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Electronic and Structural Properties of an Undoped Sodium Iodide

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ABSTRACT

This work investigated the electronic and structural properties of sodium iodide using the Density Functional Theory (DFT) method implemented in the quantum espresso code. The GGA (PBE) functional with exchange correlation was used. Convergence test for the kinetic energy cut-off, k-point and lattice parameter was carried out and the parameter generated was found to be consistent with the crystallography open data base input file of the sodium iodide. Band structure was plotted, and band gap was calculated to be 3.87 eV which was found to be in the category of a semiconductor but with high resistivity and low resolution. The plot of density of state was revealed that electrons may be scarcely found within some state in the sodium iodide crystal. The research shows that sodium Iodide can be effective as a semiconductor in the presence of dopants e.g., thallium which is often used in a radiation detection.

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1. INTRODUCTION

In the realm of materials science, the investigation of the electronic and structural properties holds the key to understanding the behavior and potential applications of various compounds [1]. One of such compounds of significant interest is the sodium iodide (NaI). It is a crystalline ionic compound with diverse applications in medicine, radiation detection and more [2,3].

In the pursuit of unraveling, its intricate characteristics, the integration of advanced computational tools has become indispensable [4]. This journal presents a collection of research endeavors centered around the utilization of the Quantum Espresso Code for probing the electronic and structural properties of sodium iodide [5]. By harnessing the power of quantum mechanics and high-performance computing researchers have embarked on a journey to decipher the underlying principles governing the behavior of NaI at the atomic and subatomic levels [6].

Through this studies,we aim to contribute to the expanding knowledge of materials science while unlocking the potential for innovative applications of sodium iodide in various technological domains [7].

Several methods have emerged in order to describe the electronic and structural properties of solid materials and molecule, one of which is the density functional theory (DFT). It has shown significant value not only in the interpretation of experiment but also in predicting important aspect of new properties and the design of new devices [8].

2. COMPUTATIONAL DETAILS

This calculation was performed using plane wave density-functional method and implemented in the QUANTUM ESPRESSO code [9,10]. The exchange correlation was used, Generalized Gradient Approximation (GGA) of Perdew, Burke and Ernzerhof [11].

Semiconductor structures has been obtained by minimization of the total energy using Hellmann Feynman forces including pulay-like corrections [12]. Structural optimizations have been performed using the conjugate gradient algorithm until the residual forces in the optimization are smaller than 0.0001 eV/angstrom. The choice of pseudopotential that was used is the ultra-soft non –relativistic and it has been used for each of the element forming the compound semiconductor, using the above pseudopotential a reasonable value of lattice parameter in (arngstrom) and Brillouin zone sampling was fixed and kinetic energy cut-off was varied unless a convergence ws reached, with the converged value of energy cut-off fixed the number of k-points and lattice parameter was also varied unless a convergence was achieved. For the purpose of this work a convergence of 10 mRy with respect to energy has been considered.

3. RESULTS AND DISCUSSIONS

The results of the simulated properties of the Sodium Iodide are presented and discussed. First of all, a convergence test with respect to kinetic energy cut-off, lattice parameter and k-points was done to confirm the fidelity of the input file. In each case the results were found to be consistent with the generated input file sourced from materials cloud. After the convergence test, band structure was plotted and band gap was calculated even the density of state which shows the number of electrons in the crystal lattice was also plotted and there seems to be agreement with the result of the band gap.

3.1. Crystal Parameters and Structures

Sodium Iodide was originally found to be in a simple cubic form with a lattice constant of 6.4728 angstrom. The crystal structure was visualized using x crysden and the atomic symbols were labelled as seen in figure 3.1

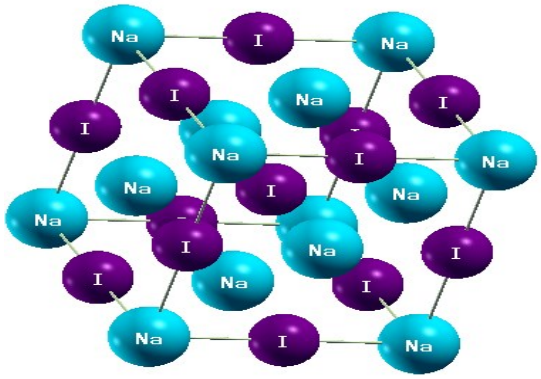


Figure 3.1 shows the structure of sodium iodide in a simple cubic

3.2. Convergence Test

3.2.1 Convergence of Kinetic energy cut-off

Kinetic energy cut-off in quantum espresso represents the maximum kinetic wave function energy of the electrons in the system [13]. It is typically given in units of Rydberg (Ry) or electron volts(eV) depending on the units chosen for the rest of the calculation.

