



(RESEARCH ARTICLE)



Study of the electronic and optical properties of undoped sodium iodide using density functional theory DFT

Mona Hermann Charly YAPI ^{1, 2, 3, *}, Koffi N'guessan Placide Gabin ALLANGBA ^{1, 2, 3, 4}, Koffi Arnaud KAMENAN ^{2, 5} and N'guessan Raymond KRÉ ²

¹ *Mathematics Physics Chemistry Department, Physics Teaching Unit, Laboratory of Environmental Sciences and Technologies, JEAN LOROUGNON GUÉDÉ University, BP 150 Daloa, Côte d'Ivoire.*

² *Laboratory of Fundamental and Applied Physics (LFAP), University Nangui Abrogoua, BP 801 Abidjan 02, Côte d'Ivoire.*

³ *Institute of Nuclear Medicine of Abidjan (IMENA), BP 917 Abidjan 08, Côte d'Ivoire.*

⁴ *Department of Medical Physics, University of Trieste and International Centre for Theoretical Physics (ICTP), ICTP-Strada Costiera 11, 34151 Trieste, Italie.*

⁵ *Mathematics Physics Chemistry Department, Physics Teaching Unit, PELEFORO GON COULIBALY University, BP 1328 Korhogo, Côte d'Ivoire.*

GSC Advanced Research and Reviews, 2025, 22(01), 059-067

Publication history: Received on 25 November 2024; revised on 02 January 2025; accepted on 04 January 2025

Article DOI: <https://doi.org/10.30574/gscarr.2025.22.1.0523>

Abstract

The electronic and optical properties of undoped sodium iodide (NaI) were investigated. This study was carried out by the method of the Density Functional Theory (DFT) implemented by Quantum Espresso. The approximation used is the GGA (Generalized Gradient Approximation). The determined lattice parameter is 4.4485 Å. According to the results obtained, the electronic and optical properties are those of an indirect-gap semiconductor. The gap obtained is 3.712 eV. The electronic properties are affected by the 2s state of iodine and the 3p state of iodine I. With regard to optical properties, the evolution of the real part of the dielectric function $\varepsilon_1(\omega)$ shows that incident electromagnetic waves are mainly reflected by the medium in a certain energy region. The material then exhibits metallic behaviour. This can provide layers of protection against radiation in these energy regions. The imaginary part $\varepsilon_2(\omega)$ of the dielectric function shows several peaks certainly due to the transitions of electrons between 3p states of sodium, 2s states of iodine and 3p states of iodine but especially 2s states of iodine and 3p states of iodine. We can therefore say that the electronic transition takes place between the 2s state of I and the 3p state of I. These studies on the electronic and optical properties prove that sodium iodide (NaI) is of considerable interest.

Keywords: Electronic properties; Optical properties; NaI; Density functional theory; Semiconductor

1. Introduction

The electronic, structural and optical properties of materials are very important for understanding their behaviour and possible applications [1,2]. One of the most widely used methods in this quest is density functional theory (DFT). DFT simplifies the description of the system by replacing the multi-electron wave function of 3N variables (N being the number of particles in the system) with the electron density, which depends on just three variables [3]. This approach considerably facilitates the mathematical and conceptual treatment of the problem.

In this work, we focused on sodium iodide (NaI). Sodium iodide (NaI) is a material widely used in medicine [4,5], especially in nuclear medicine as a scintillator. A scintillator is a material that emits light following the absorption of ionising radiation (photon or charged particle). We have studied the electronic, structural and optical properties of

* Corresponding author: Mona Hermann Charly YAPI

undoped sodium iodide to demonstrate its potential applications. We carried out this study using the DFT method implemented by the Quantum-Espresso code [6,7].

T. Tinyang *et al.* [1] also studied the electronic properties of undoped sodium iodide using DFT. They discovered that the band gap was higher than that of impure sodium iodide doped with thallium. Our study also focuses on pure sodium iodide without doping. In addition to electronic properties, we were also interested in optical properties. T. Tinyang *et al.* [1] only studied electronic properties

2. Material and methods

2.1. Material

The material used is undoped sodium iodide (NaI). We considered this material to crystallise in the cubic crystal structure ($Pm\bar{3}m$). Figure 1 shows the crystal structure of NaI. We used eight atoms per cell.

