

First-Principles Investigation of $\text{Na}_2\text{CuBiCl}_6$ as a Promising Material for High-Efficiency Optoelectronic Devices

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Abstract

This research employs first-principles calculations to explore $\text{Na}_2\text{CuBiCl}_6$, a double perovskite compound, as a promising material for high-efficiency optoelectronic devices. The structure of $\text{Na}_2\text{CuBiCl}_6$ is cubic double perovskite, with Cu^+ and Bi^{3+} positioned at the B-sites, ensuring stable charge balance and lattice integrity. The Goldschmidt tolerance factor, calculated as 1.008, suggests geometric suitability, and the negative formation enthalpy ($\Delta H = -0.187$ Ry) indicates thermodynamic stability. A Debye temperature of 223.23 K indicates strong lattice dynamics and thermal resilience. An indirect band gap of 1.3 eV is revealed by electronic structure analysis utilising the hybrid Heyd Scuseria Ernzerhof (HSE) fu

nctional. This value is consistent with values reported in the literature (1.294 eV), placing the material in the visible light range and making it suitable for optoelectronic applications. Density of states (DOS) analysis has identified orbital contributions indicative of a non-magnetic ground state, which is beneficial for minimizing electronic losses. The optical properties further underscore its potential, showing a strong dielectric function with transitions spanning the visible to ultraviolet regions. The absorption coefficient begins near 3 eV and increases at higher energies. In contrast, the elevated refractive index and extinction coefficient across the visible to near-infrared range suggest efficient light-matter interaction. Overall, $\text{Na}_2\text{CuBiCl}_6$ stands out as a structurally stable, thermally robust, and optically active semiconductor, indicating its significant potential for next-generation optoelectronic and thermoelectric applications.

Keywords: Double perovskite; $\text{Na}_2\text{CuBiCl}_6$; Structural stability; Goldschmidt.

Introduction

The increasing demand for clean, affordable, and sustainable energy has accelerated research into renewable energy technologies capable of reducing dependence on fossil fuels and mitigating environmental pollution. Among the various renewable energy sources,

solar energy has emerged as one of the most abundant and environmentally friendly options due to its wide availability and inexhaustible nature. Continuous efforts have therefore been directed toward developing highly efficient photovoltaic technologies that can convert solar energy into electricity at a lower production cost

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while maintaining long-term operational stability. In recent years, perovskite solar cells (PSCs) have become one of the most promising photovoltaic technologies because of their exceptional optoelectronic properties, solution-processable fabrication methods, and rapidly increasing power conversion efficiencies (PCEs).

Since their introduction, perovskite solar cells have demonstrated an unprecedented improvement in performance. Their power conversion efficiency has increased from less than 4% in the early stages of development to over 26% for certified single-junction devices, making them comparable to conventional crystalline silicon solar cells. This rapid progress has been attributed to the unique characteristics of perovskite materials, including high optical absorption coefficients, long charge-carrier diffusion lengths, tunable band gaps, low exciton binding energy, and balanced electron-hole transport. These outstanding properties enable efficient light harvesting and effective charge transport, making PSCs attractive candidates for next-generation photovoltaic technologies.

Despite these remarkable achievements, several challenges continue to limit the commercialization of perovskite solar cells. One of the most critical issues is the poor environmental stability of conventional lead-halide perovskites. These materials are highly sensitive to moisture, oxygen, elevated temperature, and prolonged light exposure. Under such conditions, degradation processes such as hydration, phase transition, ion migration, and chemical decomposition occur, leading to significant losses in photovoltaic performance and a reduction in device lifetime. The presence of volatile organic cations, particularly methylammonium (CH_3NH_3^+), further contributes to the instability of hybrid perovskite structures by making them more susceptible to thermal and moisture-induced degradation. Consequently, improving the stability of perovskite materials remains one of the major research priorities in the field of photovoltaic materials (1).

In addition to stability concerns, the use of lead (Pb) in conventional perovskite absorbers presents significant environmental and health challenges. Although lead-based perovskites exhibit excellent photovoltaic performance, the toxic nature of lead raises concerns regarding environmental contamination during material processing, device operation, and disposal. Leakage of lead compounds into soil and water can pose serious ecological and health risks, making large-scale commercialization increasingly difficult. These concerns have encouraged researchers to search for environmentally friendly alternatives that can maintain high photovoltaic performance while eliminating the toxicity associated with lead-based materials (1).

One of the earliest approaches to replacing lead involved the use of tin (Sn^{2+}), which belongs to the same group in the periodic table and possesses similar electronic configurations and stereochemically active lone-pair electrons. Tin-based perovskites have demonstrated encouraging photovoltaic properties and relatively high power conversion efficiencies, making them attractive candidates for lead substitution. However, their practical application has remained limited because Sn^{2+} is highly susceptible to oxidation into Sn^{4+} during material synthesis and device operation. This oxidation process introduces defects within the crystal structure, increases carrier recombination, reduces carrier lifetime, and ultimately lowers device efficiency. Furthermore, the acidification associated with SnI_2 accelerates material degradation, making long-term stability a persistent challenge (1).