The kinetic energy cut-off was varied from 25 to 60 eV in an interval of 5 eV while others were kept constant. It was found to converge at 40 eV which shows a strong agreement with the value obtained in the crystallographic open database (COD) CIF file converted to Pwscf input. Below is the plot for the convergence of kinetic energy cut-off with respect to the total energy.

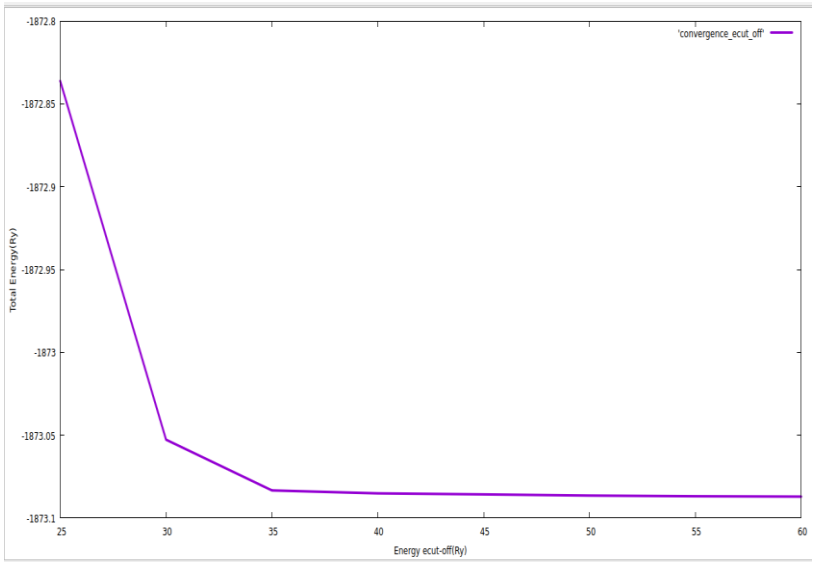


Figure 3.2 Convergence of kinetic energy cut-off

3.2.2 Convergence of Lattice Parameter

The lattice parameter is a characteristic of a crystal, sometimes they are called alat or latttice constant, it defines the structure of a crystal. For this case the lattice parameter or alat was varied between 6.00 to 7.00 angstroms in an interval of 0.05. The result obtained after the convergence was found to be consistent with theory. Below is the plot for the convergence of lattice parameter (alat) with respect to energy.

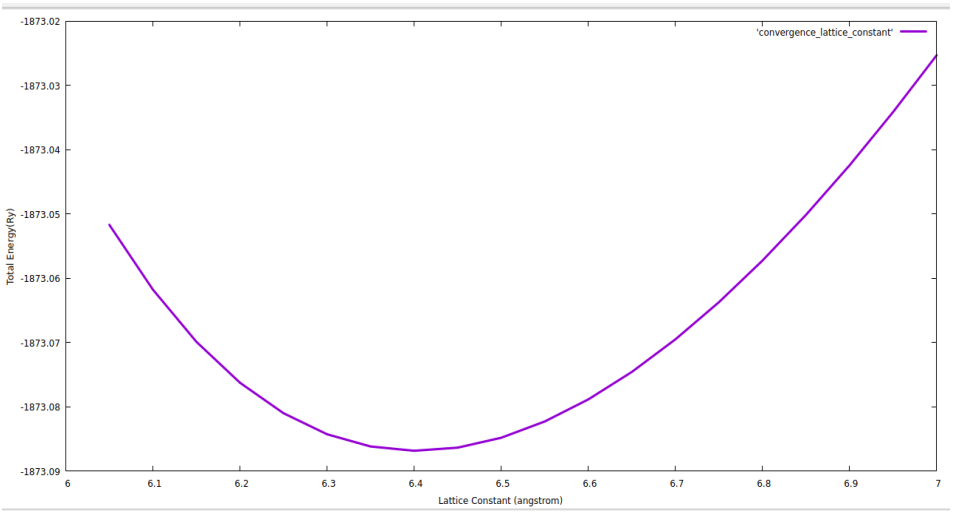


Figure 3.3 Convergence of Lattice Parameter

3.2.3 Convergence of k-point

k-point in quantum espresso is used to sample the Brillouin zone of the crystal lattice in reciprocal space [14,15]. The choice of k-point is very crucial for accurately representing the electronic structure and properties of materials. The Brillouin zone is a representation of the periodicity of the crystal lattice in reciprocal space.