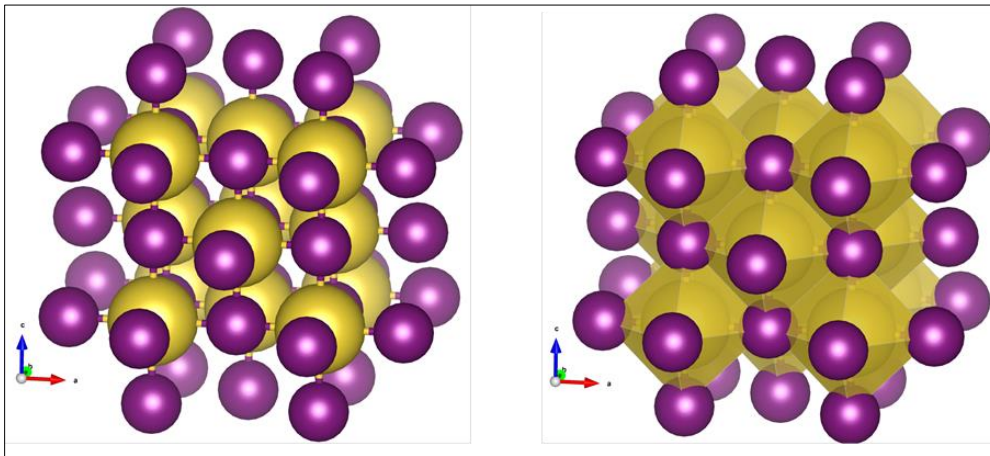


Figure 1 Typical cubic crystal structure of sodium iodide (NaI). The yellow balls are sodium atoms and the purple balls are iodine atoms

To do this work, we needed certain computer resources. We used a computer with a core i7 processor (Lenovo series) with a frequency of 2.90 GHz, 16 GB RAM, 1 TB hard disk, under Linux Ubuntu 24.04. We used Quantum Espresso software (qe-7.0 version) for ab initio calculations [6,7].

2.2. Methods

The method used in this work is density functional theory. This method is implemented in the Quantum Espresso code [6,7]. DFT has several approximations, we have used the generalized gradient approximation (GGA) of Perdew, Burke and Ernzerhof [8,9]. The GGA approximation takes into account the local electron density and its first- and second-order gradients included in the enhancement factor [10,11,12]. The GGA is available in a number of versions, all of which have demonstrated their effectiveness (in calculating electronic properties, etc.). We used a much more recent version [13]. We set the kinetic energy cut-off (*ecutwfc*) of the wave functions at 100.0 Ry. The Monkhorst-Pack [14] *k-point* sampling in the Brillouin zone used is $12 \times 12 \times 12$. The convergence level (*conv_thr*) used is 10^{-10} (1.0d-10). We have relaxed the cubic structure of sodium iodide (NaI) to obtain equilibrium parameters such as: lattice parameter, kinetic energy cut-off (*ecutwfc*), Monkhorst-Pack [14] *k-point* sampling in the Brillouin zone.

3. Results and discussion

3.1. Convergence test

Several convergence tests were performed to determine the equilibrium parameters of the sodium iodide (NaI) structure. These convergence tests concern the lattice parameter, the kinetic energy cut-off (*ecutwfc*) and the *k-points* of Monkhorst-Pack[14] in the Brillouin area. These calculations were made with a convergence level of 10^{-10} eV. This convergence study was made possible by a *vc_relax* calculation included in Quantum Espresso. To do this, several values

of the parameter concerned are submitted to the *vc_relax* calculation. The value that minimizes energy is the one for which the system is most stable. It will then correspond to the value of the parameter sought.

3.1.1. lattice parameter

Figure 2 shows the evolution of total energy as a function of the lattice parameter of cubic sodium iodide (NaI).

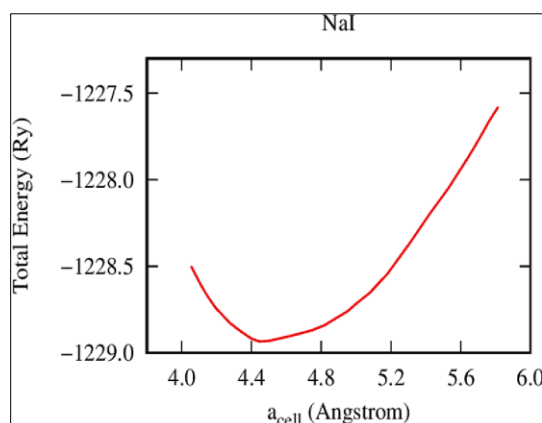


Figure 2 Convergence of Lattice Parameter a_{cell}

Table 1 shows the calculated sodium iodide (NaI) lattice parameter. We compare this with the results obtained by T. Tinyang *et al.* [1]. This lattice parameter, obtained after relaxation of the structure of sodium iodide (NaI), is 4.4485 Å. T. Tinyang *et al.* [1] obtained 6.4728 Å. We note that our results are below those obtained by T. Tinyang *et al.* [1]. This difference could be due to the term exchange-correlation that we used. Indeed, we used a more recent GGA exchange-correlation function. T. Tinyang *et al.* [1] say they also used a functional GGA, but did not specify which of its versions.