To overcome these limitations, recent studies have explored a wider range of alternative metal cations capable of forming stable lead-free perovskite materials. Elements such as silver (Ag^+), sodium (Na^+), antimony (Sb^{3+}), bismuth (Bi^{3+}), iron (Fe^{3+}), titanium (Ti^{4+}), palladium (Pd^{2+}), and several others have been investigated for the development of environmentally benign perovskite compounds. These studies have resulted in the synthesis of numerous lead-free materials with different structural configurations, offering new opportunities for improving both device stability and environmental sustainability. Nevertheless, many of these compounds possess low-dimensional crystal structures that limit charge transport, increase carrier effective mass, and enhance exciton binding energy, thereby restricting their overall photovoltaic performance (2).

These limitations have shifted research attention toward more structurally stable lead-free materials capable of preserving the favourable characteristics of conventional perovskites while eliminating their major drawbacks. Among the different classes of lead-free materials currently under investigation, halide double perovskites have emerged as one of the most promising candidates because of their excellent structural stability, improved defect tolerance, and favourable optoelectronic properties. Their three-dimensional crystal framework provides an attractive platform for developing efficient and environmentally sustainable photovoltaic devices, making them an active area of research in modern perovskite solar cell technology (2).

Computational Details

The structural, electronic, optical, and mechanical properties of $\text{Na}_2\text{CuBiCl}_6$ were investigated using first-principles calculations based on Density Functional

Theory (DFT). DFT has become one of the most reliable computational techniques for predicting the ground-state properties of materials with high accuracy while requiring relatively low computational cost. The method, originally established by Hohenberg and Kohn, provides an efficient framework for describing the electronic structure of solids using the electron density as the fundamental variable (6). Compared with other ab initio methods, DFT offers a good balance between computational efficiency and accuracy, with an energy precision typically on the order of 10^{-3} eV (7). Although DFT provides reliable predictions for structural and ground-state properties, conventional exchange-correlation functionals generally underestimate the electronic band gap of semiconductors and insulating materials because the Kohn–Sham eigenvalues do not represent true quasiparticle excitation energies (8, 9). To improve the accuracy of the electronic structure calculations, many-body perturbation theory (MBPT) within the non-self-consistent G_0W_0 approximation was employed. The G_0W_0 method provides a more realistic description of quasiparticle energies by incorporating electron-electron interactions through the Green's function (G) and the screened Coulomb potential (W). Compared with fully self-consistent GW calculations, the G_0W_0 approach significantly reduces computational cost while maintaining excellent agreement with experimental electronic properties, making it suitable for bulk semiconductor calculations (10–14). All simulations were performed using two open-source computational packages: Quantum ESPRESSO (QE) for the DFT calculations and Yambo for the quasiparticle GW calculations (16). The primitive unit cell of Na₂CuBiCl₆ consisted of 40 atoms, while a $2 \times 1 \times 1$ supercell containing 80 atoms was constructed for the calculations where necessary to improve the description of the crystal structure and its physical properties.

The structural optimization and electronic calculations were carried out using the plane-wave pseudopotential implementation of DFT within the Quantum ESPRESSO package. Exchange-correlation effects were described using three different approximations: the Local Density Approximation (LDA) with the Perdew Zunger (PZ) functional, and the Generalized Gradient Approximation (GGA) employing both the Perdew Burke Ernzerhof (PBE) and Wu Cohen (WC) functionals (17). Ultrasoft pseudopotentials obtained from the PSLibrary database were employed to describe the interaction between the valence electrons and ionic cores. The electronic wave functions were expanded using a plane wave basis set with a kinetic energy cutoff of 60 Ry. Brillouin-zone integration was performed using the Monkhorst Pack sampling scheme

to ensure accurate convergence of the total energy and electronic properties. Geometry optimization was continued until the total energy and atomic forces satisfied the predefined convergence criteria.

To obtain more accurate electronic band structures, quasiparticle calculations were subsequently performed using the Yambo package based on many-body perturbation theory within the non-self-consistent G_0W_0 approximation (18). In this approach, the Kohn Sham eigenvalues and wave functions generated from the Quantum ESPRESSO calculations were used as the initial input for the quasiparticle calculations. The Green's function and screened Coulomb interaction were then evaluated iteratively to determine the corrected quasiparticle energy spectrum. In the present study, the GGA electronic structure served as the starting point for all G_0W_0 calculations because of its computational efficiency and reliable description of the electronic wave functions. Following the DFT calculations, the initial Green's function, (G_0), was constructed from the Kohn Sham eigenvalues and wave functions according to equation 1:

$$G_0(\vec{r}, \vec{r}'; \omega) = \sum_j \frac{\Phi_n(\vec{r})^* \Phi_n(\vec{r}')}{\omega - \epsilon_n + i\eta \text{sgn}(\epsilon_n - \mu)} \quad (1)$$

