

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

3 M.A. Bilya*, M.U Sarki, and A.A. Mundi

4 Nasarawa State University, Keffi, Faculty of Natural and Applied Sciences,
5 Department of Physics.

6 Nigeria.

7 *Email: musabilya@nsuk.edu.ng

8 ABSTRACT

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

16 **KEYWORDS:** DOS , Energy Band-Gap, Photovoltaic, Pseudopotential, Quantum
17 Simulation,

18 1.0 INTRODUCTION:

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

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

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

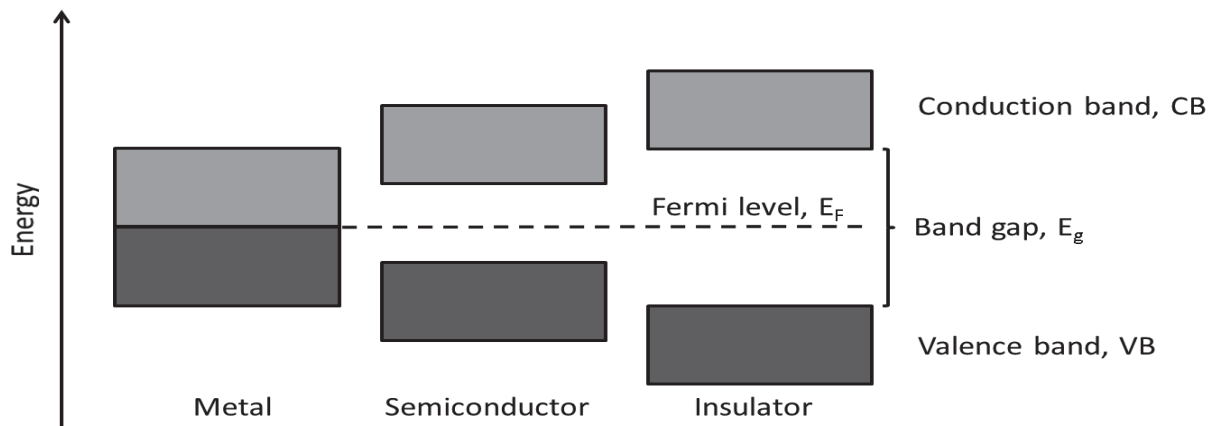
38 capable of absorbing larger part of solar spectrum and hence exhibiting higher
39 photocurrent values, have lower energy conversion efficiency in the range of high
40 energy photons and exhibit lower output voltage.

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

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

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

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



67
68

69 **Fig 3:** Conductor: Partially filled conduction band and Valence band (Callister &
70 Rethwisch, 2007)

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

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

83 **Silicon as material found wide applications in electronics and it is still a**
84 **subject of intense research. Nevertheless, the indirect band gap nature of**
85 **the band structure of bulk silicon has always been the major obstacle for its**
86 **employment in light-emitting devices since momentum conservation**
87 **requires additional momentum transfer mechanisms involved in the light**
88 **emission processes. The situation changed dramatically in the last two**
89 **decades due to the emergence of the possibility of preparing Si-based**
90 **structures with nanometer size, where quantum effects begin to play a**
91 **dominant role. In particular, large effort has been devoted to the study of**

92 **the optical properties of Si nanocrystals in the last years, with a perspective**
93 **of potential for real-life applications such as e.g. light emitting diodes, next-**
94 **generation solar cells and biomedical devices. The discovery of efficient**
95 **visible photoluminescence and optical gain from silicon nanocrystals has**
96 **demonstrated the possibility of partially overcoming the limitations of the**
97 **indirect band gap of silicon by exploiting the quantum phenomena at the**
98 **nanoscale. Despite the large amount of papers published on this subject,**
99 **there are still many aspects which are not fully understood and are subject**
100 **of intense dispute. (Prokop H., Kateřina K., Ivan P., & Pavel J., 2019)**

101
102
103 Thus, in this research, we shall study the Density of state, and the Electronic band
104 structure of Silicon.