Table 1 Lattice parameter

	Our results	T. Tinyang <i>et al.</i> [1]
a_{cell} en Å	4.4485	6.4728

3.1.2. Convergence of kinetic energy cut-off (*ecutwfc*)

Kinetic energy cut-off (*ecutwfc*) is the maximum value of the kinetic energy of the electron wave function in the crystal [15]. The kinetic energy cut-off (*ecutwfc*) is the limit energy fixed in the calculation that each iteration must not exceed [6,7]. It is set in rydberg for each file of the calculation. Figure 3 shows the different variations in total energy as a function of the kinetic energy cut-off (*ecutwfc*) of sodium iodide (NaI). We started iteration from 25 Ry up to 120 Ry. It is important to recognize that the bigger this parameter becomes, the more the calculation becomes cumbersome and will use more computer resources. Conversely, when the latter is low, the results obtained will not be as precise.

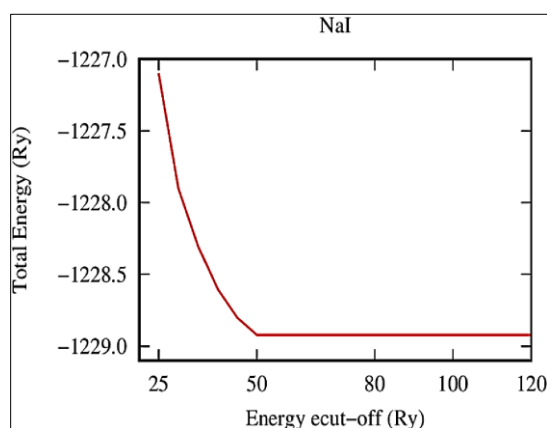


Figure 3 Convergence of kinetic energy cut-off (*ecutwfc*)

From 25 Ry, the energy decreases very considerably to 50 Ry. From 50 Ry, we notice that the energy stabilizes at -1228.90 eV. This energy remains constant for the other values of the kinetic energy cut-off (*ecutwfc*). It is therefore deduced that 50 Ry is the cut-off energy required for these calculations. We therefore choose to set the kinetic energy cut-off (*ecutwfc*) at twice this value to achieve a very good precision, that is to say 100 Ry. T. Tinyang *et al.* [1] have selected a kinetic energy cut-off (*ecutwfc*) of 60 Ry [1], all of which are shown in Table 2.

Table 2 *k*-points of the brillouin zone and calculated kinetic energy cut-off (*ecutwfc*)

	k-point	Kinetic energy cut-off <i>ecutwfc</i> (eV)
Our results	12 12 12	100
T. Tinyang <i>et al.</i> [1]	8 8 8	40

3.1.3. Convergence of *k*-point

The Brillouin zone of sodium iodide (NaI) is sampled using the Monkhorst-Pack method [14]. Through a relaxation of the structure, the optimal *k*-point sampling parameter was determined. Figure 4 shows the different variations of special *k*-point values according to total energy. According to the graph, convergence is observed from the 8×8×8 Monkhorst-Pack points (*k*-points). We therefore chose to carry out our calculations with a 12×12×12 grid. This choice is significantly superior to the 6×6×6 grid used by T. Tinyang *et al.* [1] in their work on NaI materials.

This choice of 12×12×12 *k*-point sampling is admittedly very high. This high choice is justified by the precision required in the calculations. However, it should be pointed out that the calculation will be heavier, i.e. the calculation time will be longer than with a 6×6×6 sampling. The computer resources to be used for this will be much greater.

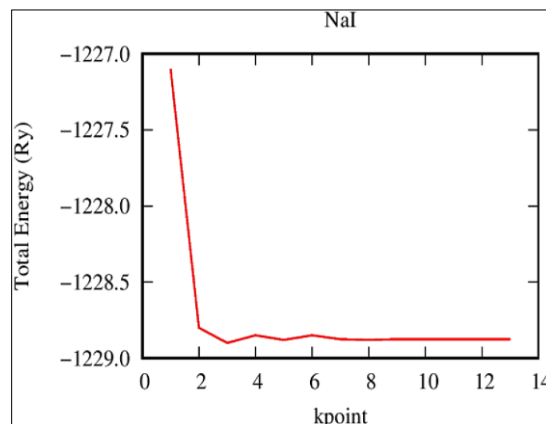


Figure 4 Evolution of total energy as a function of the number of special *k*-point points

3.2. Electronic properties

In this section, we present the electronic properties of sodium iodide (NaI) calculated using the GGA approximation in the DFT framework. The electronic properties determined in this work are: the electronic band structure, the total density (TDOS) and the partial densities of states (PDOS) of the NaI cubic structure in the directions of high symmetries of the first Brillouin zone. We also present the gap energy and gap type of sodium iodide (NaI).