In this picture, the G_0W_0 self-energy can be computed by performing Fourier transformation as:

$$\Sigma_{G_0W_0}(\vec{r}, \vec{r}'; \omega) = \frac{i}{2\pi} \int G_0(\vec{r}, \vec{r}'; \omega + \omega') W_0(\vec{r}, \vec{r}'; \omega') e^{i\omega'\eta} d\omega' \quad (2)$$

where η is a small positive infinitesimal constant, W_0 is the dynamical screened Coulomb potential, and G_0 is the single particle Green's function of the KS system. The bare Coulomb potential V is related to the screen Coulomb potential W_0 through the inverse of the dielectric function $\epsilon^{-1}(\vec{r}, \vec{r}''; \omega)$.

$$W_0(\vec{r}, \vec{r}'; \omega) = \int \epsilon^{-1}(\vec{r}, \vec{r}''; \omega) V(\vec{r}, \vec{r}'') d^3\vec{r}'' \quad (3)$$

The dielectric function is given as:

$$\epsilon(\vec{r}, \vec{r}''; \omega) = \delta(\vec{r} - \vec{r}'') - \int V(\vec{r}, \vec{r}''') \chi(\vec{r}'', \vec{r}'; \omega) d^3\vec{r}''' \quad (4)$$

where $\chi(\vec{r}'', \vec{r}'; \omega)$ is polarizability, and the Fourier transformation of the polarizability is given as:

$$\chi(\vec{r}'', \vec{r}'; \omega) = \sum_i^c \sum_j^v \Phi_i^0(\vec{r}) \Phi_j^{0*}(\vec{r}) \Phi_i^{0*}(\vec{r}') \Phi_j^0(\vec{r}') \times \left(\frac{1}{\hbar\omega - \epsilon_i^0 - \epsilon_j^0 + i\eta} - \frac{1}{\hbar\omega - \epsilon_i^0 - \epsilon_j^0 - i\eta} \right) \quad (5)$$

where ϵ_i^0 is KS energies, Φ_i^0 is the KS wave-function and c and v are band indexes of conduction and valence bands. Then finally, QP energies are obtained via the solution of the Dyson equation perturbatively as:

$$\varepsilon_n^{QP} = \varepsilon_n^0 + Z_n(\Sigma(\varepsilon_n^0) - V_{XC}) \quad (6)$$

where QP renormalization factor Z_n is given by :

$$Z_{nk} = \left[1 - \frac{d\Sigma_n(\omega)}{d\omega} \right]_{\omega=\varepsilon_n^0}^{-1} \quad (7)$$

and then the self-energy is split into the screened-exchange and correlation part (19).

$$\Sigma_{GW} = \Sigma_X + \Sigma_C \quad (8)$$

2200 bands and 28 Ry plane wave cut-offs were used for screening the dielectric matrix, G_0W_0 self-energy, and dielectric function. The generalized Godby-Needs Plasmon model has been used for screening the dynamic dielectric function in all G_0W_0 calculations (18). For optical properties, it is well known that an accurate description of optical absorption involves interactions between the excited electron and the hole it leaves behind in the valence state.

Results and Discussion

Elastic and structural properties

The structural stability of $\text{Na}_2\text{CuBiCl}_6$ was investigated through geometry optimization using the Birch Murnaghan equation of state (EOS), which is widely employed to determine the equilibrium lattice parameters, ground-state energy, bulk modulus, and

equilibrium volume of crystalline materials (20). During the optimization process, the total energy of the crystal was calculated as a function of unit-cell volume, and the equilibrium structure was obtained by locating the minimum point on the energy volume curve. The optimized structure corresponds to the most energetically stable configuration of the material. In addition to the Birch Murnaghan equation of state, the structural stability of halide double perovskites can be assessed using the Goldschmidt tolerance factor or by evaluating the bond lengths based on the effective ionic radii of the constituent ions (21). These structural descriptors provide useful information on the geometric compatibility of the cations and anions within the perovskite lattice and help predict whether a stable crystal structure can be formed. Halide double perovskites generally possess the chemical formula $\text{A}_2\text{B(I)B'(III)X}_6$, where A is a monovalent cation, B(I) is a monovalent metal cation, B'(III) is a trivalent metal cation, and X represents the halide ion. The interaction between the B(I) and B'(III) cations plays a significant role in determining the electronic band structure, while the arrangement of these cations within the octahedral framework contributes to the structural stability of the crystal.

The optimized crystal structure of $\text{Na}_2\text{CuBiCl}_6$ was obtained by fitting the calculated energy volume data to the Birch Murnaghan equation of state. The optimization

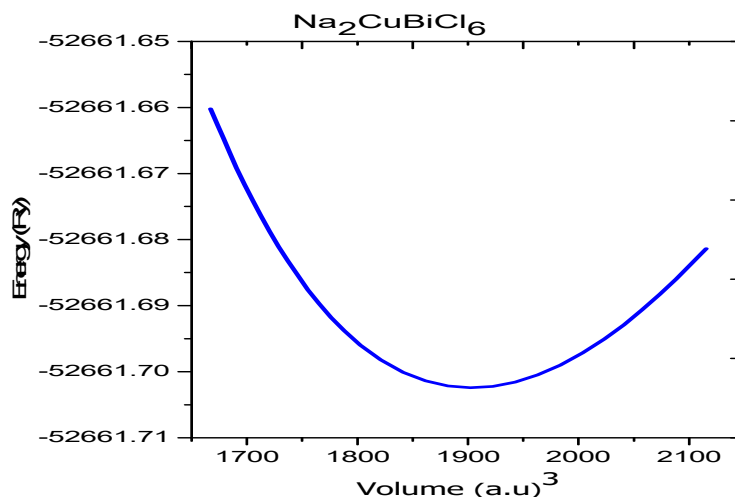


Figure 1. Showing the graph of Energy against Volume optimization of $\text{Na}_2\text{CuBiCl}_6$

Table 1. The optimized cubic lattice parameters of $\text{Na}_2\text{CuBiCl}_6$ with Fm-3m space group.

