



RESEARCH ARTICLE

First-Principle Calculations of Structural, Electronic, Elastic, and Optical Properties of XBaCl_3 ($\text{X} = \text{In}, \text{Tl}$) Chloro-Perovskites

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Abstract: To investigate the potential of barium-based halide perovskites for optoelectronic applications, we performed first-principles density functional theory calculations on XBaCl_3 ($\text{X} = \text{In}, \text{Tl}$). These calculations were performed using the WIEN2k package, which provides detailed insights into the materials' characteristics. The code provides a silent insight into materials' characteristics and potential improvements. We employed the Full-Potential Linearized Augmented Plane Wave (FP-LAPW) approximation to study the optimized structure, electronic, elastic, and optical properties of XBaCl_3 chloro-perovskite compounds. To assess the structural stability, we are applying the Birch–Murnaghan fitting curves, confirming that each compound is structurally stable in its optimal or ground states. The IRelast Package is utilized for evaluating the elastic properties, revealing that the materials are anisotropic, brittle, and mechanically stable. In the analysis of electronic structure, the density of states and band structure were examined. It was discovered that the compounds have an indirect bandgap of 4.9 eV for InBaCl_3 and 5.6 eV for TlBaCl_3 . Examining the total and partial density of states allowed us to trace how individual atomic orbitals shape the overall band structure. Furthermore, we also studied the optical response that comprises the dielectric function, refractive index, absorption coefficient, and reflectivity across an energy range of 0–13.5 eV. The materials are transparent to low-energy photons, absorbing light and exhibiting optical conductivity only in the ultraviolet range. This provides critical insight for developing more efficient and functional high-tech electronics and motivating further experimental investigation.

Keywords: chloro-perovskites, dielectric function, ultraviolet absorption, wide bandgap, WIEN2k

1. Introduction

Materials scientists investigate compounds that are crucial to modern technology, primarily through theoretical research. They intend to advance technologies in sectors such as semiconductors, energy storage, and optics. Despite the vast body of existing scientific knowledge, perovskites continue to offer new and surprising properties [1–4]. Perovskite, a mineral first identified by Gustav Rose in 1839 and named for Lev Perovski, has the basic composition CaTiO_3 but follows an ABX_3 structural pattern, with two cations A and B of dissimilar sizes and an anion (X). Perovskites fall into two main categories, oxide (with oxygen as X) and halide (with halogens as X), created by swapping the X-site anion. This substitution at the X-site is the primary source of perovskite diversity, and the distinct traits of oxide versus halide perovskites largely determine their functions and applications [5–7]. Perovskite compounds have elevated

noteworthy devotion across diverse scientific and technological domains due to their remarkable and tunable physical properties. Notably, their characteristics such as tunable laser emission [8], ferroelectric behavior [9], phase transition phenomena [10], strong electron–phonon coupling [11], and pronounced crystal field effects [12] are extensively reported. Perovskites also parade an array of cutting-edge functionalities, including high dielectric permittivity [13], piezoelectricity [14], superconductivity [15], and excellent charge transport properties [16]. They also demonstrate intriguing optoelectronic features such as high absorption coefficients [17], extended carrier diffusion spans [18], and imperfection tolerance [19], rendering them effective for solar cells and LEDs. Furthermore, their structural flexibility allows for compositional engineering, enabling the tailoring of electronic band structures and enhancing their applicability in next-generation energy and electronic devices.

Besides the mentioned properties, their ability to act as semiconductors [20], anti-ferromagnetism [21], and usage as scintillating materials have also been reported [22]. Scintillation detectors are widely used for radiation sensing, with ongoing efforts to develop new inorganic scintillators for physics, medical

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imaging, and materials science. The operation of a radiation detection device using a single-crystal scintillator is contingent strongly on the physical and scintillation characteristics of the crystal [23, 24]. Scintillators are widely used for their brightness, directivity, and energy sensitivity [25, 26], while chloro-perovskites are gaining interest as promising candidates due to their favorable bandgaps, high absorbance, and low-cost synthesis [27–30]. Alkali-metal doping (Li, Na, K, Rb, Cs) boosts perovskite solar cell performance and efficiency [31, 32]. Furthermore, the incorporation of these metals induces significant modifications in the electronic and thermodynamic properties, resulting in enhanced generation and diffusion of photo-induced charge carriers. This, in turn, contributes to improved long-term stability under ambient conditions [33–37].

The incorporation of alkali metal ions into halide perovskites has been reported to produce structural and optoelectronic adjustments, resulting in superior charge dose, increased luminance, improved humidity resistance, and optimized band orientation in nanocrystalline as well as polycrystalline perovskite thin films [38–40]. Perovskites are studied for solar applications via density functional theory (DFT), a well-established computational tool [41].

In this paper, the fundamental physical properties of ternary XBaCl_3 ($X = \text{In, Tl}$) chloro-perovskites have been theoretically studied through the DFT framework. These materials are useful in energy storage, scintillators, and modern devices. To date, no experimental studies on InBaCl_3 or TlBaCl_3 have been reported, nor have any theoretical investigations using the same method (WIEN2k) been published. However, analogous chloro-perovskites such as CsCaCl_3 , CsCaI_3 , and CsBaCl_3 have been successfully synthesized, suggesting that InBaCl_3 and TlBaCl_3 are likely also synthetically feasible [42–44].

The selection of InBaCl_3 and TlBaCl_3 is motivated by the need for a systematic comparison of how the A-site cation influences the properties of chloro-perovskites. Although both In and Tl belong to Group 13, they differ significantly in ionic radius, electronegativity [45], and relativistic effects [46], enabling a meaningful structure–property correlation. Additionally, while lead-based perovskites raise toxicity concerns [47], In- and Tl-containing chloro-perovskites remain underexplored despite their potential for optoelectronic and radiation detection applications [48, 49]. This study therefore investigates these two compounds to establish their fundamental structural, electronic, and optical characteristics.