3.2.1. Electronic band structure

The electronic properties of materials are derived from their band electronic structures. The electronic structure of bands in a material is strongly influenced by the energy states of the electrons of this material [16,17]. Two very important bands are highlighted by the electronic band structure: the conduction band and the valence band [18,19]. The valence band is the energy band occupied by electrons in the zero-absolute temperature material. It constitutes states where electrons are closely related to the atoms of the crystalline network. The conduction band is positioned above the valence band. It includes the energy levels in which electrons are free to move through the crystal, thus participating in electrical conductivity. The difference between the bottom of the conduction band and the top of the valence band is the gap. The gap of semiconductors is between 0.1 and 4.0 eV [16,17,18,19].

Figure 5 shows the electronic band structure of sodium iodide (NaI) along the axes of points of high symmetry in the first Brillouin zone. The conduction band and valence band can be distinguished. The path of points of high symmetry followed in the Brillouin zone of the cubic structure is: Γ -R-X-M- Γ .

There are two types of semiconductors: direct gap semiconductors and indirect gap semiconductors [16,17,18,19]. A material is of direct gap when the maximum of the valence band and the minimum of the conduction band are at the same values of wave vectors \vec{k} . Materials with indirect gap have their valence band maximums and conduction band minimums located at different k values [16,17,18,19]. Direct gap materials are suitable for optoelectronic applications, indirect gap materials have electronic applications.

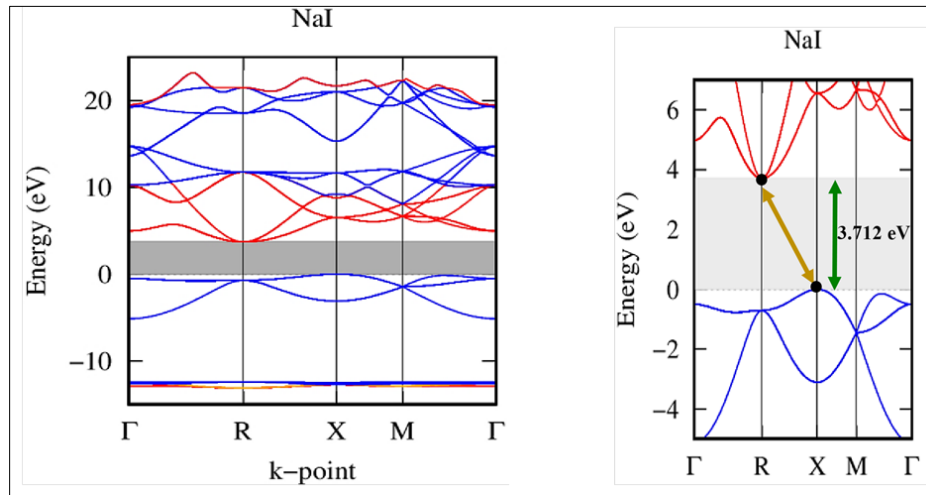


Figure 5 Electronic band structure of sodium iodide. The band structure on the right and the band gap on the left

The gap of the sodium iodide obtained is 3.712 eV (Table 3). Sodium iodide (NaI) is therefore a semiconductor material. T. Tinyang *et al.* [1] obtained a gap value of 3.870 eV. Our result is therefore close to theirs, with a very slight difference of about 0.158 eV. However, it should be noted that A. Jain *et al.* [20], who studied thallium-doped sodium iodide, obtained a gap value of 3.0 eV. This value is very low compared with those obtained by us and by T. Tinyang *et al.* [1]. This can be explained by the influence of the presence of thallium in the crystal structure. The same observation was also made by T. Tinyang *et al.* [1].

Table 3 Gap width obtained

	Our result	T. Tinyang <i>et al.</i> [1]
gap en eV	3.712	3.870

Through the electronic band structure, we obtain that sodium iodide (NaI) has an indirect gap on the R-X path. We deduce that the electronic transitions are less efficient, so sodium iodide is inefficient in terms of energy resolution. Since the conduction band minimum and valence band maximum are not at the same values of \vec{k} wavevectors, optical transmissions from the valence band to the conduction band will be difficult. Nevertheless, it will be very useful in electronic applications and less so in optoelectronic applications.