S/N	COMPOUND	a(A ⁰)	B (GPa)	B'	Eg(eV)
1	$\text{Na}_2\text{CuBiCl}_6$ (present work)	10.3849	32.251	4.700	1.3(using HSE)
	Previous reported	10.385(material project 2020)			1.294 (23)

confirmed that the material is energetically stable in its cubic crystal phase, indicating that the optimized lattice parameters correspond to the equilibrium ground state configuration. Figure 1 presents the optimized crystal structure together with the energy volume curve, while Table 1 summarizes the optimized lattice parameters. The calculated structural parameters show good agreement with previously reported theoretical results, confirming the reliability of the present computational approach and validating the optimized crystal structure of Na₂CuBiCl₆ for subsequent electronic and optical property calculations (22).

Table 1, shows these materials' ground state lattice parameters, which agreed well with previous findings (Material Project 2020). These two compounds were recently added to the Material Project; therefore, only preliminary information was made available. To investigate the structural stability, the enthalpy of formation was calculated (22, 24). The calculated ΔH value for Na₂CuBiCl₆ is -0.187 Ry. The negative sign of the endothermic phase decomposition shows the structural stability. The cubic stability was obtained from the tolerance factor (t). The Goldschmidt formula; $t = \frac{(r_A + r_X)}{2\sqrt{(r_X + r_{BB'})}}$ where r_A and r_X are the ionic radii of A and X, $r_{BB'}$ is the average of the ionic radii of B and B', was used to determine t of both double perovskite A₂BB'X₆ compounds (10, 25, 26). Perovskites with t within the range of $0.81 < t < 1.11$ were considered stable (27). The t of Na₂CuBiCl₆ was found to be 1.008, therefore it is stable (Figure 2, Table 2).

The average velocity (v_m) was calculated using both the longitudinal velocity and the transverse velocity given by

$$v_l = \left(\frac{B + \frac{4G}{3}}{\rho} \right)^{1/2} \quad (9)$$

$$V_t = \left(\frac{G}{\rho} \right)^{1/2} \quad (10)$$

$$V_m = \left(\frac{1}{3} \left(\frac{2}{v_l^2} + \frac{1}{v_t^2} \right) \right)^{-1/2} \quad (11)$$

(28). The longitudinal and transverse velocities play a significant role in determining an object's average velocity, providing insights into its speed, direction, and overall motion. Using average velocity, scientists and engineers can analyze and optimize the motion of objects across various applications, leading to improved efficiency and performance. To understand the thermal and mechanical properties of a material, the average velocity was used to calculate the Debye temperature (θ_D) of Na₂CuBiCl₆ using the equation

$$\theta_D = \frac{h}{K_B} \left[\frac{3n}{4\pi} \left(\frac{N_A \rho}{m} \right) \right]^{\frac{1}{3}} v_m \quad (12)$$

(5) where h = plank's constant, ρ = density, K_B = Boltzman's constant and N_A = Avogadro's constant. The Debye temperature value of 223.23K was obtained for Na₂CuBiCl₆, confirming the anisotropic nature and stability at high temperature, which is important in fabricating devices.

