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Research Article

Density Functional Theoretical Calculations for Evaluation of Electronic Properties of Silicon

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Abstract

In the current work, we present a study on the structural and electronic properties of Silicon, using density functional theoretical calculations performed using the local density approximation (LDA) and the PBE generalized gradient approximations for the exchange-correlation functional by density functional theory based QUANTUM ESPRESSO. The lattice parameter of the structure was obtained by total energy minimization of the crystal. The equilibrium lattice constant for Silicon agrees well with the experimental result. The obtained band structure calculations suggest that the Silicon semiconductor is an indirect band gap semiconductor. The density of states and charge density studies were also performed for silicon to understand the nature of bonding.

Keywords: *Quantum Espresso, electronic structure, Band Gap, density functional theory*

1. Introduction

Silicon belongs to the IVA family in the periodic table and the important use of elemental silicon is as a semiconductor. There are lot more applications of Silicon, for electronic applications, we are interested in elemental silicon as a conductor of electricity. By adding controlled amounts of impurities we can determine the sign of the charge carriers and their density. By doing this in few areas, we can construct electronic devices that rectify, amplify and move electric charge.

Silicon crystallizes in the same pattern as diamond, The lines between silicon atoms in the lattice illustration indicate nearest-neighbor bonds as seen in figure 1.

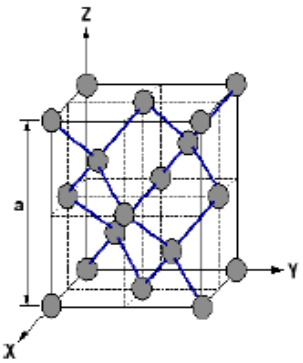

Fig.1 Silicon in Diamond Structure

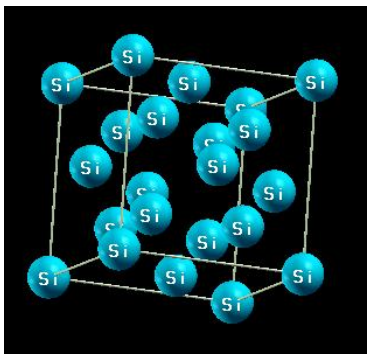

Fig.2 (Silicon as seen in XcrysDen)

Figure 2 provides us with the structure of silicon generated with XCrysDen. Density Functional theory related studies of the structural and electronic properties of semiconducting materials are done by means of first principle studies. These methods allow us to obtain the total energy of the system to accurate values, under local density approximation.

In the current work, we put forward a systematic study of the structural properties, electronic properties using the local density approximation (LDA) and PW91 based gradient approximations for the exchange-correlation functional using QUANTUM ESPRESSO (open source).

The rest of the paper is presented as follows. In section 2, we mention about the methods that we have followed, In Section 3, we present and discuss our results, we present the conclusions from the current work.

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2. Computational Methods

We use the QUANTUM ESPRESSO (P. Giannozzi, *et al*, 2009) which is a computer package to study the electronic structure and optimization using the molecular dynamics simulation. The Quantum ESPRESSO distribution contains the main packages PWscf (Plane-Wave Self-Consistent Field) for obtaining electronic-structure properties by Density-Functional Theory (DFT), using a Plane-Wave (PW) basis set and pseudopotentials. It has in it more packages for specific purpose calculations.

We have also used XCrySDen which is a crystalline- and molecular-structure visualisation program. The name of the program stands for Crystalline Structures and Densities and X because it runs under the X-Window environment. It facilitates a display of iso-surfaces and contours, which can be superimposed on crystalline structures and interactively rotated and visualized.

In order to calculate the ground state properties of Silicon, the total energies are calculated in the Si (diamond) structure, The cutoff energy is calculated first and then the lattice parameter is obtained by total energy minimization of the crystal.

3. Results and Discussion

3.1 Structural Properties of Silicon

Now we will study the structural properties of Silicon. At ambient conditions Si is in the diamond structure.