3.2.2. Total density (TDOS) and partial densities of states (PDOS) of the NaI.

To determine the nature of the electronic band structure of a material, it is necessary to evaluate the total density of states (TDOS or DOS) and partial density of states (PDOS) [21]. The DOS gives the number of allowed states of electrons at a given energy per volume. The PDOS gives the projection of the DOS onto each atomic orbital. The density of states provides an understanding of the nature of electronic properties [21]. The total density of states (TDOS) and partial densities of states of sodium iodide (NaI) are shown in figure 6.

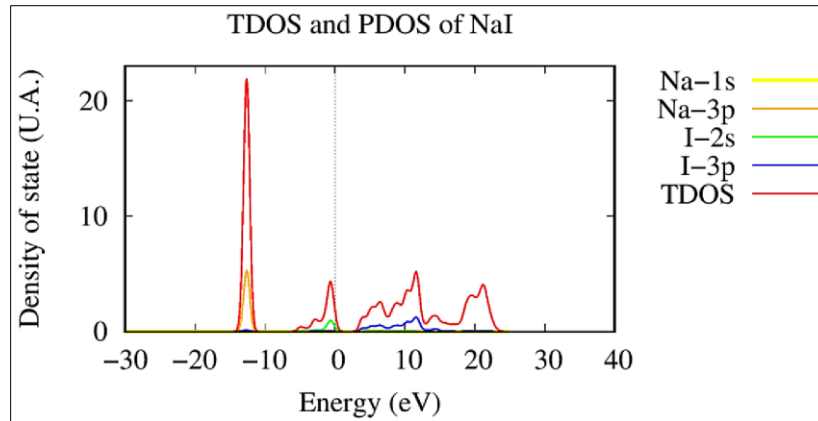


Figure 6 Total density of DOS states and partial densities of PDOS states of sodium iodide (NaI)

Examination of the total density of states (TDOS or DOS) and partial densities of states (PDOS) of sodium iodide (NaI) shows that the valence band is dominated by the 3p sodium states and 2s iodine states. The conduction band is dominated only by the 3p iodine state. In reality, the gap is characterised by the distance between the 2s state of iodine and the 3p iodine state. We can therefore say that the electronic transition takes place between the 2s state of iodine and the 3p state of iodine. It should be noted that T. Tinyang *et al.* [1] have not performed calculations on the partial densities of state (PDOS) of sodium iodide (NaI).

3.3. Optical properties

3.3.1. Complex dielectric function

The complex dielectric function is the basic property for calculating the optical properties of a material. It corresponds to the response of electrons in a solid to electromagnetic radiation. The complex dielectric function $\tilde{\epsilon}$ is written:

$$\tilde{\epsilon}(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega) \dots \dots (1)$$

ϵ_1 represents the real part of the dielectric function and ϵ_2 represents the imaginary part of the dielectric function. The imaginary part ϵ_2 reflects the absorption of the material, while the real part ϵ_1 is linked to the polarisation of the medium. Through ϵ_1 and ϵ_2 , we can evaluate various optical functions in this case: the refractive index $n(\omega)$, the extinction coefficient $k(\omega)$, the reflection coefficient $R(\omega)$, the absorption coefficient $\alpha(\omega)$ and the optical conductivity $\sigma(\omega)$. The real and imaginary parts of the dielectric function of sodium iodide (NaI) were calculated between 0 and 30 eV. They are shown in figure 7.

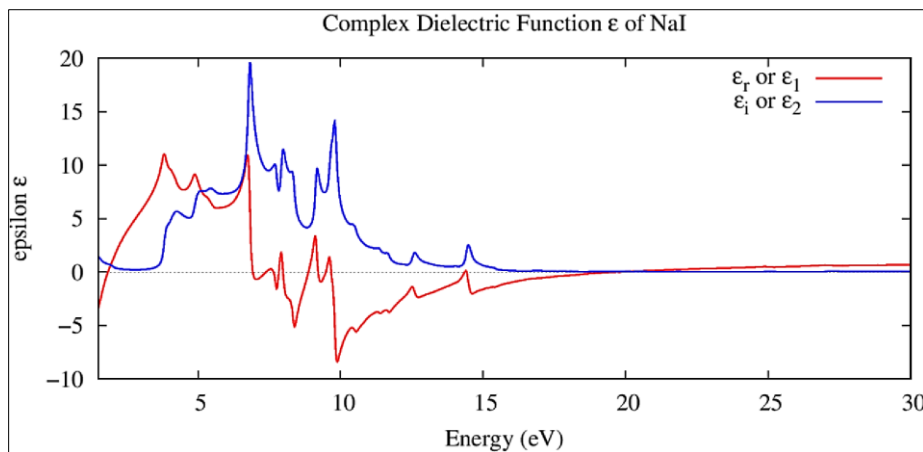


Figure 7 Real part ϵ_1 and imaginary part ϵ_2 of the dielectric function

It should be recalled, however, that T. Tinyang *et al.* [1] did not carry out studies on optical properties, that is to say the real and imaginary parts of complex dielectric function of sodium iodide (NaI).