2. Computational Method

This study employs first-principles computational analysis. Calculations were performed using the FP-LAPW method within

DFT, as implemented in WIEN2K [50]. Structural optimization and elastic properties were obtained using the Perdew-Burke-Ernzerhof Generalized Gradient Approximation (PBE-GGA) functional [51, 52]. Lattice parameters were derived by fitting the energy-volume curve to the Birch–Murnaghan equation (BME) of state [53]. Elastic constants (ECs) were computed using the IRLast package [54]. The TB-mBJ potential was used for exchange-correlation to improve electronic and optical property accuracy. TB-mBJ is an advanced DFT functional that enhances bandgap accuracy [55]. A total of 2000 k-points was employed to sample the first Brillouin zone (BZ) in reciprocal space. The RMT values for each atom were determined with the condition of no overlap. In this study, the muffin-tin radii are 2.72 a.u. (Ba), 2.5 a.u. (X, where $X = \text{In}$ or Tl), and 2.4 a.u. (Cl). The self-consistent field calculations met the convergence criterion, with a total energy threshold set to 0.001 mRy. For both compounds, the selected cut-off energy, which divides the valence and core states, is set at -6.0 Ry. Molecular dynamics (MD) calculations were conducted with the Dynamics module in Materials Studio. The compound simulation was run in the microcanonical (NVE) ensemble, starting at 298 K without pressure coupling. Initial atomic velocities were assigned randomly, and the system was propagated with a 1.0 fs integration time step over 15.0 ps (1000 steps). To improve numerical stability, all covalent bonds were constrained using the Fix Bonds setting, and atomic positions were saved only at the final time step. All other force-field choices and simulation settings are provided in the methodology section. To determine the materials' optical characteristics, the study uses the basic complex dielectric function, which is $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$.

3. Results and Discussion

This section presents the results for XBaCl_3 ($X = \text{In, Tl}$) chloro-perovskites obtained from the methods described above. Different physical properties of the materials are considered separately.

3.1. Structural properties

We examined the structural properties of the XBaCl_3 ($X = \text{In, Tl}$) chloro-perovskites, which have lattice constants of 5.64 Å and 5.88 Å, respectively, and crystallize in the Pm-3m (#221) space group. This study takes advantage of the WIEN2K program. Figure 1 displays the cubic crystal structures of the XBaCl_3 ($X = \text{In, Tl}$). Thus, in these compounds, “Ba” is placed at (0.5, 0.5, 0.5), “Cl” atoms are positioned at (0, 0.5, 0.5), and “X = “In” and “Tl” atoms are at coordinates (0, 0, 0). We decided to employ the BME to obtain the most important struc-

Figure 1
The optimized crystal structures of ternary XBaCl_3 ($X = \text{In, Tl}$)

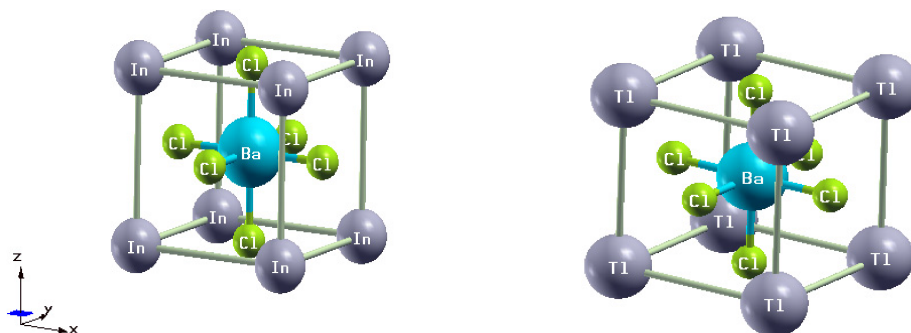


Table 1
The computed optimized lattice constants ($a = b = c$), bulk modulus (B_0), pressure derivative of bulk modulus (B'), volume at ground state (V_0), and ground state energy (E_0)

Optimized lattice parameters	InBaCl ₃	TlBaCl ₃	Zhang et al. [56]	Ullah et al. [57]
Lattice constant (a_0) in Å	5.64	5.98	5.98	5.98
Bulk modulus (B_0) in GPa	17.9641	17.7631	–	17.95
Pressure derivative of bulk modulus (B') in GPa	4.9418	4.6240	–	5.88
Volume at ground state (V_0) in (a.u.) ³	1446.0378	1448.0941	1443.08	1445.63
Ground state energy (E_0) in Ry	−30814.949	−59626.200	–	−59626.2

tural parameters in this work. These parameters comprise the bulk modulus, its pressure derivative, lattice constant, equilibrium unit cell volume, and ground state energy. As seen in the figure, the process is completed by fitting the primitive cell's energy to its volume characteristics.

$$E(V) = E_0 + \frac{B}{B'(B' - 1)} \left[V \left(\frac{V_0}{V} \right)^{B'} - V_0 \right] + \frac{B}{B'} (V - V_0) \quad (1)$$

In Equation (1) B , E_0 , V , B' , and V_0 refer to the optimum values for bulk modulus, total energy, optimal unit cell volume, bulk modulus pressure derivative, and total unit cell volume, respectively. The values of the structural characteristics for the XBaCl_3 chloro-perovskite (where $X = \text{In}$ or Tl) are given in Table 1 [43]. Figure 2 displays optimization curves obtained from the generalized gradient approximation (GGA) approximation for structural analysis. Table 1 lists the optimal parameters that were discovered when these curves were fitted using the BME. As the unit cell volume increases, the total energy decreases until reaching a minimum at the equilibrium volume, which corresponds to the ground state. The unit cell volume increases when the lattice constant rises.

