

1 DETERMINATION OF THE ENERGY BAND GAP OF SILICON USING 2 QUANTUM SIMULATION FOR PHOTOVOLTAIC ENERGY 3 APPLICATIONS

4 ABSTRACT

5 *This research deals with the study of the band structure, and density of state of*
6 *silicon, using the first-principles pseudopotential method, based on the density*
7 *functional theory (DFT) and the plane-wave method as implemented into Quantum*
8 *Espresso (this is an open source software for Research of the Electronic Structure,*
9 *Simulations, and Optimizations of materials) package. The value of the band gap*
10 *found ranges between -0.2 to +0.6eV. From the DOS graph we can observe the*
11 *peaks from - 3.0 eV to - 3.5eV, and 5.50eV to 7.5eV for Si Material.*

12 **KEYWORDS:** DOS , Energy Band-Gap, Photovoltaic, Pseudopotential, Quantum
13 Simulation,

14 1.0 INTRODUCTION:

15 The key property of each solar cell is its capability to absorb effectively wide
16 spectrum of photons contained in solar radiation reaching its active surface. This
17 feature depends on intrinsic optical and electronic properties of semiconductor
18 material used as an absorber layer in a cell and is described by wavelength
19 dependent value of the absorption coefficient, the parameter being directly related
20 to semiconductor's energy band gap and energy band structure.

21 As it is well known photons with energy lower than the absorber band gap cannot
22 be absorbed and so they do not contribute to energy conversion. On the other hand
23 one photon, even if its energy exceeds doubled value of that of the band gap,
24 cannot generate more than single electron-hole pair, dissipating all its excess
25 energy as a heat in the cell. With these limitations, the role of the absorber in the
26 conventional solar cells are briefly explained as follows.

27 When using wide band semiconductor light absorption becomes limited only to
28 high energy photons while for the sub-band gap photons solar cell practically
29 remains transparent. This results in lower photocurrent of such cell but the
30 advantages in this case are more efficient energy conversion of the absorbed high
31 energy part of solar spectrum due to the fact that higher fraction of photons energy
32 is being converted into electricity, and higher value of the output voltage of the
33 cell. Contrary to that, solar cells made of narrow band semiconductors, though
34 capable of absorbing larger part of solar spectrum and hence exhibiting higher
35 photocurrent values, have lower energy conversion efficiency in the range of high
36 energy photons and exhibit lower output voltage.

37 The above discussion leads to obvious conclusion that to achieve maximum
38 conversion efficiency for a specified solar spectrum, absorber material with
39 optimum band gap could be use for any solar cell fabrication (Andreas, 2018).

40 In addition, the Band Structure is one of the most important concepts in Solid State
41 Physics. It provides the electronic levels in (ideal) crystal structures, which are
42 characterized by two quantum numbers, the Bloch vector, \mathbf{k} and the band index, n .
43 Here, the Bloch vector is an element of the reciprocal space (in units 1/length) and
44 the energy of the electron $E_n(\mathbf{k})$ is a continuous function of \mathbf{k} , so that one obtains a
45 continuous range of energies referred to as the energy band. Many electrical,
46 optical, and even some magnetic properties of crystals can be explained in terms of
47 the band structure. Hence, of particular importance is the location of the Fermi
48 energy, until which all levels are occupied at zero temperature. If the Fermi energy
49 is located in a band gap, the material is insulating (or semiconducting) while it is
50 metallic if otherwise. (Zdanowicz *et al.*, 2005).

51 Furthermore, the energy band concept is a great help in understanding several
52 properties of solids. The nature of the energy bands determines whether the
53 material is an electrical insulator, a semiconductor, or a conductor. In particular,
54 what matters are the extent to which the states in each band are occupied and the
55 spacing, or energy gap between adjacent bands. A crucial factor is the exclusion
56 principle which states that only one electron can occupy a given quantum
57 mechanical state. In an insulator at absolute zero temperature, the highest band that
58 is completely filled, called the valence band, is also the highest band that has any
59 electrons in it. The next higher band, called the conduction band is completely
60 empty, and there are no electrons in its states.