3.3.2. Real part of the complex dielectric function

The real part of the complex dielectric function is represented by the red graph in figure 7. There are several peaks. The curve has three parts. The first part, located between 0 eV and 6 eV, corresponds to the positive part with several peaks, the most important on the curve. The second part, between 6 eV and 20 eV, is where the curve varies between positive and negative values. The last part is between 20 eV and 30 eV. In this part, the curve is practically zero. The principal peak is in the first zone. It is 11.04 eV at 3.83 eV. The second peak is from 10.90 eV to 6.75 eV. The real part of the dielectric function ϵ_1 decreases to negative values and then rises to positive values. The negative values of ϵ_1 in this region show that the incident electromagnetic waves are mainly reflected by the medium in this energy region, i.e. between 6 eV and 20 eV. The material therefore exhibits metallic behaviour between 6 eV and 20 eV. It can be used as a protective layer against radiation in energy regions where the real part of the complex dielectric function is negative.

3.3.3. Imaginary part of the complex dielectric function

The variation of the imaginary part of the complex dielectric function ϵ_2 as a function of energy is shown in Figure 7. The curve of the imaginary part of the complex dielectric function ϵ_2 reflects the absorption of the material. From it, we can get the different interband transitions. It is shown in blue in figure 7.

This curve has several peaks. There are two distinct parts to the curve. The first part is between 0 and 16 eV and the second part between 16 eV and 30 eV. The second part is practically zero, while the first part has several peaks and is non-zero. In the first part, the main peaks are 19.0 at 6.82 eV and 14.05 at 9.80 eV. These peaks are certainly due to the transitions of the electrons between the 3p Na, 2s I and 3p I states, but above all between the 2s I and 3p I states. We can therefore say that the electron transition takes place between the 2s of I and 3p of I states. We can therefore say that the electronic transition takes place between the 2s states of I and the 3p states of I. The two peaks corresponding to the ϵ_2 peaks at 6.82 eV and 9.80 eV show energy absorption due to the π - π^* interband transition and due to the σ - σ^* interband transition respectively.

3.3.4. Energy loss function EELS

The energy loss spectrum is given by the loss function $L(\omega) = \text{Im}[-1/(\tilde{\epsilon}(\omega))]$. It therefore depends on the complex dielectric function $\tilde{\epsilon}(\omega)$, and is therefore a function of the angular frequency ω of an external electric field [22,23]. The energy loss function EELS is expressed through relation 2.

$$L(\omega) = \text{Im} \left[-\frac{1}{\tilde{\epsilon}(\omega)} \right] = \frac{\tilde{\epsilon}_2}{\epsilon_1^2 + \epsilon_2^2} \dots (2)$$

The spectrum of the energy loss function is related to the spectrum of the real part ϵ_1 and the imaginary part ϵ_2 of the complex dielectric function.

The calculation of the energy loss function calculated in this work was from 0 eV to 30 eV. Figure 8 shows the energy loss spectrum due to valence electron excitations in sodium iodide (NaI). The EELS spectrum in a low-energy region (from 0 to 50 eV) is called the valence loss spectrum. This energy region corresponds to the dielectric response for frequencies $\omega = \sim 10^{15}$ Hz. In this region, the valence electrons cause resonant oscillations. When the value of ϵ_2 is very low and ϵ_1 is zero or very close to 0, the loss function shows a sharp peak [22,23]. The frequency at which this occurs is the plasma frequency ω_p , the energy corresponding to this plasma frequency is $E = \hbar\omega_p$.