Table 1 displays the bottom volume state (E_0) corresponding to a specific unit cell volume. It is important to note that the findings of this study cannot be directly compared to any experimental. Substituting In with Tl expands the lattice constant significantly from 5.64 Å to 5.98 Å (~5.6%), reflecting the larger ionic radius of Tl. Mechanically, however, the materials remain remarkably similar, both exhibiting soft compressibility with bulk

moduli hovering near 18 GPa. While TlBaCl_3 shows a marginal reduction in bulk modulus and pressure derivative (4.94 and 4.62), suggesting slight softening, the overall elastic response is preserved across both compounds. Nonetheless, the accuracy of our findings is supported by the dense sampling of 2000 k-points within the Brillouin zone, a methodology that aligns with established high-precision research.

The MD curves shown in Figure 3 for InBaCl_3 (black) and TlBaCl_3 (red) show potential energy, non-bonded interaction energy, kinetic energy, and instantaneous temperature fluctuating around approximately constant mean values over 0–15 ps, with no sustained upward/downward drift; such stationary fluctuations are characteristic of dynamically stable systems in which the structure remains intact and the simulation is well behaved [58]. The comparable fluctuation amplitudes in potential and non-bond energies indicate that both compounds maintain similar ionic packing and long-range electrostatic balance under the applied conditions, while the stable kinetic energy and temperature bands suggest consistent thermal equilibration and absence of numerical instability. Overall, the curves support short-timescale dynamical stability for both InBaCl_3 and TlBaCl_3 , with no clear evidence from these diagnostics alone that one is markedly less stable than the other.

In brief, the absence of any significant energy drift or catastrophic failure over the simulation timescale confirms that both the XBaCl_3 ($X = \text{In}, \text{Tl}$) crystal structures have stable energy and temperature profiles, validating the structural integrity and dynamic robustness of these compounds under the simulated environment.

Figure 2
Optimized curve fitting using the Birch–Murnaghan equation of state for (a) InBaCl_3 and (b) TlBaCl_3

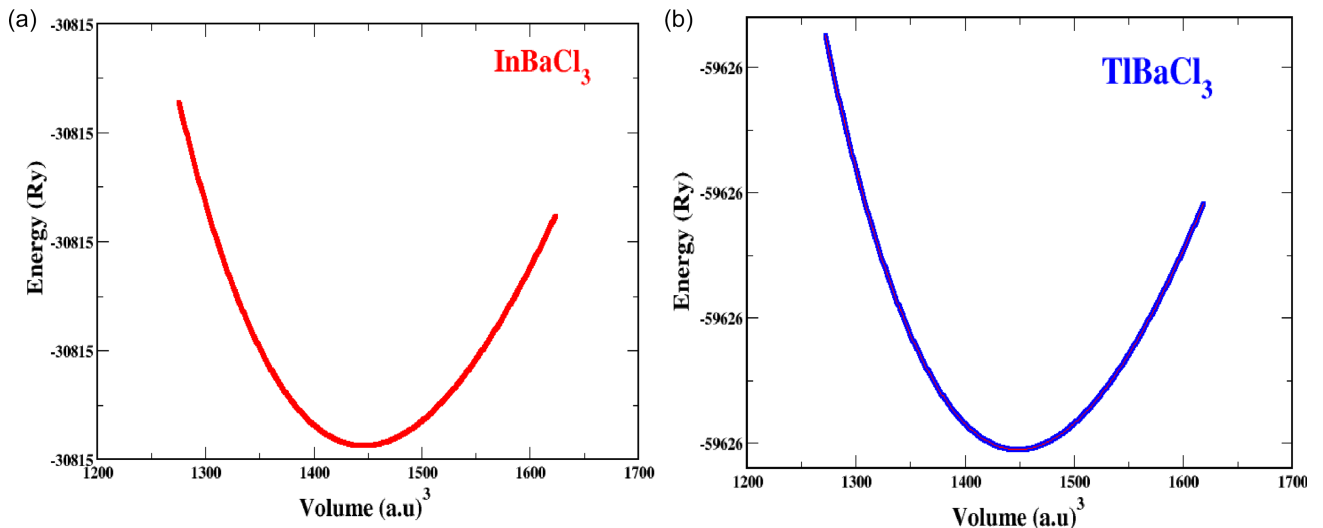
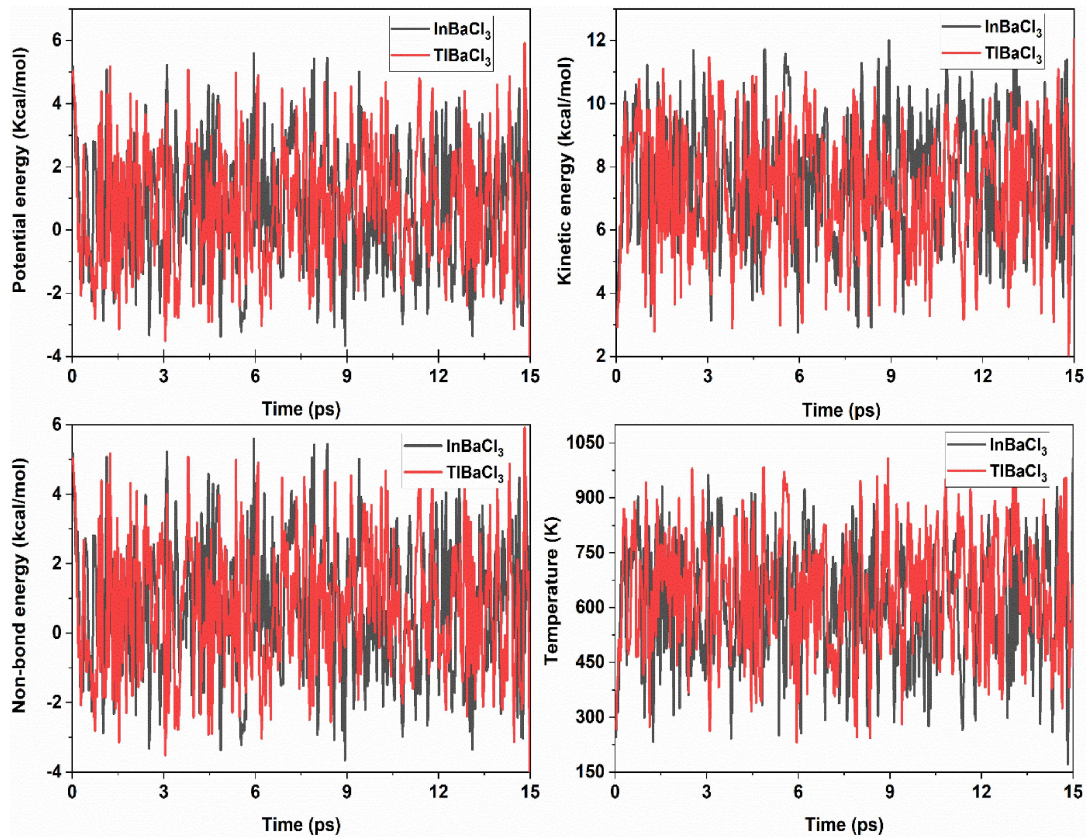