Electronic Properties

The electronic properties of solids are largely

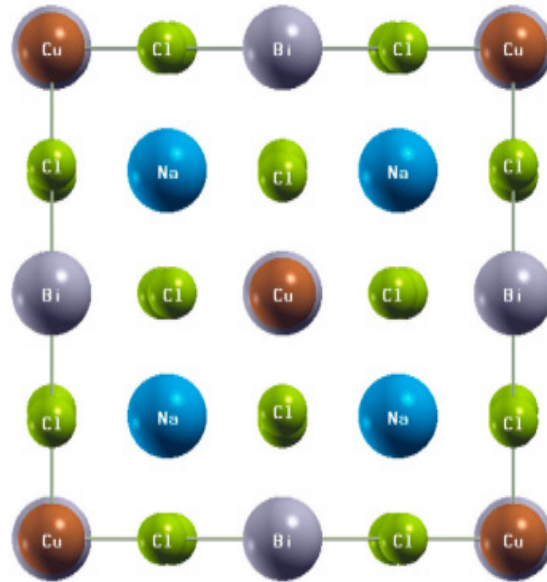


Figure 2. Showing the crystal structure of Na₂CuBiCl₆

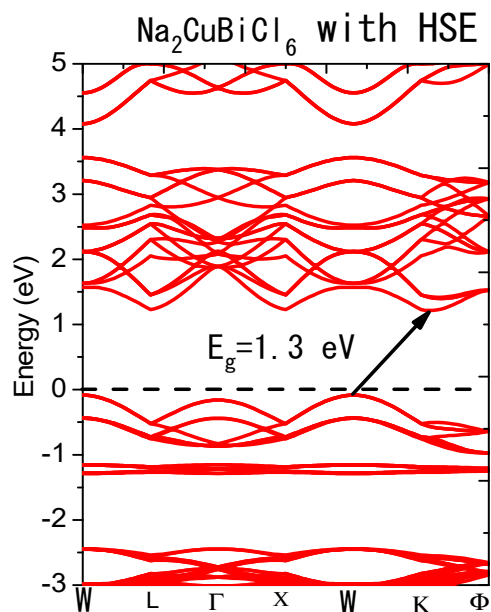
Table 2. SOECs were obtained using the GGA-PBE approach for Na₂CuBiCl₆.

S/N	Parameters	Na ₂ CuBiCl ₆
1	C ₁₁	59.57
2	C ₁₂	17.46
3	C ₄₄	9.31
4	B (GPa)	31.50
5	G (GPa)	12.99
6	B/G	2.42
7	Y (GPa)	34.27
8	ν	0.32
9	A	0.44
10	C ₁₁ – C ₄₄	8.15
11	νl (m/s)	3951.61
12	νt (m/s)	2038.66
13	νm (m/s)	2282.60
14	θD (K)	223.23

determined by their band structure and electron distribution (29). The band structure of Na₂CuBiCl₆ was calculated using the Heyd-Scuseria hybrid functional, which integrates Hartree-Fock exchange with Perdew-Burke-Ernzerhof (PBE) methods. The HSE approach accounts for both long-range and short-range correlation effects, making it particularly effective for accurately predicting the characteristics of materials that exhibit strong electronic correlations or semiconductor band gaps. As illustrated in Figure 3, the band structure of Na₂CuBiCl₆ shows that the Fermi level is unoccupied, highlighting its semiconducting nature. Additionally, the conduction band's minimum does not coincide with the valence band's maximum, indicating that this material has an indirect band gap. The calculated band gap for

Na₂CuBiCl₆ is 1.3 eV, which aligns well with the value of 1.294 eV reported by (23).

To further investigate the nature of band gap configuration and arrangement of the orbitals in the electronic structure of Na₂CuBiCl₆, the total and partial density of states (DOS and PDOS) have been studied. The results of total and partial densities of states (DOS and PDOS) of Na₂CuBiCl₆ are shown in Figure 4. The valence band of Na₂CuBiCl₆ is composed of p and s-orbitals of Na, d-orbital of Cu, s, p, and d-orbital of Bi, and p-orbital of Cl. While the conduction band is mainly composed of the s-orbital of Na, the s-orbital of Cu, the p-orbital of Bi, and s-orbital of Cl. D-orbital of Cu, p-orbital of Bi, and s-orbital of Cl are the most vital states close to the Fermi level. The presence of unpaired electrons in the constituent atoms confirms the non-magnetic nature of these compounds, already established by the structural optimization. The materials will have a great impact on optoelectronics and thermoelectric applications because of their semiconducting nature and small bandgap.

**Figure 3.** Showing the band structure of Na₂CuBiCl₆ was calculated using HSE methods.

The Optical Properties

Optical properties investigations play a crucial role in the better understanding of the optoelectronic behavior of any material under investigation for its technological applications. (30). The optical characteristics of Na₂CuBiCl₆ are determined using the G_0W_0 methodology. The G_0W_0 band aligns well with the experimental data because it considers the interactions between electrons. The frequency-dependent microscopic dielectric function's real and imaginary components are illustrated in Figures 5 and 6, respectively. The real component of a macroscopic dielectric function indicates the extent to which a material becomes polarized due to the creation of induced electric dipoles from an external electric field, while the imaginary component represents the material's ability to