After obtaining the cutoff energy after a few computations, the method of minimizing the total energy of the crystal was followed to obtain the lattice parameter value of Silicon.

The equilibrium lattice parameters obtained for Silicon is 5.42 Å.

3.2 Electronic Properties of Silicon

Fig - 3 shows the electronic energy band structure calculated at ambient pressure for Silicon at the high-symmetry points in the Brillouin zone. Here for reference, the top of the valence band is considered as zero energy.

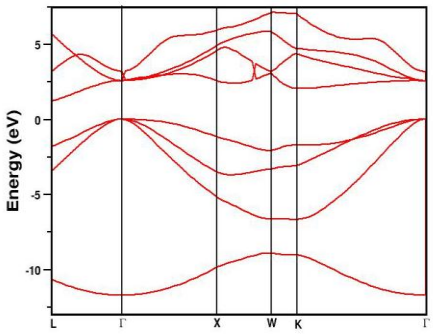

Fig.3 Band Structure of Silicon

By above plot we conclude that Si is an indirect band gap semiconductor because the maximum of the valence band (at Γ) does not coincide with the minimum of the conduction band (to the left of L). Silicon is actually a indirect band-gap semiconductor, the band gap here is observed to be 1.1 eV.

3.3 Density of States of Silicon

The density of states for Silicon is plotted in figure 4.

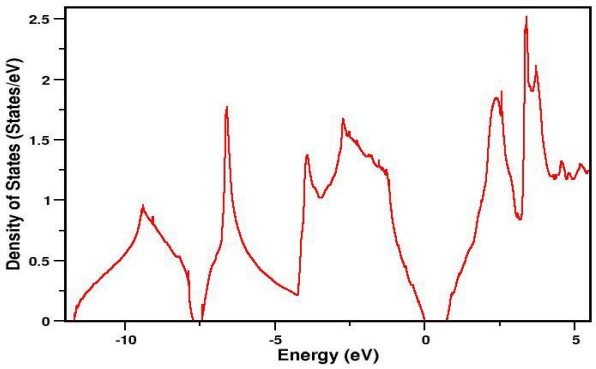

Fig.4 Density of States of Silicon

Here in the Density of States of Silicon plot we find three regions, > 0e.v which corresponds to the conduction band electrons and 0 to -7 e.v. which corresponds to Valence band and it is a hybrid of s and p orbitals, another region around -10 e.v. which corresponds to s orbital.

3.4 Charge density of Silicon

The Charge density for Silicon is plotted in figure 5.

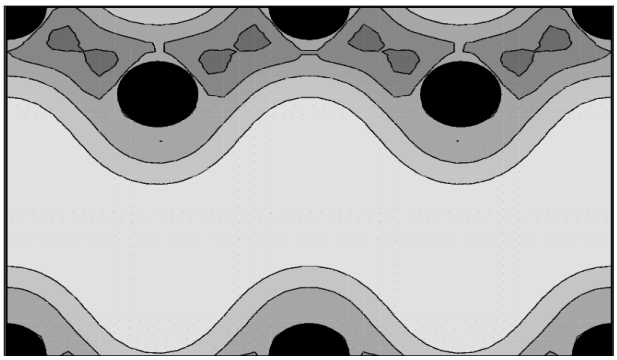

Fig.5 Charge density of Silicon

The Charge Density plot shows the density of electrons around Si atoms and this also provides an understanding about the nature of covalent bonding of Silicon.

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Conclusions

To conclude, we have done an investigation on the structural properties of Silicon using First-Priniciples calculations.

The calculated equilibrium lattice constant (a) of Silicon in the present work it is 5.42 Å.

From the Electronic band structure obtained, we conclude that Silicon is an indirect band gap semiconductor with an obtained value for band gap of 1.1 eV. The density of states and the charge densities obtained provide information regarding the orbitals and nature of bonding in Silicon.

References

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Kokalj: J. Mol. Graphics Modelling, 1999, Vol. 17, 176--179. Code available from http://www.xcrysden.org.