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67 In a conductor such as metal, there are electrons in the conduction band even at
68 absolute zero. The metal sodium, Na is an example. (Young & Freedman, 2008)

Empty conduction band

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Large Energy Gap, E_g

Filled Valence Band

71 **Fig 1: Insulator: Empty Conduction Band, Large Energy Gap**

Empty conduction band

72 Small Energy Gap, E_g

Filled Valence Band

73 **Fig 2: Semiconductor: Empty conduction Band, Small Energy Gap**

Partially Filled conduction band

74 Energy Gap

Filled Valence Band

75 **Fig 3: Conductor: Partially filled conduction band and Valence band.**

76 When an electrical field is applied across the material, electrons would move into
77 different quantum state with slightly different energy. That is, the electron would
78 jump across the energy gap, into the conduction band, where there are plenty of
79 nearby unoccupied states. At any temperature above absolute zero, there is high
80 probability that this jumping of the electrons can take place, because an electron
81 can gain energy from thermal motion or agitation. (Young & Freedman, 2008)

82 In an insulator, however, the energy gap between the valence band, and the
83 conduction bands can be 5eV or more, and that much thermal energy is not
84 ordinarily available, hence, little or no current flow in response to an applied
85 electric field, and low electrical conductivity. In a conductor, such as a metal,
86 there are electrons in the conduction band even at the absolute zero temperature.
87 (Young & Freedman, 2008).

88 Thus, in this research, we shall study one of the semiconductor material, Silicon, Si
89 including its Density of state, and the Electronic structure.

90 **COMPUTATIONAL METHODS**

91 In this study research, we consider the Silicon Semiconductor Material. All
92 arithmetical calculations were carried out using First-Principles Pseudopotential
93 method, based on the Principle of the Density Functional theory (DFT), and the
94 Plane-Wave method as implemented in the Quantum Espresso (which is an
95 acronym for an opEn-Source Package for Research in Electronic Structure,
96 Simulation, and Optimization) Application Package. Exchange and correlation
97 effects are treated under the generalized-gradient-approximation with Perdew-
98 Burke-Ehrenk of (PBE) function. The Ultrasoft Pseudopotential (USP) method was
99 used to treat valence electron configuration. The cut-off of W.F. was set at
100 25.000Ry and the Cut-off of the Charge is at 225.000Ry.

101 For the Band structure calculations, current dimensions of program PWSCF are:
102 Max number of different atomic species (ntypx) = 10, Max number of k-points
103 (npk) = 4000, Max angular momentum in pseudopotentials (lmaxx) = 3.

104 For the Density of States calculation, XC Functional Enforced from input Program
105 file, Exchange-Corellation = SLA PW PBE PBE (1 4 3 4 0 0), any further DFT
106 definition will be discarded.

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108 **3.0 THE MODEL**

109 We model a Si material as shown in the Fig.4 below. The convergence of the SCF
110 curve calculation is set, and the geometry of the system is fully relaxed.

111 The Si electronic structure is calculated via the plane wave projector-augmented
112 wave method implemented in the Quantum Espresso (QE) package. In the QE
113 package, the approach is based on an iterative solution of the Kohn-Sham equation
114 of the DFT theory. In the DFT approach, the generalized gradient approximation
115 (GGA) method, and the exchange-correlation functions are realized in the non-
116 relativistic Perdew-Burke Emzerhof pseudo-potential (PBE). In addition, The plane
117 wave basis is arranged to a kinetic energy cut-off equal to 490 eV. The DFT
118 scheme was then used to investigate the band structure, the density of state (DOS),
119 and the charge density distribution of the system.

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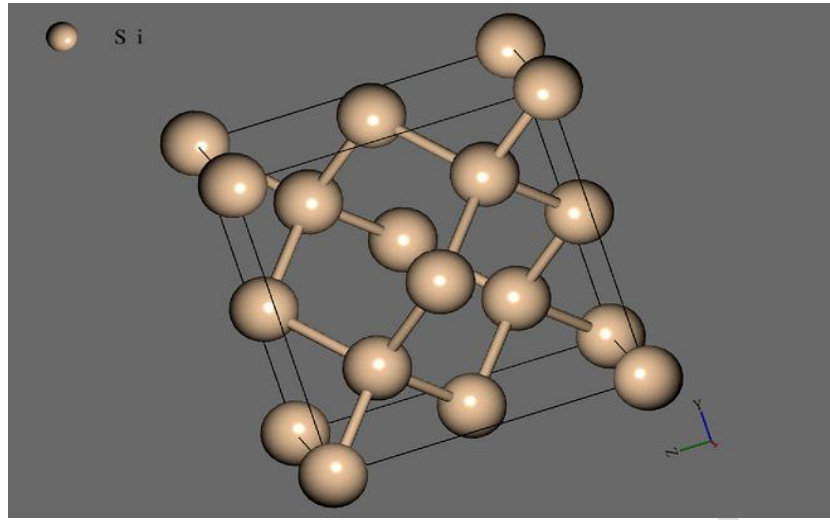


FIG 4: Molecular Structure for the Si Material.