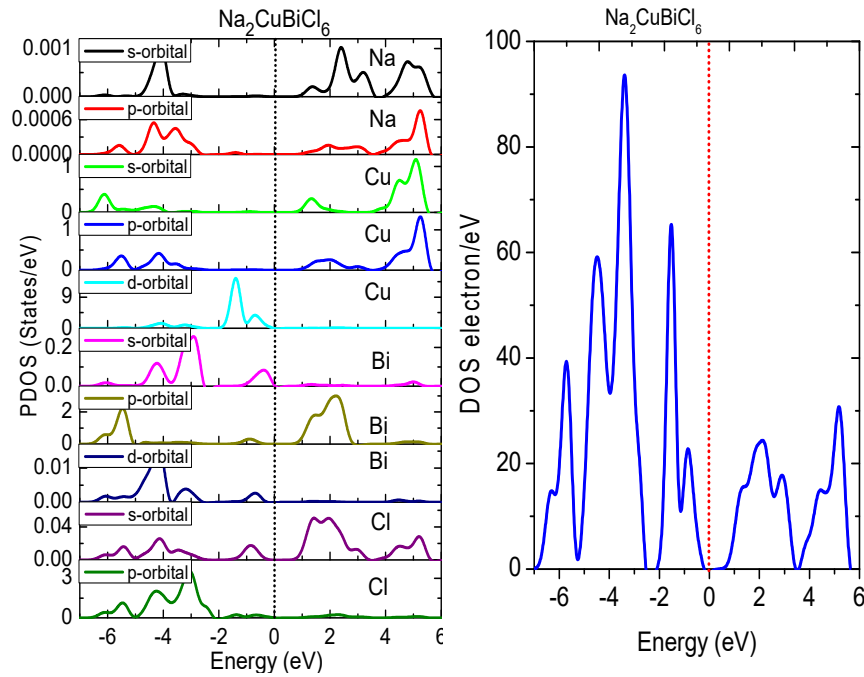


Figure 4. Showing the density of states and partial density of states of $\text{Na}_2\text{CuBiCl}_6$

absorb photon energy. The static dielectric permittivity tensor $\epsilon(0)$ encompasses electronic contributions at high frequencies and ionic contributions typical of a non-polar material. The static dielectric permittivity tensor and plasma energy are crucial for calculating the band gap energy, E_g , using the Penn Model equation. (31). The optical gap in the imaginary component of the dielectric function reflects the inter-band transitions between the conduction band minimum and the valence band maximum, which correspond to the material's fundamental band gap.

The dielectric function of the material shown in Figure 6 is a response to an external electric field, particularly when interacting with light. It consists of two parts: the real part and the imaginary part represented by both ϵ_1 and ϵ_2 . The real part in Figure 6 shows initial peaks and a plateau (0 to 3 eV). The sharp peak indicates strong electronic polarization and likely corresponds to resonance with specific electronic transitions. Decreasing trend (3 to 8 eV) shows reduced polarization due to transition reaching saturation or the dominance of other processes. The fluctuation likely indicates complex interaction at higher energies involving different electronic transitions or inter band interactions. The imaginary part in Figure 6 shows that the primary broad peak of (2 to 4 eV) corresponds to strong absorption, which aligns with the optical transition between

electronic states critical for determining optical band gap. The dielectric function also shows a significant electronic transition in the visible to ultraviolet range, indicating it optical activity in those regions. These findings are crucial for application in optoelectronic or other technologies (optical properties).

Figure 7 shows that the absorption begins around 3 eV, indicating the energy threshold required for electronic transition in this material, which is related to the band gap. The notable absorption peaks at approximately 4 eV and 6 eV, with an additional increase in absorption above 10 eV. These peaks show the presence of multiple electronic transitions or excitations within the material. The absorption coefficient above 10 eV indicates strong absorption in the high-energy region. $\text{Na}_2\text{CuBiCl}_6$ has distinct optical characteristics with an onset absorption around 3 eV and increasing absorption at higher energies, useful for applications requiring precise light absorption.

The extinction coefficient is a measure of how strongly a material absorbs light at a given energy. It's a component of the complex refractive index.

$$\tilde{n} = n + ik \quad 4.4$$

The peak value of $K \approx 1.6$ around 2.5 eV indicates strong absorption of light in this region (visible range, near green light). It remains low, which indicates reduced absorption of high photon energies. The fundamental

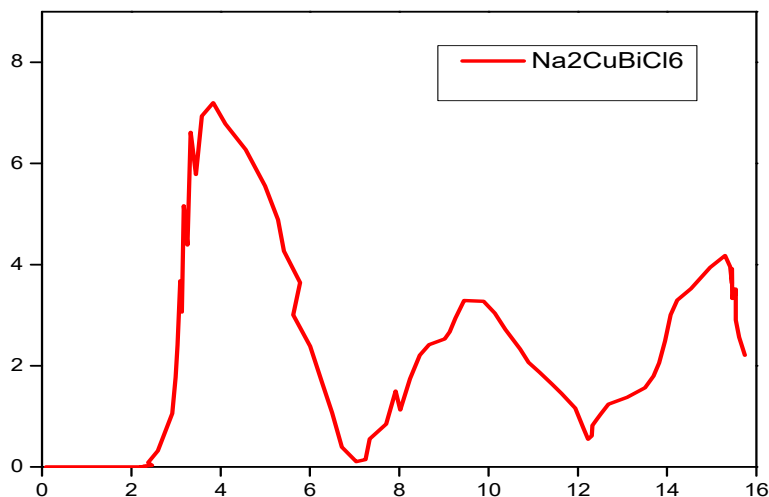


Figure 5. The imaginary part of the dielectric function of $\text{Na}_2\text{CuBiCl}_6$ using G_0W_0

