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

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ABSTRACT

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

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

1.0 INTRODUCTION:

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

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

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

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

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

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

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

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

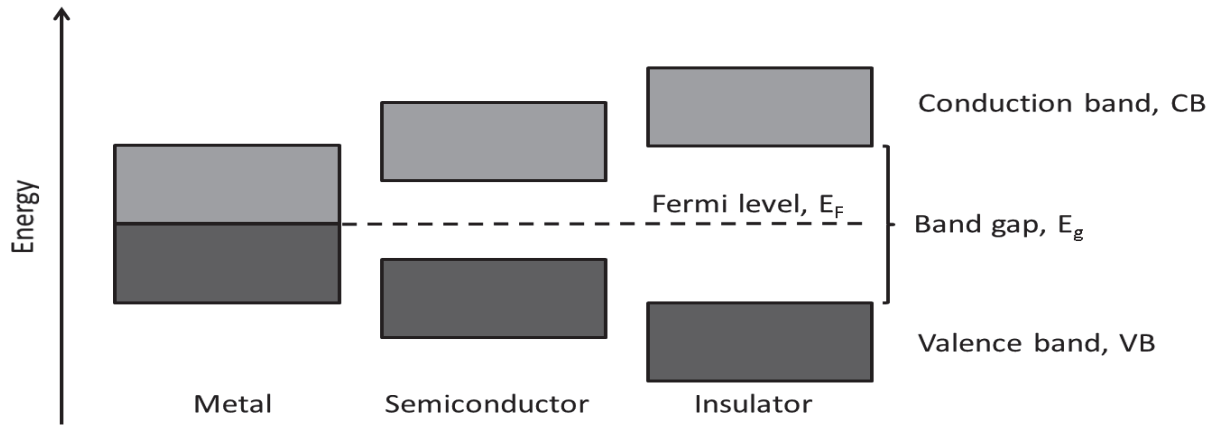

Fig 1: Conductor: Partially filled conduction band and Valence band (Callister & Rethwisch, 2007)

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

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

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

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

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

COMPUTATIONAL METHODS

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

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

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

3.0 THE MODEL

We model a Si material as shown in the Fig.2 below. The convergence of the SCF curve calculation is set, and the geometry of the system is fully relaxed.

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

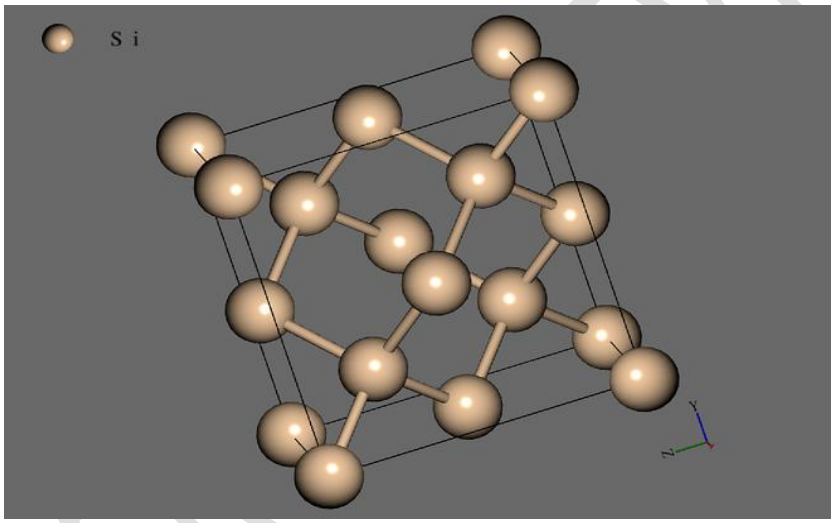

FIG 2: Molecular Structure for the Si Material.

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

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

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

$$k^o_{i,j}(T,\mu) = \frac{1}{C^2 T\Omega} \int \delta_{i,j}(\epsilon)(\epsilon - \mu)^2 \left[-\frac{\partial f\mu(T;\epsilon)}{\partial x} \right] d\epsilon \qquad 3.2$$