Figure 3
Stability analysis of XBaCl_3 ($X = \text{In, Tl}$) using ab initio molecular dynamics



3.2 Electronic properties

The electronic properties of XBaCl_3 ($X = \text{In, Tl}$) were explored using band structure and density of states (DOS) calculations. The GGA approximation has been used to compute these characteristics.

1) Bands structure

The band structure and DOS determine the electronic properties of chloro-perovskite materials, such as how well they are semiconducting, metallic or insulating, as well as the bonding type and gap energies. The band structure gives valuable evidence about material conductance and acts as a vital connection between electronic and optical capabilities and crystal structure. DFT calculations allow you to establish the band pattern of a material, along the high-symmetry paths in the first BZ using 2000 k-points. The approximation of TB-mBJ predicts that the band structures of the inspected ternary XBaCl_3 ($X = \text{In, Tl}$) chloro-perovskite compounds would lie inside the BZ, ranging from -2 eV to $+10$ eV, as demonstrated by the high-symmetry sites “M-X” depicted in Figure 4. For both compounds, the conduction band minima are positioned at the X symmetry point, while the valence band maxima are at the M symmetry point [59]. InBaCl_3 and TlBaCl_3 have calculated bandgaps of 4.9 eV and 5.6 eV, showing that they are both indirect bandgap insulators. For InBaCl_3 , Zhang et al. [56] reported an HSE06 bandgap of 4.178 eV (direct), differing by $\sim 17\%$ from our TB-mBJ value of 4.9 eV (indirect). This discrepancy likely arises from differences in computational code, functionality, and bandgap character. For TlBaCl_3 , our TB-mBJ bandgap (5.6 eV) agrees within 2% of Ullah et al. [57] (5.51 eV),

confirming reproducibility across independent WIEN2k/TB-mBJ calculations. Wide-bandgap semiconductors (e.g., diamond, SiC, $\text{CuAlS}_2 \sim 3.49$ eV, $\text{Ga}_2\text{O}_3 \sim 4.66$ eV) enable higher power, frequency, temperature, and UV operation, with Ga_2O_3 exhibiting the widest tunable spectral range. They are used in transparent electronics, gas sensors, optoelectronics, UV emitters, and as window layers in cascade solar cells to improve UV quantum efficiency [60].

2) Density of states (DOS)

In order to deeply comprehend the electronic properties of a solid, analysis of the DOS is essential. This analysis, depicted in Figure 5 for XBaCl_3 ($X = \text{In, Tl}$) chloro-perovskites, reports energy from -4 eV to 7 eV. A comparative analysis of the total density of states (TDOS) and partial density of states (PDOS) in Figure 5 reveals that while InBaCl_3 and TlBaCl_3 share fundamental bonding characteristics, they differ markedly in their deep valence electronic structures. In both compounds, the region immediately surrounding the Fermi level ($E_F = 0$ eV) in the valence band is enormously dominated by chlorine p-states hybridizing with barium orbitals, forming the primary valence band maximum. Additionally, both materials exhibit a common, sharp resonance in the conduction band at approximately $+5.64$ eV, driven by unoccupied high-energy states.

However, a critical distinction appears in the lower valence band (-1 to -3 eV). TlBaCl_3 displays substantial spectral weight from thallium d-states and f-states that overlap precisely with the secondary Cl-p peaks in this region. This indicates substantial p-d(f) hybridization involving the heavy Tl cation. In contrast, InBaCl_3 shows negligible contribution from indium d-states in this energy range, resulting in a spectrum dominated almost exclusively by the

Figure 4
The electronic band structure of XBaCl_3 ($X = \text{In, Tl}$) chloro-perovskites