Similarly, the k-point was varied while other parameters were kept constant, and the k-point was found to converge at 5. See the plot below for details

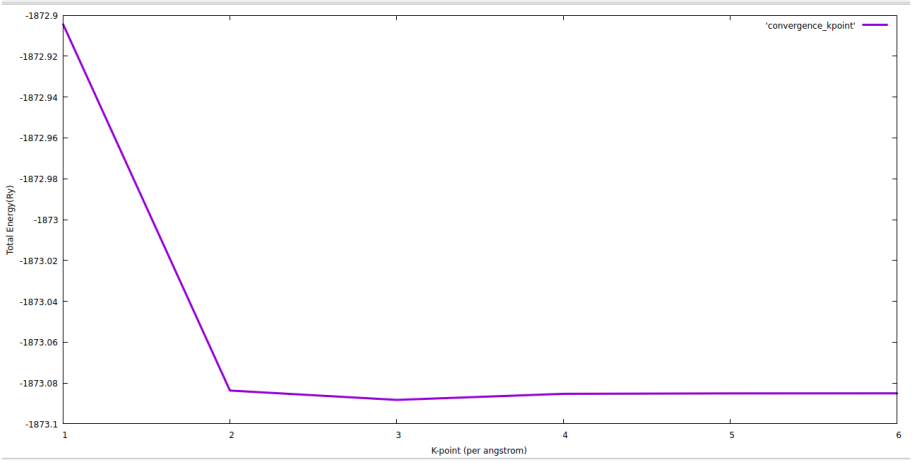


Figure 3.4 Convergence of k-point

3.4 Band Structure

Band structure describes the energy levels of electrons in the materials as a function of their momentum in reciprocal space. It provides valuable insight into the behavior of electrons and their interaction with photons in semiconductors. The band structure is characterized by two key energy bands, the valence and the conduction band. The valence band is the highest energy band that is fully occupied by electrons at absolute zero temperature. It represents the bound states of electrons tightly bound to atoms in the crystal lattice. The conduction band on the other hand, lies above the valence band and represent the energy levels where electrons can move freely and contribute to electrical conductivity. In the energy band the difference between the valence band and the conduction band is called the band gap. In general, the band gap of semiconductors falls within the range of approximately 0.1 eV to 4.0 eV. Semiconductor materials are classified into two main categories based on their band gap energies. In the direct band gap materials, the energy minimum of the conduction band and the maximum of the valence band occur at the momentum point in the Brillouin zone. These materials typically have band gaps in the range of 0.1 eV to 2.0 eV and in the indirect band gap material, the energy minimum of the conduction band and the energy maximum of the valence band occur at different momentum points in Brillouin zone. This makes the electron transitions less efficient compared to direct band gap materials, these materials have band gaps in the range of 1.0 eV to 4.0 eV. The plot shows that sodium iodide band gap 3.87ev falls within the range of the indirect band gap material and therefore this makes sodium iodide inefficient in energy resolution