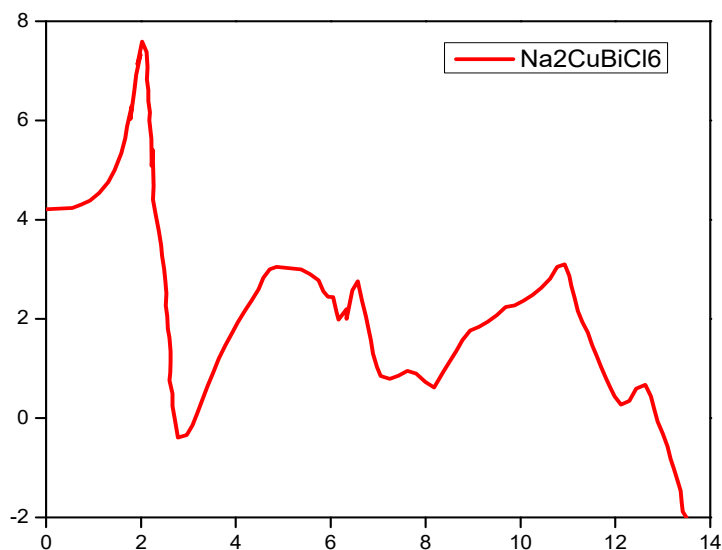


Figure 6. The real part of the dielectric function of $\text{Na}_2\text{CuBiCl}_6$ using G_0W_0

absorption edge is found to be in the region of 2-3eV. The transparent region where K is equal to zero was found within 4 – 6eV. Figure 8 shows the calculated refractive index $n(\omega)$ dispersion curves for a perpendicular electric field. Refractive index describes the phenomenon of the bending of the incident light when it enters a material. The refractive index $n(\omega)$ has a peak value between 1.5 – 3eV Which indicate strong interaction of light with the material in the near infrared/visible region. A high refractive index implies strong light bending and slower light propagation through the material. The drop to about

1.0 around 2-4eV indicates the reduced optical density in the mid-energy region. However, the fluctuation from 4-12eV shows multiple peaks and valleys between 1.0 and 1.6, which indicates complex dispersion.

The energy range in Figure 9 covers from 0 to 14eV, indicating the range of photon energies over which the optical properties are being measured. The rising region from 10 eV indicates strong absorption features or an electronic transition. Multiple peaks show the presence of a complex electronic structure with several allowed electronic transitions. The low energy level shows a lack

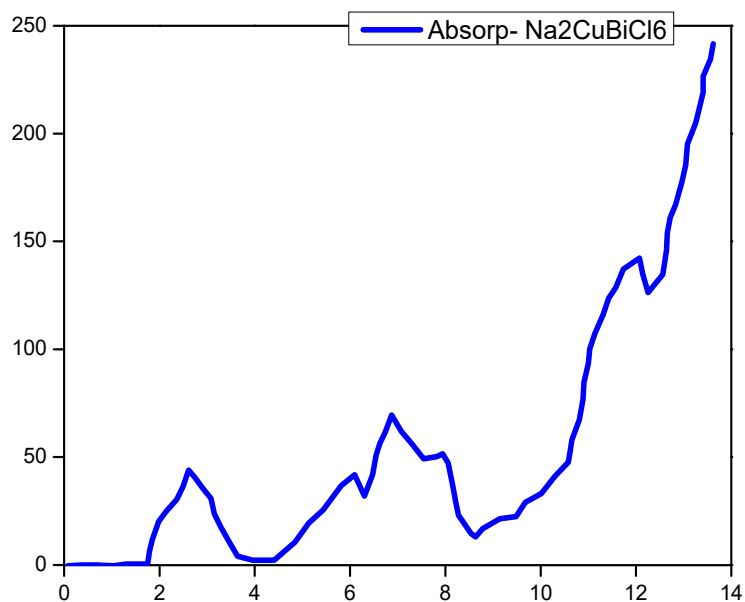


Figure 7. Absorption coefficient ($10^4/\text{cm}$) of $\text{Na}_2\text{CuBiCl}_6$ using G_0W_0

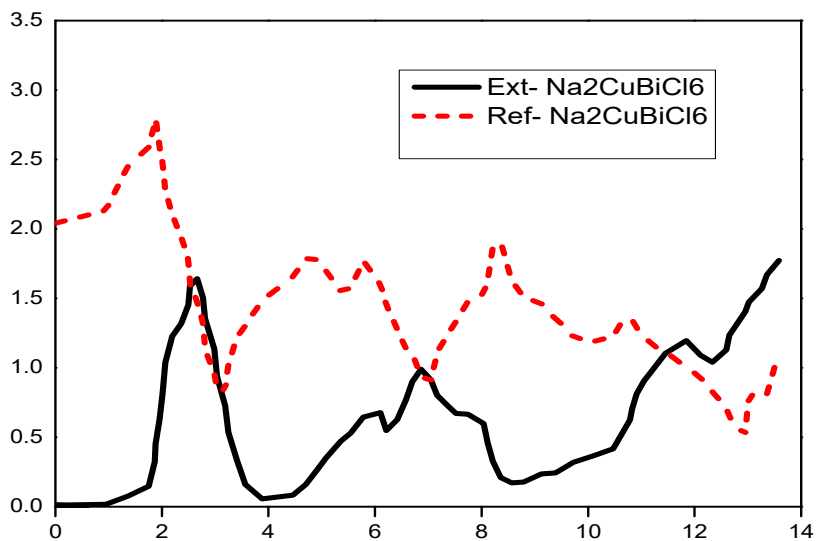


Figure 8. The refractive index and the exchange coefficient $\text{Na}_2\text{CuBiCl}_6$ using G_0W_0

of available states for optical transition in this energy range. This might imply an optical band gap below the threshold.