105 **COMPUTATIONAL METHODS**

106 In this study research, we consider the Silicon Semiconductor Material. All
107 arithmetical calculations were carried out using First-Principles Pseudopotential
108 method, based on the Principle of the Density Functional theory (DFT), and the
109 Plane-Wave method as implemented in the Quantum Espresso (which is an
110 acronym for an open-Source Package for Research in Electronic Structure,
111 Simulation, and Optimization) Application Package. Exchange and correlation
112 effects are treated under the generalized-gradient-approximation with Perdew-
113 Burke-Ehrenk of (PBE) function. The Ultrasoft Pseudopotential (USP) method was
114 used to treat valence electron configuration. The cut-off of W.F. was set at
115 25.000Ry and the Cut-off of the Charge is at 225.000Ry.

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

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

122

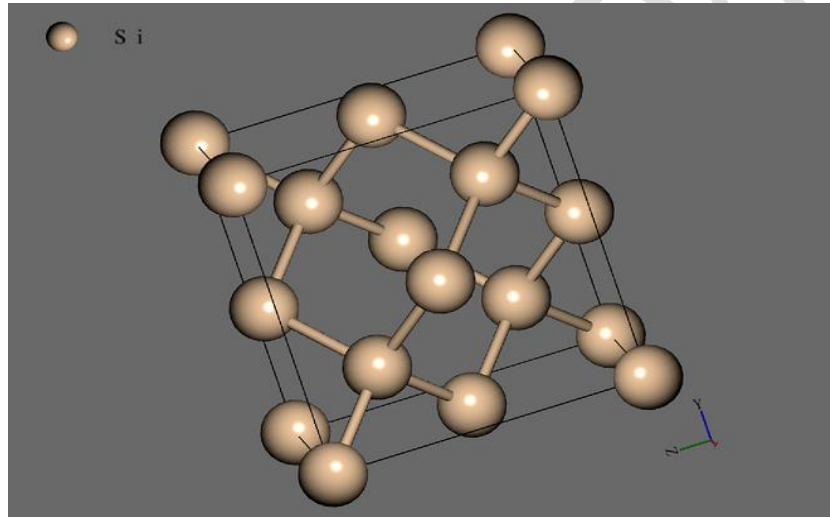
123

124 **3.0 THE MODEL**

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

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

136



137

138 **FIG 4:** Molecular Structure for the Si Material.

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

141
$$c(T,\mu) = \int n(\epsilon)(\epsilon - \mu)^2 \left[-\frac{\partial f_{\mu}(T;\epsilon)}{\partial x} \right] d\epsilon \quad 3.1$$

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

143
$$k_{i,j}^0(T,\mu) = \frac{1}{c^2 T \Omega} \int \delta_{i,j}(\epsilon)(\epsilon - \mu)^2 \left[-\frac{\partial f_{\mu}(T;\epsilon)}{\partial x} \right] d\epsilon \quad 3.2$$

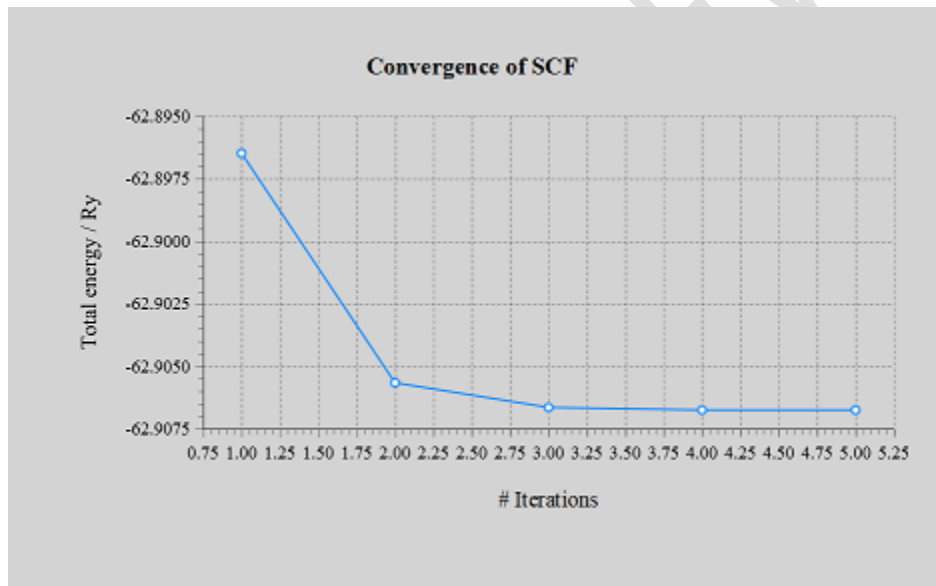
144 where $\sigma_{i,j}(\varepsilon)$ indicates the conductivity tensors, and Ω is the number of K point
145 which are sampled in Brillouin zone. (Rashid *at al.*, 2019).