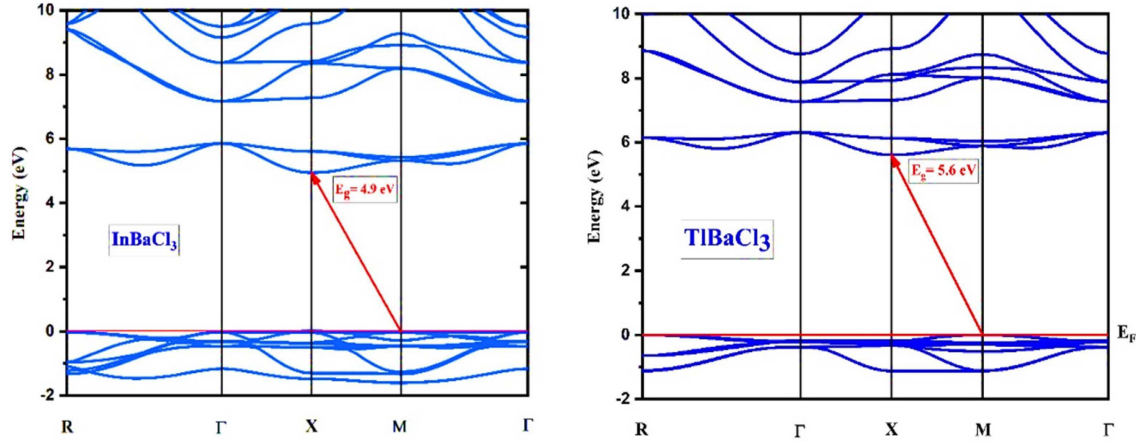
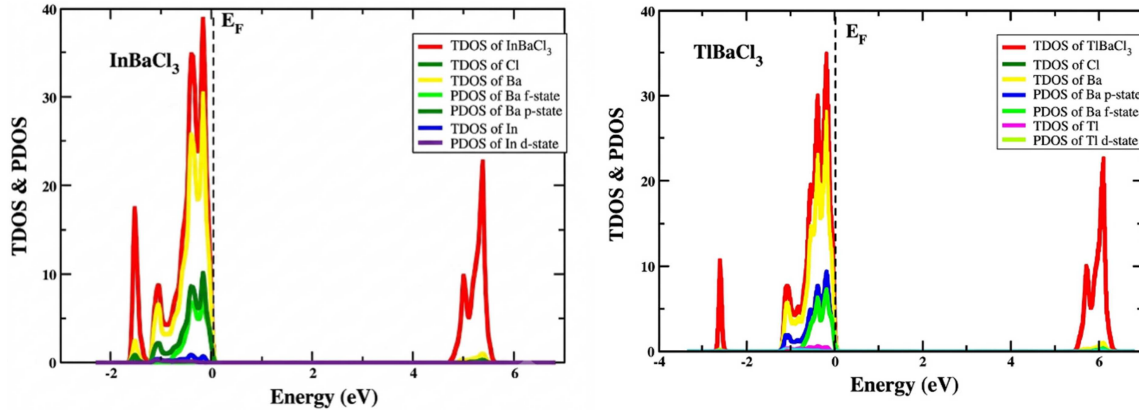


Figure 5
The calculated density of states (DOS) for InBaCl_3 and TlBaCl_3 chloro-perovskites



halide and alkaline earth framework without the complex multi-orbital mixing seen in the Tl counterpart.

3.3. Elastic properties

ECs are crucial parameters for understanding a material's mechanical behavior, hardness, and strength, with three independent constants governing the elastic behavior of any cubic crystal. The ECs in this work were found using the IR-Elast program from the Wien2k Package. The calculated EC values for the barium-based perovskite XBaCl_3 ($X = \text{In, Tl}$) are shown in Table 2. Based on the Born–Huang criteria, both compounds are mechanically stable, as evidenced by the positive estimated values of the ECs: $(C_{11} - C_{12}) > 0$; $(C_{11} + 2C_{12}) > 0$; $C_{44} > 0$, and the bulk modulus $B = (2C_{12} + C_{11}) / 3 > 0$ must also fulfill the requirement: $(C_{12} < B < C_{11})$ for mechanical stability, confirming the mechanically stable state of both compounds [61]. Additionally, the C_{11} value is higher than C_{12} and C_{44} , indicating that the compounds are resistant to compression along the x-axis. The hardness of a material is indicated by the bulk modulus (B). A higher B value corresponds to greater hardness. The higher bulk modulus of InBaCl_3 shows that it is harder than TlBaCl_3 . Consequently, when the compounds undergo compression, InBaCl_3 withstands greater volume change from all directions than TlBaCl_3 . InBaCl_3 can withstand greater transverse deformation than TlBaCl_3 because of its high shear modulus (G) [62]. In order to ascertain “B” and “G” generally, the estimations

of Voigt and Reuss are frequently employed [63]. One may assess a material's ductility and brittleness using Pugh's ratio (B/G). The material will be ductile if the B/G is farther than 1.75; otherwise, it will be brittle [64]. The Pugh's ratio computation results are shown in Table 2. The brittleness of the materials under investigation is shown by the calculated Pugh's ratio values. The anisotropy factor (A) provides an explanation for the material's anisotropic nature [65]. The estimated value of “A” differs from “1,” indicating that both compounds are anisotropic [66, 67]. The Cauchy pressure parameter ($C_{12} - C_{44}$) determines a material's bonding behavior; a positive value specifies ionic bonding, whereas a negative value directs covalent bonding. The negative results of the Cauchy pressure for InBaCl_3 indicate the covalent nature of bonding, while the positive value of the Cauchy pressure for TlBaCl_3 indicates the ionic nature of bonding [68]. Formulas for the anisotropy factor, Young's and Reuss approximations, Poisson's ratio, compressibility, and shear moduli are listed below:

$$G = \frac{1}{2}(G_V + G_R) \quad (2)$$

$$G_V = \frac{1}{5}(C_{11} - C_{12} + 3C_{44}) \quad (3)$$

$$G_R = \frac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3(C_{11} - C_{12})} \quad (4)$$

$$E = \frac{9GB}{3B + G} \quad (5)$$

$$\nu = \frac{3B - 2G}{2(3B + G)} \quad (6)$$

$$A = \frac{2C_{44}}{(C_{11} - C_{12})} \quad (7)$$

$$B = \frac{(2C_{12} + C_{11})}{3} \quad (8)$$

Shear modulus, Vogt's G_V and Reuss G_R , Young's modulus Y , Poisson's ratio ν , anisotropy factor A , and bulk modulus B are in Equations (2)–(8), respectively.

In comparing the mechanical properties of InBaCl₃ and TlBaCl₃ in Table 2, significant differences emerge regarding their elasticity and structural stability. InBaCl₃ exhibits much higher longitudinal stiffness, with a C_{11} of 84.15 GPa compared to 43.91 GPa for TlBaCl₃. The exceptional feature of InBaCl₃ is its negative C_{12} (−14.47 GPa) and negative Poisson's ratio (−0.102), identifying it as an auxetic material [69, 70], whereas TlBaCl₃ behaves traditionally with a positive ratio of 0.364. While both materials share nearly identical bulk moduli ($B \sim 18$ GPa), InBaCl₃ is significantly more rigid in terms of shear (G) and Young's modulus (E), being roughly six and four times stiffer than TlBaCl₃, respectively. Furthermore, the B/G ratio classifies InBaCl₃ as a brittle material (0.497), while TlBaCl₃ is highly ductile (3.33).