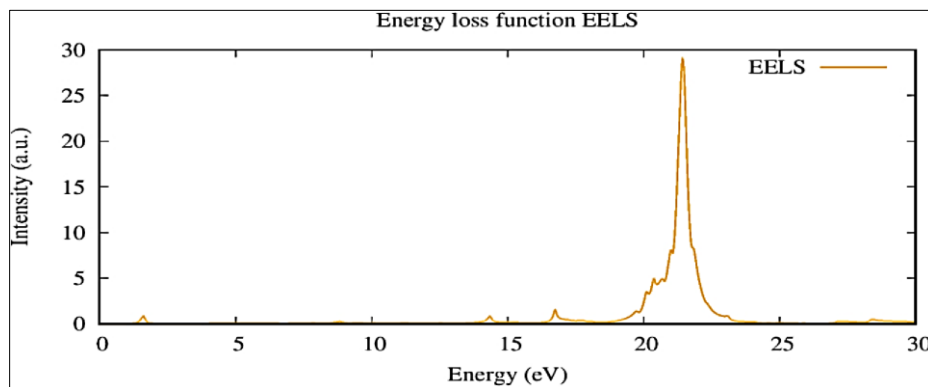


Figure 8 Energy loss function spectrum

In the graph in figure 8, the spectral peak of 29 a.u. at 21.43 eV (i.e. the sharp peak) is due to the collective longitudinal oscillation of the valence electrons (all the π and σ electrons) of sodium iodide (NaI). And indeed, at this energy value

of 21.43 eV, the value of ϵ_2 and the value of ϵ_1 are so small that they are practically zero as proved by Raether H. *et al.* [22]. This is shown in figure 9. The valence electrons cause resonant oscillations at or around this energy.

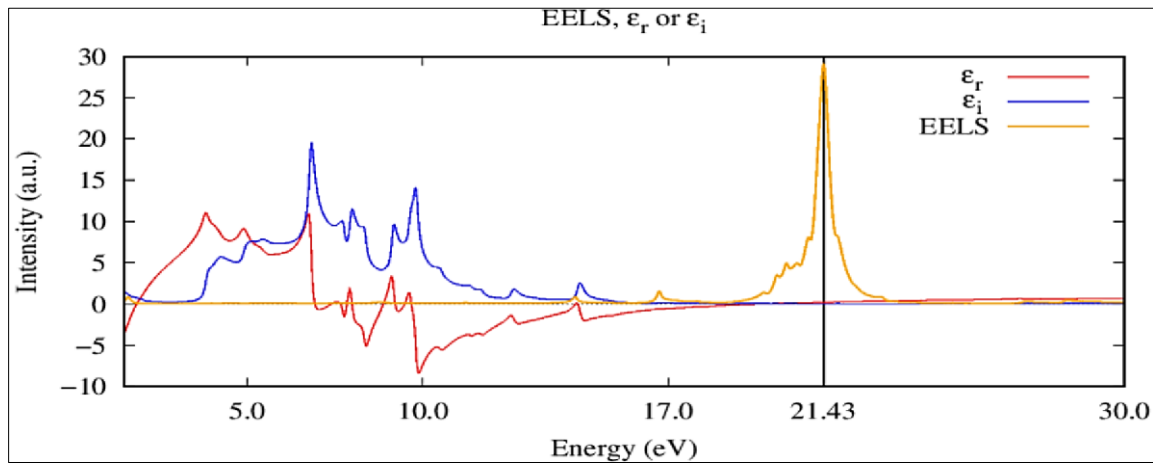


Figure 9 Real and imaginary parts of the complex dielectric function and Energy loss function spectrum

4. Conclusion

The electronic, structural and optical properties of undoped sodium iodide (NaI) have been calculated using the DFT method in the GGA approximation. The calculated lattice parameter is 4.4485 Å. The electronic band structure confirms that undoped sodium iodide (NaI) is a semiconductor with a band gap of 3.712 eV. The gap is indirect. In terms of optical properties, observation of the real part of the complex dielectric function shows that the material exhibits metallic behaviour between 6 eV and 20 eV. It can be used as a protective layer against radiation in this energy region. The imaginary part shows main peaks at 6.82 eV and 9.80 eV. These peaks are certainly due to the transitions of the electrons between the 3p Na, 2s I and 3p I states, but above all between the 2s I and 3p I states. This shows that the electron transition takes place between the 2s of I and 3p of I states.

This work shows that undoped sodium iodide (NaI) is of great interest. Its semiconductor properties could be exploited for the development of different applications in various fields. It could also be doped not only with thallium but also with other chemical elements. This could amplify the properties of sodium iodide (NaI).

Compliance with ethical standards

Acknowledgments

Our thanks go to the Physics teaching unit of JEAN LOROUGNON GUEDE University (UJLoG) of Daloa, Physics teaching unit of PELEFORO GON COULIBALY University of Korhogo and to the Fundamental and Applied Physics Laboratory (LPFA) of the NANGUI ABROGOUA University (Abidjan, Ivory Coast), where the work was carried out.

Disclosure of conflict of interest

The authors declare that there are no conflicts of interest that is relevant to the content of this article.