146

147

148 **4.0 Density of State for Silicon (DOS)**

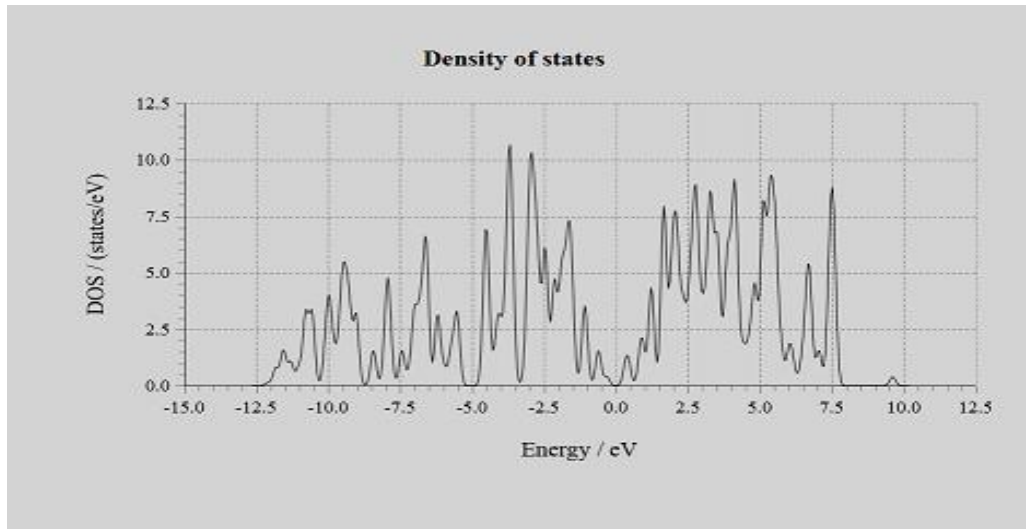
149 The Density of State (DOS), $g(E)$ can be defined as the number of states, dn per
150 unit energy range, dE . Thus, to determine this Density of State, we ran the
151 simulation, using quantum expressor. In doing so, series of iterations were ran, and
152 five points were obtained as the points of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



154

155 **Fig 5:** Convergence of the Self-consistent curve

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



159

160

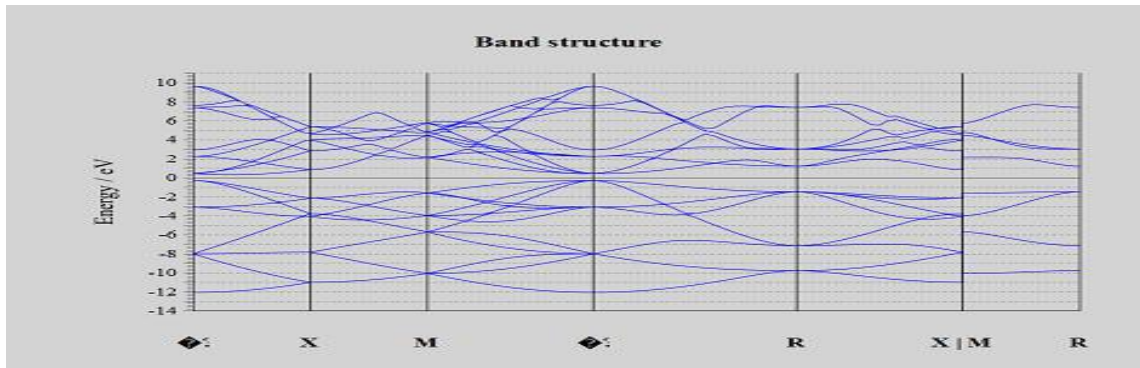
Fig 6: Graph of the Density of State For Silicon (DOS)

161 From the Density of State DOS graph as shown in the **Fig 6** above, is a plot of the
 162 Density of State in electron volt, per unit energy in the electron volts. Thus, we can
 163 observe that the peaks are between -3.5 to -3.0 eV. This result corresponds to the
 164 valence bands occupied by the electrons of Silicon Material.