Figure 10 is a measure of how much light is reflected by a material surface; it ranges from zero (no reflection) to one (total reflection). The reflectivity reaches a high value of 0.35 around 1.5 eV indicating strong reflection in

the lower energy (infrared to visible) region. Due to the interband transition, several smaller peaks and valleys appear, showing complex interaction. The dips in reflectivity suggest energy where the material absorbs more light, which are typically linked to an electronic transition.

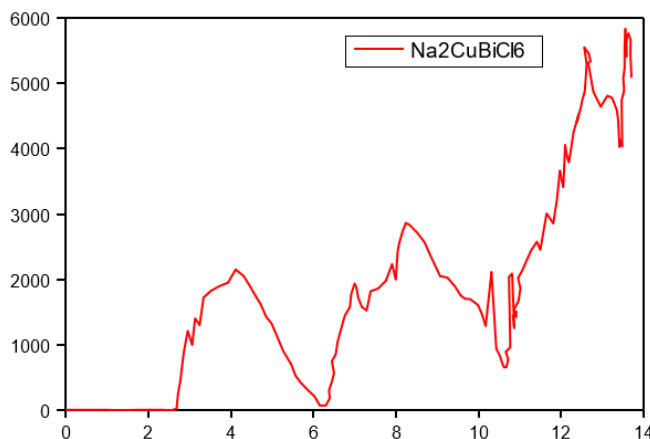


Figure 9. The optical conductivity of $\text{Na}_2\text{CuBiCl}_6$ using G_0W_0

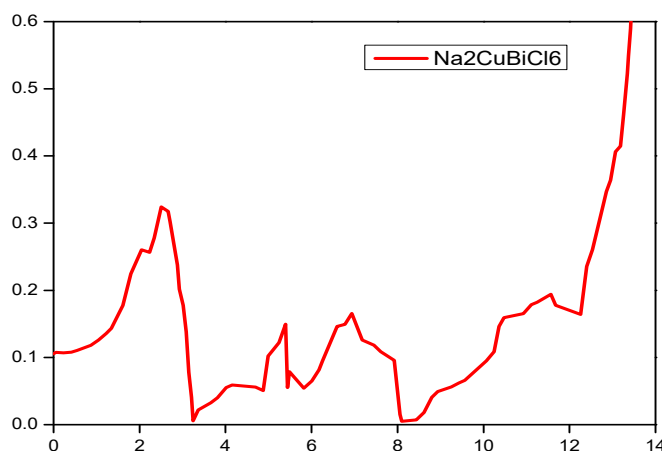


Figure 10. The reflectivity of $\text{Na}_2\text{CuBiCl}_6$ using G_0W_0

Conclusion

This research work contributes to the search for a better alternative to a lead-free double perovskite. Sodium-hexachloro-bismuthate III ($\text{Na}_2\text{CuBiCl}_6$) adopts the double perovskite structure because of the presence of different metal cations (Cu^+ and Bi^{3+}) occupying the B-site of the classic perovskite lattice. The cubic crystal structure is ordered to balance charge and maintain stability. Using the Goldschmidt formula, the tolerance factor was found to be 1.008, and the calculated ΔH value for $\text{Na}_2\text{CuBiCl}_6$ is -0.187 Ry. The negative sign of the endothermic phase decomposition shows the structural stability. The Debye temperature value of 223.23K was obtained for $\text{Na}_2\text{CuBiCl}_6$, confirming the anisotropic nature and stability at high temperature, which is important in fabricating devices. The band structure of $\text{Na}_2\text{CuBiCl}_6$ was computed using Heyd-Scuseria, which is a hybrid function; it combines Hartree-Fock exchange

with the Perdew-Burke-Ernzerhof (PBE). The HSE includes both the long-range and short-range correlation effects, making it more accurate for predicting properties of materials with strong electronic correlations or band gaps of semiconductors. The indirect band gap of $\text{Na}_2\text{CuBiCl}_6$ was found to be 1.3, which is in agreement with 1.294 reported by (23). The density of states and the partial density of states show the presence of unpaired electrons in the constituent atoms, confirming the non-magnetic nature of these compounds already established by the structural optimization. The materials will have a great impact on optoelectronics and thermoelectric applications because of their semiconducting nature and small bandgap. To analyze the optical properties, the real and the imaginary part of the dielectric function were calculated, which shows significant electronic transition in the visible to ultraviolet range, indicating its optical activity in those regions. These findings are crucial for

application in optoelectronic or other technologies (optical properties). The absorption coefficient of the Na₂CuBiCl₆ has distinct optical characteristics with an onset absorption around 3eV and increasing absorption at higher energies, useful for applications requiring precise light absorption. The refraction index and the exchange coefficient Na₂CuBiCl₆ indicates strong interaction of light with the material in the near infrared/visible region. A high refractive index implies strong light bending and slower light propagation through the material.

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