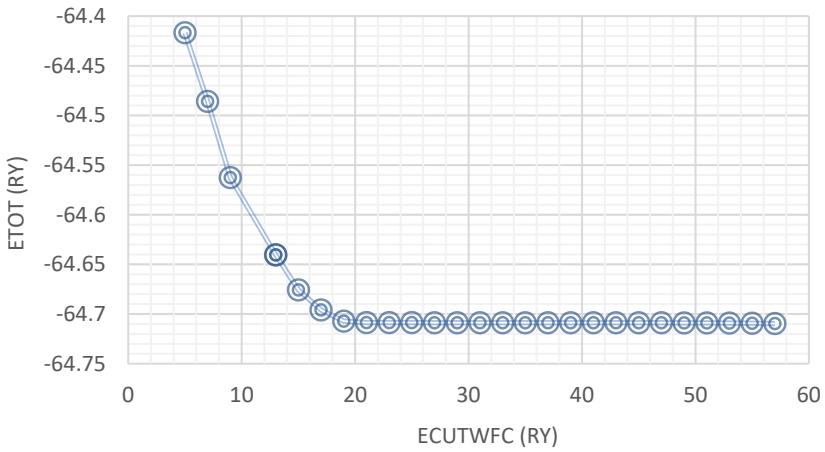

Figure 6. Convergence graph of total energy (E_{tot}) *vs*. cutwfc energy (E_{cut}) in Ry.

4. Conclusions

In this research, we have investigated the BS, DOS, k-resolved DOS, and convergence calculations for optimized SiC crystal using the DFT method with PBE function via the QE package. In addition, figures and graphs have been plotted using VESTA, GNUplot, Matplotlib, and Excel programs. The PAW method has been applied to the PPs. The E_{cut} and charge density has been set at 60.00 and 244.00 Ry, respectively, with a mixing beta of 0.70. Finally, the convergence of the SCF calculation has been achieved for the fully relaxed crystal. The E_F and E_g of SiC crystal have been calculated as 9.80 and 1.41 eV, respectively. Therefore, our scrutinized SiC crystal turns out to be a notable semiconductor that can promise a new generation of solar cells.

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Conflicts of Interest

The author declares no conflict of interest.

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Supplementary material

☑ SCF Calculation Results:

Total energy	=	-64.70966345 Ry
Total all-electron energy	=	-655.818811 Ry
Estimated scf accuracy	<	4.4E-09 Ry

The total energy is the sum of the following terms:

One-electron contribution	=	-0.05413590 Ry
Hartree contribution	=	3.33000031 Ry
XC contribution	=	-10.13721452 Ry
Ewald contribution	=	-16.13009979 Ry
One-center paw contrib.	=	-41.71739878 Ry

☑ SiC Crystal properties:

Chemical compound source	Synthetic	Symmetry space group name H-M	'F -4 3 m'
Chemical formula structural	'Si C'	Cell length a	4.348
Chemical name mineral	'Moissanite 3C'	Cell length b	4.348
Chemical name systematic	'Silicon carbide'	Cell length c	4.348
Space group IT number	216	Cell volume	82.2
Symmetry cell setting	cubic	Exptl crystal density meas	3.2
Symmetry Int Tables number	216	Cod database code	1010995