Zhang et al. [56]'s results align nearly perfectly with TlBaCl₃, describing a soft, ductile material, while Ullah et al. [57] report a much stiffer, stronger compound with a different elastic preference. InBaCl₃ stands apart as a rigid auxetic material. Overall, the three studies reveal distinct mechanical profiles ranging from ductile to stiff and auxetic behavior.

3.4. Optical properties

The optical properties of XBaCl₃ ($X = \text{In, Tl}$) chloro-perovskites are extensively discussed in this section, focusing on various parameters. It has been established that both InBaCl₃ and TlBaCl₃ compounds are insulators with an indirect bandgap, determined through their electronic properties and band structure.

Consequently, these materials are well-suited for photosensitive applications. The following equations were used to calculate the optical properties using the dielectric constant [71, 72].

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \quad (9)$$

$$n(\omega) = \left[\frac{\varepsilon_1(\omega)}{2} + \frac{\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}}{2} \right]^{\frac{1}{2}} \quad (10)$$

$$k(\omega) = \left[\frac{-\varepsilon_1(\omega)}{2} + \frac{\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}}{2} \right]^{\frac{1}{2}} \quad (11)$$

$$I(\omega) = \frac{2\omega}{c} k(\omega) \quad (12)$$

$$R(\omega) = \frac{(1 - n)^2 + k^2}{(1 + n)^2 + k^2} \quad (13)$$

$$\sigma(\omega) = \frac{\hbar\omega\varepsilon_0\varepsilon_2(E)}{\hbar} \quad (14)$$

1) Dielectric function

Analyzing the dielectric function reveals key optical properties of InBaCl₃ and TlBaCl₃. This complex function, including real and imaginary parts, depicts how materials retort to electromagnetic fields and how light propagates through them. Both materials show consistent spectral patterns in their real dielectric functions, and the function is essential for assessing optical performance across all energies [73, 74]. In Figure 6, the “ $\varepsilon_1(\omega)$ ” curves extend from 0 eV to 13 eV of incoming photon energy, exhibiting an aggregate positive peak of 4.9 for InBaCl₃ and 5.6 for TlBaCl₃ at low photon energy limits. Between 8 eV and 13 eV input photon energy, both XBaCl₃ ($X = \text{In, Tl}$) reach negative highest values of approximately −1 for InBaCl₃ and −2 for TlBaCl₃, suggesting total reflection within these energy ranges. InBaCl₃ has a real static “(0)” dielectric function of 2.3, while TlBaCl₃ has a

Table 2
The investigated mechanical parameters for XBaCl₃ ($X = \text{In, Tl}$) ternary chloro-perovskites

Mechanical properties	InBaCl ₃	TlBaCl ₃	Zhang et al. [56]	Ullah et al. [57]
C_{11} (GPa)	84.15	43.91	42.61	115.41
C_{12} (GPa)	−14.47	5.21	4.71	63.22
C_{44} (GPa)	30.83	1.43	1.91	47.29
B (GPa)	18.40	18.11	17.78	21.32
ν	−0.102	0.364	0.35	0.30
$C_{12} - C_{44}$ (GPa)	−45.29	3.78	2.8	16.18
G (GPa)	36.99	5.43	5.86	37.26
E (GPa)	66.45	14.80	15.80	96.89
A	0.618	0.074	0.10	1.81
B/G	0.497	3.33	2.96	2.16

value of 2. The imaginary component $\varepsilon_2(\omega)$ is crucial for evaluating optical conversions from the VB to the CB [75]. Figure 6 depicts the “ $\varepsilon_2(\omega)$ ” spectrum for the examined substances. The maximum peaks of InBaCl₃ and TlBaCl₃ in the 0 to 13 eV photon energy range are 4 and 6.8, respectively. The “ $\varepsilon_2(\omega)$ ” begins at zero at 4.9 eV for InBaCl₃ and 5.6 eV for TlBaCl₃, indicating the absorption threshold. It achieves its extreme magnitude of 4 at 5 eV for InBaCl₃ and 6.8 at 8.7 eV for TlBaCl₃; consequently, this implies that the ultraviolet (UV) range is where absorption is supreme. Due to their UV absorption, these materials have intriguing applications in optoelectronics, such as scintillators.

2) Optical conductivity

Optical conductivity relates the applied electric field amplitude to the induced current density at a given frequency [76]. Figure 6 shows the optical conductivity spectra calculated for both chloro-perovskite compounds XBaCl₃ (X = In, Tl) over a spectrum of incoming photons from 0 eV to 13.5 eV. Figure 6 clearly shows that optical conductivity begins at incoming photon matching the electronic bandgap. The maximal optical conductivity of InBaCl₃ is 3300 $\Omega^{-1}\text{cm}^{-1}$ at a photon energy of 6.8 eV, whereas TlBaCl₃ is 8000 $\Omega^{-1}\text{cm}^{-1}$ at an input photon intensity of 8.5 eV. Both InBaCl₃ and TlBaCl₃ have strong optical conductivity at

high energy levels, indicating that they might be used in UV-based optical systems.

3) Absorption coefficient

Figure 6 shows the computed absorption coefficient, representing light absorbed per unit length [77]. The absorption coefficient spectrum produced by the TB-mBJ method is shown in this diagram. It illustrates the behavior of $I(\omega)$ (absorption coefficient) and its resemblance to the dielectric strength $\varepsilon(\omega)$. It is discovered that there was no light absorption beyond the threshold energy, as predicted, since electronic band transitions from the VB to the CB cannot be produced beneath the bands. The critical ranges of $I(\omega)$ for both InBaCl₃ and TlBaCl₃ chloro-perovskites exceed the bandgap values determined from the band structure calculations. At incoming photons of 12 eV and 8.8 eV, the maximal peak values of absorption for InBaCl₃ and TlBaCl₃ are at $115 \times 10^4/\text{cm}$ and $172 \times 10^4/\text{cm}$, respectively, which renders them a better choice for scintillators in the UV range and for lenses at low frequencies [78].