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

4.0 Density of State for Silicon (DOS)

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

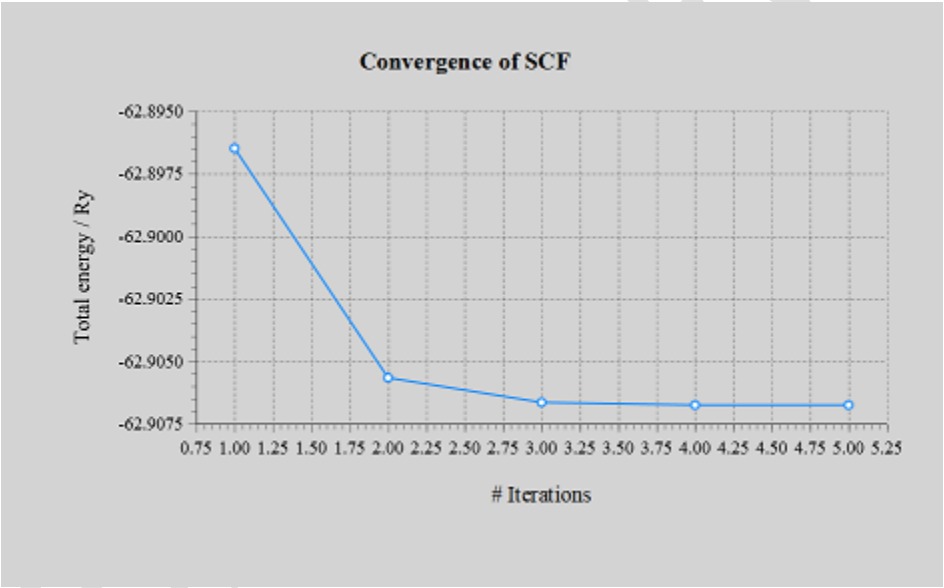

Fig 3: Convergence of the Self-consistent curve

It is at the convergence, that the graph of the Density of State was obtained. This DOS graph gives the electronic band structure of the Si material. Thus, the DOS graph is as shown in **Fig 4** below:

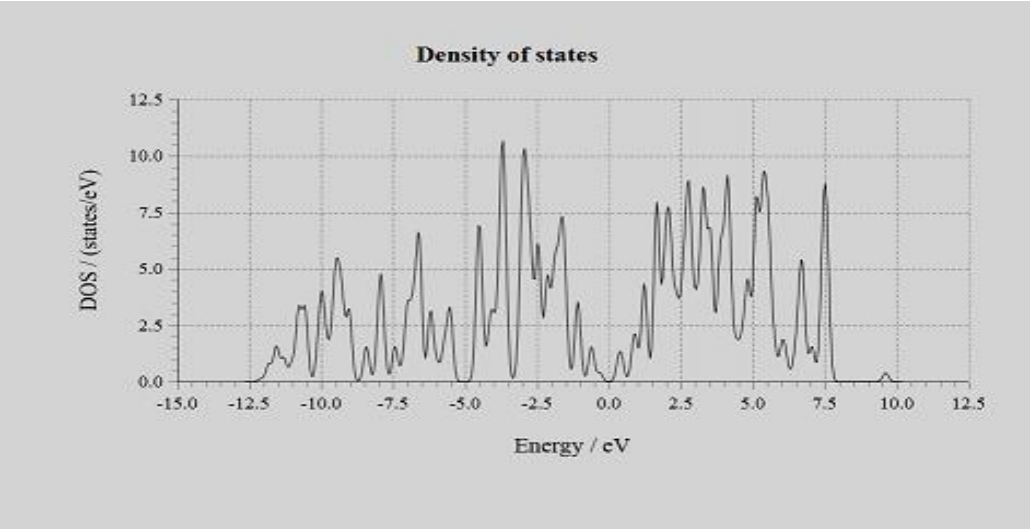

Fig 4: Graph of the Density of State For Silicon (DOS)

From the Density of State DOS graph as shown in the **Fig 4** above, is a plot of the Density of State in electron volt, per unit energy in the electron volts. Thus, we can observe that the peaks are between -3.5 to -3.0 eV. This result corresponds to the valence bands occupied by the electrons of Silicon Material.

5.0 Electronic Band Structure for Silicon, Si

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

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

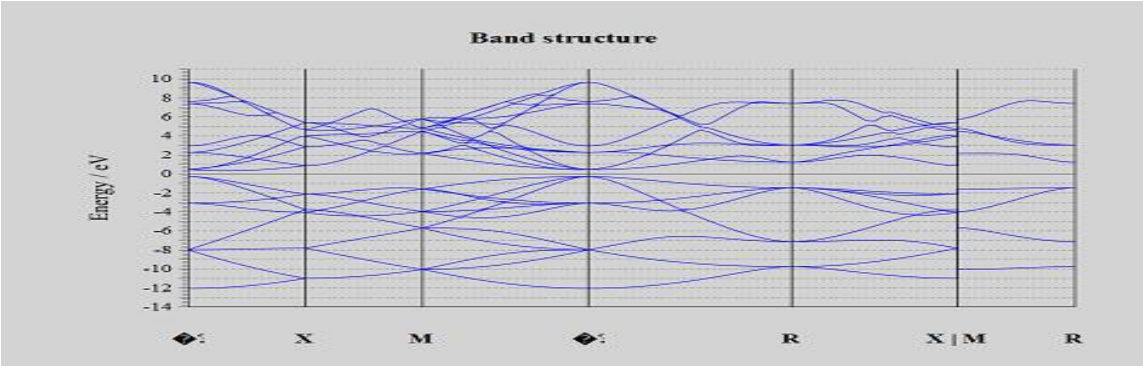

FIG 5. Electronic Band Structure For Silicon

CONCLUSION

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

Ethical: NA

Consent: NA

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