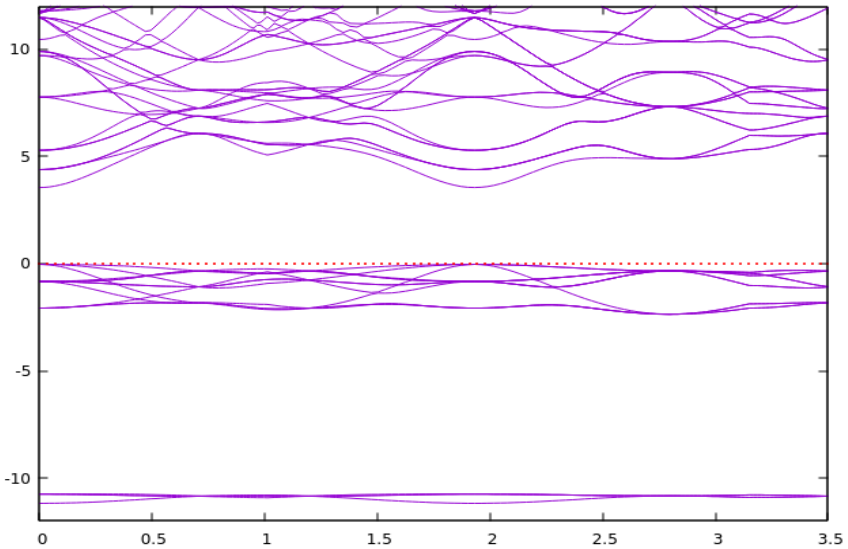


Figure 3.5 Band structure of sodium iodide

3.1 Comparison of result obtain with the theory [16]

	Lattice parameter)	k-point (per arngstrom)	Kinetic energy cut-off(eV)	Band gap(eV)
Results	**6.47**	**8 8 8**	**40**	**3.87**
Theory	**6.44**	**4 4 4**	**40**	**3.90**

From table 3.1

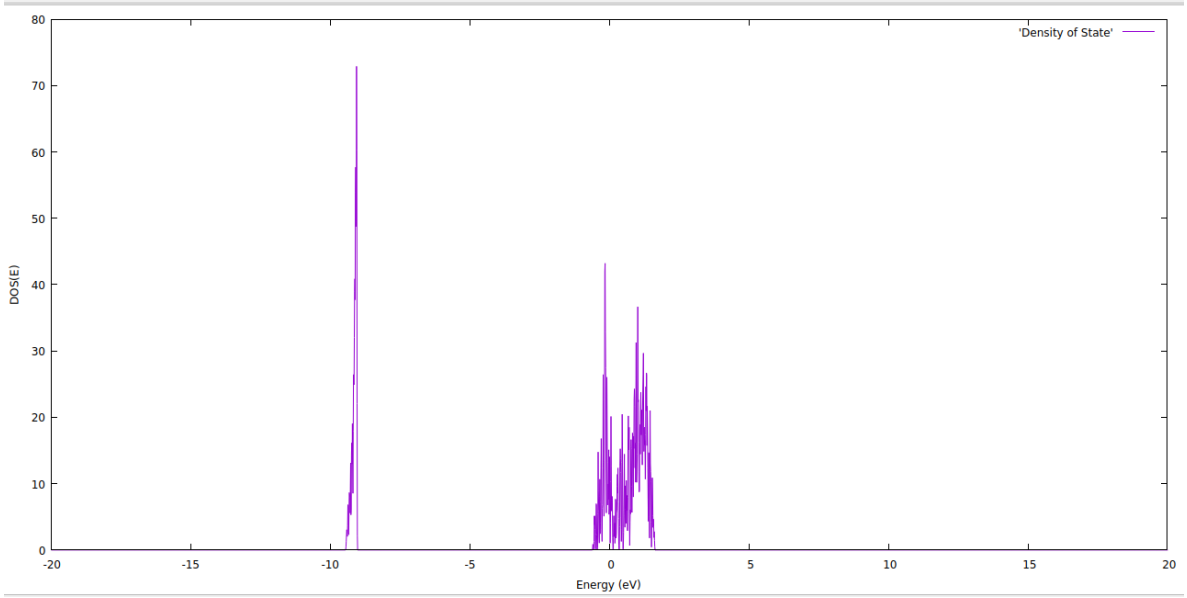
a) There's an agreement between the experimental and theory result.

b) Band gap was obtained to be 3.87 eV for sodium iodide. This is a clear indication that the presence of thallium in semiconductor detector resulted in its efficiency and add up its conductivity because sodium iodide with thallium has a band gap of 3.0 eV [17]

3.6 Density of State

Density of state refers to the number of available quantum state per unit energy range per unit volume in a system.

The plot of the density of state below simply shows that there are some state in which electrons are less occupied this could have similar explanation with the band gap which clearly shows some unoccupied



state.

4. CONCLUSION

The convergence test of k-point, kinetic energy cut-off and lattice parameter was done and the convergence test result corresponds with the input file generated.

The density of state and band gap revealed that electrons may be scarcely found within some state in the sodium iodide crystal.

In this study Sodium Iodide electronic properties was investigated, and the band gap was discovered to be higher compared to impure thallium doped. This means that, presence of an impurity in a sodium iodide will increase its conductivity by reducing its energy gap which allows electrons to move from its valence band to conduction band with less restriction.

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