4) The refractive index

The refractive index $n(\omega)$, derived from the dielectric function, quantifies light bending and improves understanding of

Figure 6
The calculated optical properties for XBaCl₃ (X = In, Tl) chloro-perovskites

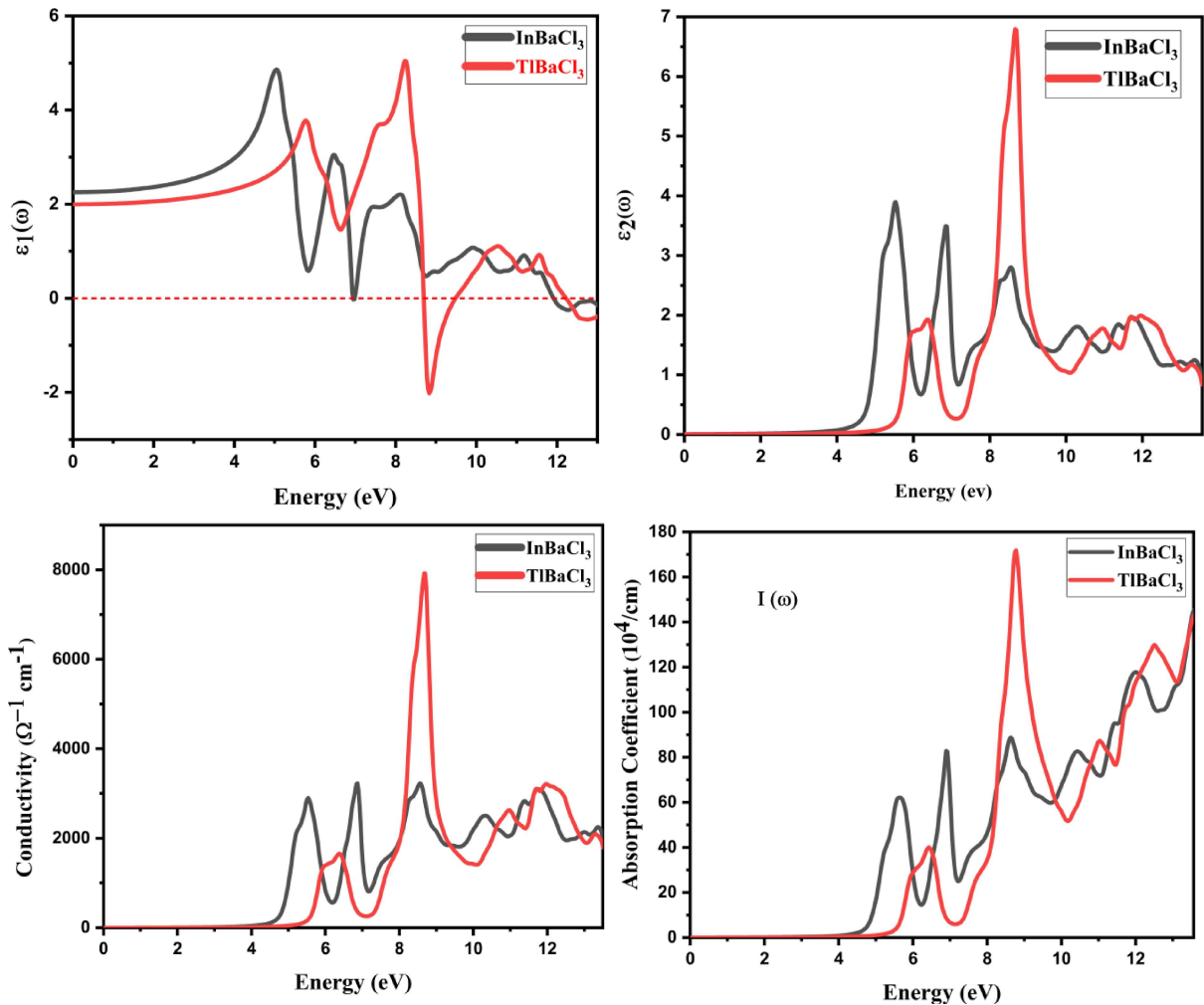
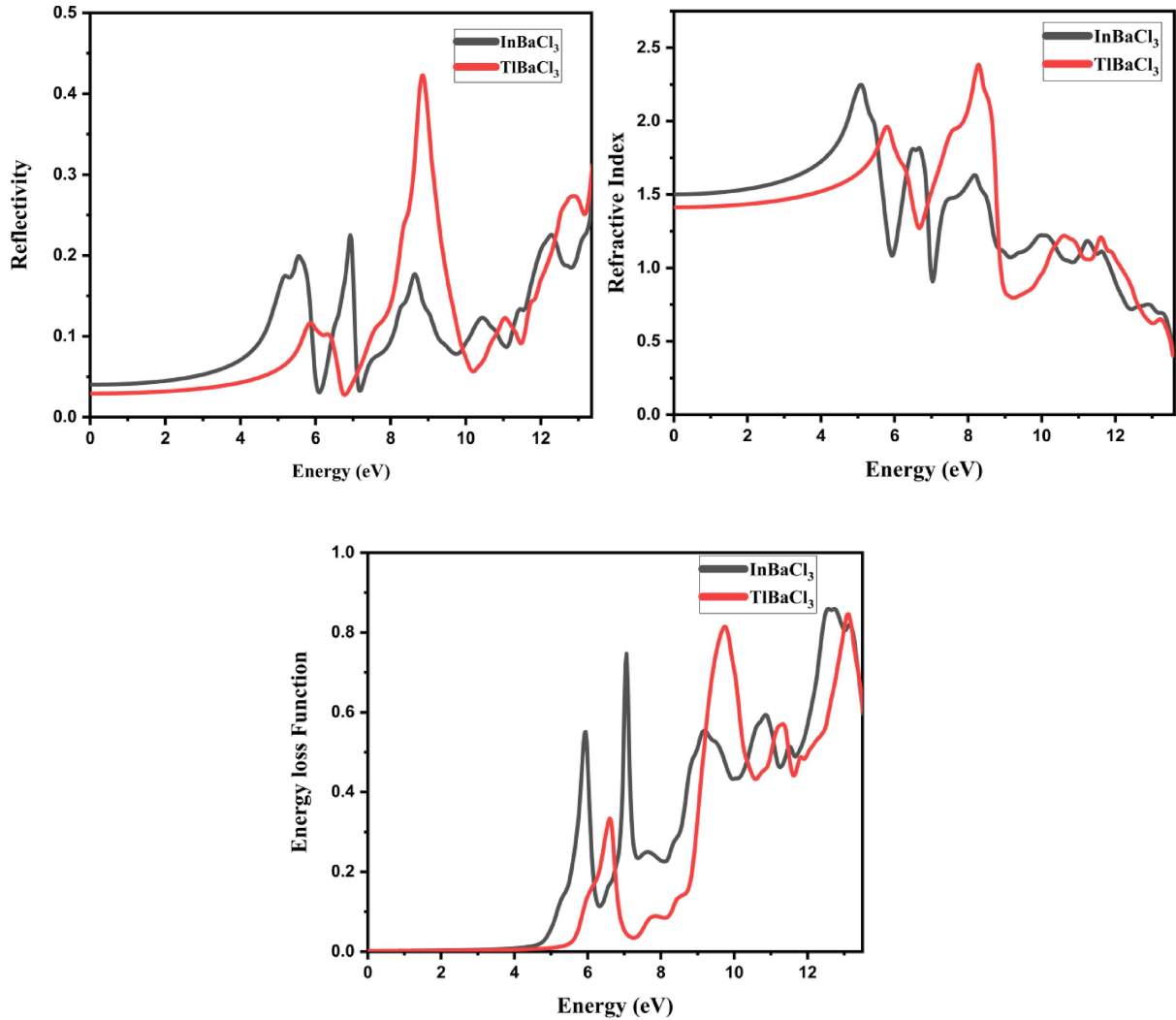