References

- [1] T. Tinyang, S. T Tonga, I. Isah3 L.P Kenda, "Electronic and Structural Properties of an Undoped Sodium Iodide ", International Journal of Engineering and Applied Physics (IJEAP), Vol. 4, No. 2, May 2024, pp. 971~976, ISSN: 2737-8071
- [2] Milman, V., *et al.* "Electronic structure, properties, and phase stability of inorganic crystals: A pseudopotential plane-wave study." International Journal of Quantum Chemistry 77.5 (2000): 895-910.
- [3] W. Kohn and L. J. Sham; Self-Consistent Equations Including Exchange and Correlation Effects. In: Physical Review, (1965), Vol. 140, No. 4A, p. A1133-A1138.

- [4] Lecoq, Paul. Development of new scintillators for medical applications. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 809 (2016): 130-139.
- [5] Kakavelakis, George, *et al.* Metal halide perovskites for high-energy radiation detection. *Advanced Science* 7.22 (2020): 2002098.
- [6] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. Fabris, G. Fratesi, S. de Gironcoli, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P. Umari, and R. M. Wentzcovitch, *QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials*, *Journal of Physics: Condensed Matter*, (2009), 21(39), p. 395502.
- [7] P. Giannozzi, O. Andreussi, T. Brumme, O. Bunau, M. N. Buongiorno, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, M. Cococcioni, N. Colonna, I. Carnimeo, A. Dal Corso, S. De Gironcoli *et al.* ; Advanced capabilities for materials modelling with Quantum Espresso. *Journal of Physics: Condensed Matter*, (2017), 29(46), 465901.
- [8] A. M. Rappe, K. M. Rabe, E. Kaxiras and J. D. Joannopoulos, Optimized pseudopotentials, *Phys. Rev. B* 44, (1991), 13175.
- [9] J. P. Perdew, K. Burke, K. and M. G. Ernzerhof, Generalized Gradient Approximation Made Simple, *Phys. Rev. Lett.*, 77, (1996), 3865 and *Phys. Rev. Lett.*, 78, (1997), 1396.
- [10] A. D. Becke; Density-functional exchange-energy approximation with correct asymptotic behavior. In: *Physical Review A*, (1988), 38(6), p. 3098–3100.
- [11] J. P. Perdew, K. Burke & M. Ernzerhof. Generalized Gradient Approximation Made Simple [*Phys. Rev. Lett.* 77, 3865 (1996)]. In: *Physical Review Letters*, (1997), 78(7), p. 1396-1396.
- [12] C. Adamo & V. Barone; Exchange functionals with improved long-range behavior and adiabatic connection methods without adjustable parameters: The mPW and mPW1PW models. *The Journal of Chemical Physics*, (1998), 108(2), p. 664-675.
- [13] A. D. Becke and E. R. Johnson ; A Simple Effective Potential for Exchange, *J. Chem. Phys.*, (2006), Vol. 124, p. 221101.
- [14] H. J. Monkhorst and J. D. Pack. Special Points for Brillouin-Zone Integrations. *Physical Review B*. (1976), Vol. 13, pp. 5188-5192.
- [15] Sapkota, Dhruva. Study of structural and electronic properties of sodium and potassium. Diss. Department of Physics Birendra Multiple Campus. 2020.
- [16] Mathilde Bouchard. AMX₃ halogenated perovskites: synthesis, cationic substitution and structural study. [University doctoral thesis]. Speciality: Molecular and Structural Physical Chemistry. France: Grenoble Alpes University. 2018. 119 p.
- [17] Yacine Marouf. Study and simulation of multi-junction solar cells based on III-V semiconductor materials. [University doctoral thesis]. Speciality: Electronic. Algeria: Mohamed Khider-Biskra University. 2019. 140 p.
- [18] S. Norvez. Electronic properties in solids: energy bands, semiconductors. ESPCI : Paris. 2017. 54 p.
- [19] Lédée F. Crystallization and functionalization of 2-dimensional halogenated hybrid perovskites for photovoltaics and light emission. [University doctoral thesis]. Speciality: Physics and chemistry of matter and materials. France, Paris : Paris-Saclay University. 2018.
- [20] Jain, A., Ong, S. P., Hautier, G., Chen, W., Richards, W. D., Dacek, S., ... & Persson, K. A. The materials project: A materials genome approach to accelerating materials innovation, *APL Mater.* 2013.
- [21] Charles Kittel. *Solid state physics*. 7th edition. Paris: Dunod. 1998.
- [22] H. Raether, *Springer Tracts in Modern Physics*, 88 (1980), *Excitation of Plasmons and Interband Transitions by Electrons* (Springer-Verlag Berlin Heidelberg GmbH, 1980)
- [23] R.F. Egerton. *Electron Energy-Loss Spectroscopy in the Electron Microscope*. Third Edition (Springer, 2011)