165 **5.0 Electronic Band Structure for Silicon, Si**

166 **The Electronic Band Structure of Solid describes the range of energies an**
 167 **electron within the solid may have, called band structure and the ranges of**
 168 **energies the electron may not have, called band gaps or the forbidden band**
 169 **gaps (Wikipedia, 2019).**

170 To have a clear view understanding of the electronic structure of Silicon. We
 171 consider the graph below. In this graph, is a black colored horizontal line that
 172 divides into half the lower part called the valence band, and the other half the upper
 173 part, that is the conduction band. This gap that separates between the valence band
 174 and the conduction band, is called the band gap. The minimum amount of energy
 175 required for electron to jump across this band gives the band gap energy, or the
 176 energy band gap. Thus, for this silicon material, the band gap obtained is from -
 177 0.2eV to 0.6 eV.



178

FIG 7. Electronic Band Structure For Silicon

179

180 CONCLUSION

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

188 REFERENCE

189 Andreas, W. (2018). An Introduction to the Concept of Band Structure.
 190 Mathematical Physics, Lund University.

191 Rashid, H.O, Abdullah, N.R, and Gudmundsson V. (2019). Silicon on a graphene
 192 nanosheet with triangle and dot-shape: Electronic structure, specific heat, and
 193 thermal conductivity from first-principle calculations.KOmar Research Center,
 194 KOmar University of Science and Technology, Sulaimani,
 195 Iraq.ArXiv:1908.10614v 1[cond-mat.mess-hall].Pp.1-7.

196 Vos, M., Bowles, C., Kheifets A.S., and Went, M.R. (2006). Band Structure of
 197 Silicon as Measured in Extended Momentum Space. Physical Review B73, 085207.
 198 Pp.1-7.

199 Young and Freedman, (2008). University Physics. Pearson International. Pearson
200 Education, Inc., Publishing, 12th Ed. 1301 Sansome St., San Francisco, CA94111.
201

202 Zdanowicz, T., Rodziewicz, T., & Waclawek, Z.M., (2005). Theoretical Analysis
203 of the Optimum Energy Band Gap of Semiconductors for Fabrication of Solar
204 Cells for Applications in Higher Latitudes Locations. Solar Energy Materials, and
205 Solar Cells. Elsevier. Sciencedirect.com. Pp.757-769.
206

207 Abdullahi, Z., Isa A., Egba A.C., Noble A., Babalola O.A., and Buba A.D.A
208 (2019). Band Structure and Density of States Studies of Licoo₂ and Cu Doped
209 Licoo For Energy Storage Applications. Physics Advanced Research Centre,
210 (PARC), Sheda Science and Technology Complex (SHESTCO), Abuja

211 **Federico, M., Chin-Yi, C., Rajib, R., Xie-Gang, Z., Craig, M.P., Thiagarajan,
212 B., Phil, D.C., Philip, H., Jili, A.M., and Justin, W.W. (2019). The Sub-band
213 Structure of Atomically Sharp Dopant Profiles in Silicon.
214 arXiv:1904.10929v1[cond-mat.mes-hall]**
215

216 **Wikipedia (2019). Electronic band structure. Content available under CC BY-
217 SA 3.0. en.m.wikipedia.org/wiki/Electronic_band_structure**

218 **Prokop H., Kateřina K., Ivan P., and Pavel J., (2019). Theoretical analysis
219 of electronic band structure of 2-to-3-nm Si nanocrystals. *Institute of
220 Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10, 162 00
221 Prague, Czech Republic. arXiv:1204.0421v2 [cond-mat.mes-hall] 25 Jan 2013***

222 **Andreas, S. (2019). Advanced Physical Models for Silicon Device Simulation .
223 Institut für Integrierte Systeme, ETH Zurich, Schweiz. Springer book archive.
224 Link.springer.com**
225
226
227
228