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123 The thermal properties of the system are studied using the Boltzmann's Theory,
 124 where the specific heat, c , of the system can be calculated using:

$$125 \quad c(T, \mu) = \int n(\epsilon) (\epsilon - \mu)^2 \left[-\frac{\partial f_{\mu}(T; \epsilon)}{\partial x} \right] d\epsilon \quad 3.1$$

126 In addition, the electronic thermal conductivity, κ^0 , is determined using:

$$127 \quad \kappa_{i,j}^0(T, \mu) = \frac{1}{c^2 T \Omega} \int \delta_{i,j}(\epsilon) (\epsilon - \mu)^2 \left[-\frac{\partial f_{\mu}(T; \epsilon)}{\partial x} \right] d\epsilon \quad 3.2$$

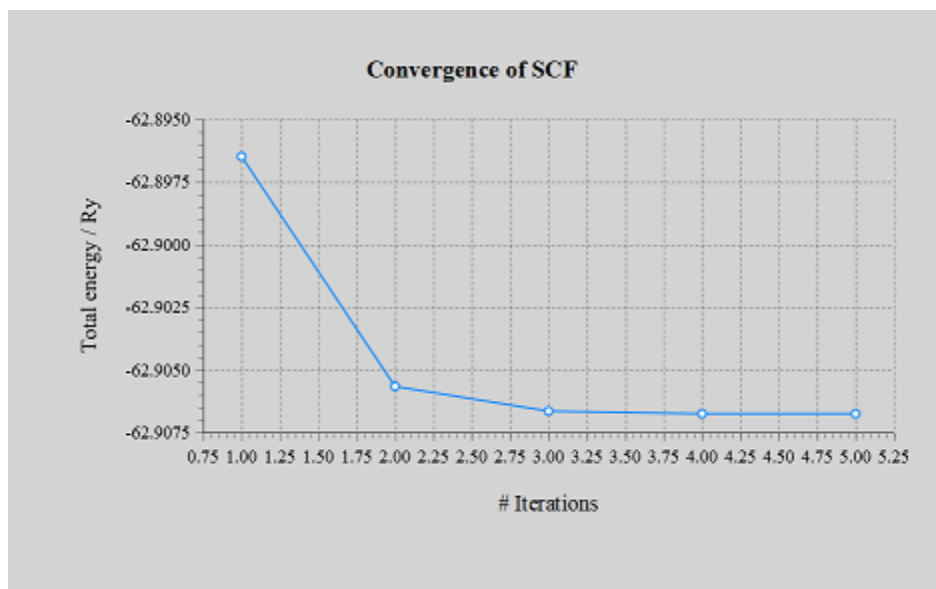
128 where $\sigma_{i,j}(\epsilon)$ indicates the conductivity tensors, and Ω is the number of K point
 129 which are sampled in Brillouin zone. (Rashid *at al.*, 2019).

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132 **4.0 Density of State for Silicon (DOS)**

133 The Density of State (DOS), $g(E)$ can be defined as the number of states, dn per
 134 unit energy range, dE . Thus, to determine this Density of State, we ran the
 135 simulation, using quantum expessor. In doing so, series of iterations were ran, and
 136 five points were obtained as the points of convergence as shown in the following
 137 graph below:

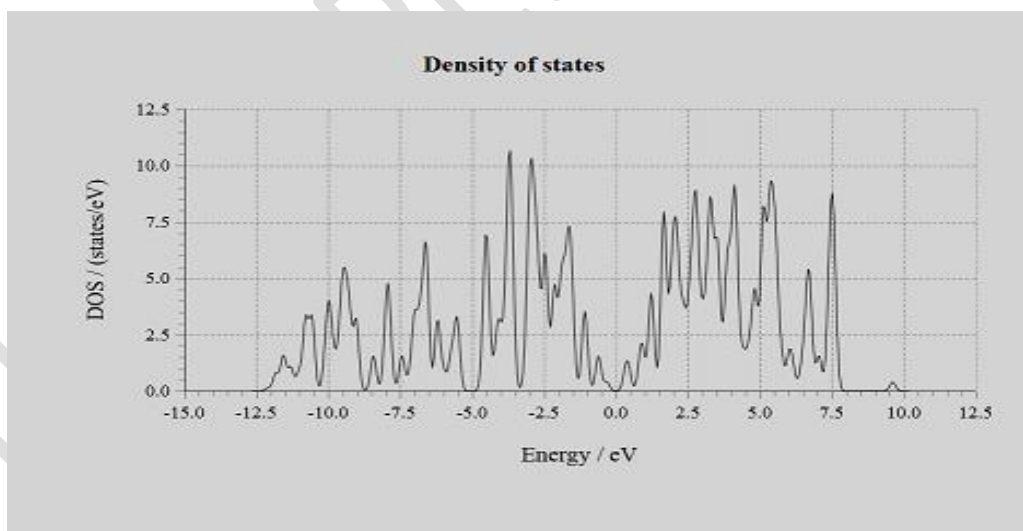


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Fig 5: Convergence of the Self-consistent curve

140 It is at the convergence, that the graph of the Density of State was obtained. This
 141 DOS graph gives the electronic band structure of the Si material. Thus, the DOS
 142 graph is as shown in **Fig 6** below:



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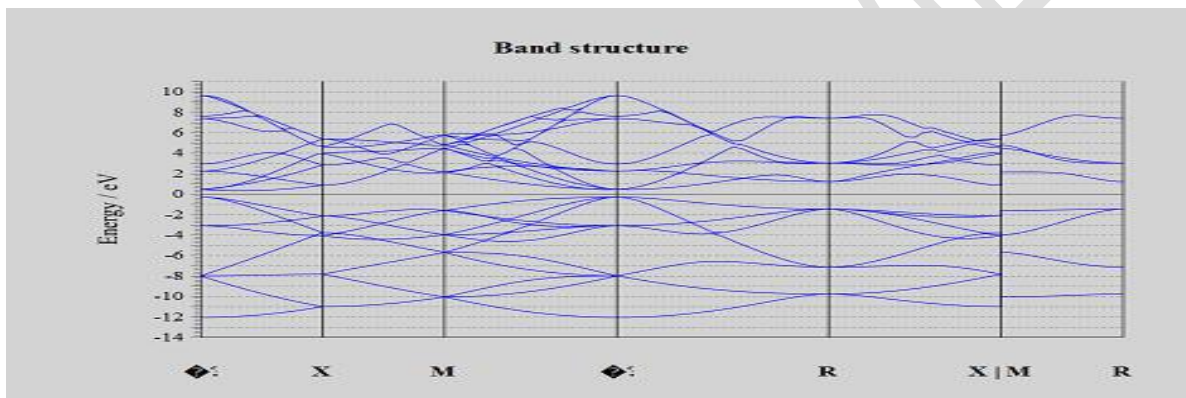
Fig 6: Graph of the Density of State For Silicon (DOS)

145 From the Density of State DOS graph as shown in the **Fig 6** above, is a plot of the
 146 Density of State in electron volt, per unit energy in the electron volts. Thus, we can

147 observe that the peaks are between -3.5 to -3.0 eV. This result corresponds to the
148 valence bands occupied by the electrons of Silicon Material.

149 **5.0 Electronic Band Structure for Silicon, Si**

150 To have a clear view understanding of the electronic structure of Silicon. We
151 consider the graph below. In this graph, is a black colored horizontal line that
152 divides into half the lower part called the valence band, and the other half the upper
153 part, that is the conduction band. This gap that separates between the valence band
154 and the conduction band, is called the band gap. The minimum amount of energy
155 required for electron to jump across this band gives the band gap energy, or the
156 energy band gap. Thus, for this silicon material, the band gap obtained is from -
157 0.2eV to 0.6 eV.



158

159 **FIG 7.** Electronic Band Structure For Silicon

159

160 **CONCLUSION**

161 In this research, we have studied the Band Structure and the Density of State
162 (DOS) using First-Principles Pseudopotential method based on the Density
163 Functional Theory (DFT) and the Plane Wave Method as implemented in the
164 Quantum Espresso. We are able to determine the DOS and the Band gap of the Si
165 material. *The value of the band gap found ranges between -0.2 to +0.6eV, and the*
166 *DOS peaks between - 3.0 eV to - 3.5eV, and 5.50eV to 7.5eV.* Thus, the electronic
167 structure property of silicon for possible photovoltaic applications is achieved.

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