Figure 6
(Continued)

light-material interactions [79]. Figure 6 displays the refractive indices for XBaCl_3 ($X = \text{In, Tl}$) chloro-perovskites. The static refractive index $n(0)$ is 1.5 for InBaCl_3 and 1.4 for TlBaCl_3 . The maximum values of 2.26 for InBaCl_3 and 2.38 for TlBaCl_3 were achieved above the zero frequency. The refractive index exceeds one due to photon deceleration from electron interactions. A material's refractive index determines the delay in photon travel time through the material. This shows that both compounds are good optical refractors.

5) Optical reflectivity

Reflectivity is a measure of a material's ability to reflect incident energy from its surface [80]. According to Equation (13), the spectrum curves for $R(\omega)$ (reflectivity) of XBaCl_3 ($X = \text{In, Tl}$) chloro-perovskites are depicted in Figure 6. The static standards of $R(0)$ for InBaCl_3 and TlBaCl_3 compounds are 0.04 and 0.03 at 6.8 eV and 8.7 eV, respectively. As photon energy increases, photons are more likely to be reflected from the material's surface. As photon energy increases, both InBaCl_3 and TlBaCl_3 exhibit increased optical reflectivity, as seen in Figure 6. In the 0–5 eV photon energy range, optical reflectivity is modest, and as photon energy rises, the $R(\omega)$ spectra for the two substances climb, achieving maximum values of 0.45 for InBaCl_3 and

0.48 for TlBaCl_3 in the high-photon-energy UV range (13.5 eV), showing that both compounds have relatively low reflectivity at low photon frequencies.

6) The energy loss function

The energy loss function (ELF) measures electron energy lost through collisions with other electrons or the lattice [81]. It is computed using the imaginary component of the inverted dielectric functions and provides useful information related to a material's plasmonic, intra-band, and inter-band characteristics. The ELF for InBaCl_3 and TlBaCl_3 is presented in Figure 6, demonstrating the different energy loss properties of the materials. The ELF remains zero from 0 eV up to the bandgap energy (4.9 eV for InBaCl_3 and 5.6 eV for TlBaCl_3), indicating no energy loss below the absorption edge. Above these thresholds, the ELF increases, peaking at 12.6 eV for InBaCl_3 and 13 eV for TlBaCl_3 . ELF indicates material response to fields and reveals plasmonic features.

4. Conclusion

DFT, as implemented in WIEN2k, was employed to determine the materials' structural, elastic, electronic, and optical properties. By fitting the BME of the state, it has been ascertained

that InBaCl₃ and TlBaCl₃ exhibit stable cubic structures. The computed optimized lattice constants for XBaCl₃ (X = In, Tl) are 5.64 Å and 5.98 Å, respectively, demonstrating the structural stability at the optimized lattice constants. The ground state energy and lattice characteristics, including bulk moduli and derivatives of bulk moduli, decrease when the metallic cation changes from In to Tl. The computed anisotropy factor “A” confirms that XBaCl₃ exhibits significant elastic anisotropy. While the Born criteria verify their mechanical stability, the calculated B/G ratios (Pugh’s criterion) classify that InBaCl₃ is brittle while TlBaCl₃ is ductile in nature. The results of these compounds’ band structure calculations show wide indirect energy bandgaps, resulting in insulating properties: 4.9 eV (*M* – *X*) for InBaCl₃ and 5.6 eV (*M* – *X*) for TlBaCl₃. The role of various elemental states in the band structure was determined using PDOS and TDOS. The insulating properties of these compounds facilitate the investigation of their optical properties, which include strong reflectivity at high energies, high absorption coefficients, and high refractive indices. The analysis of their optical characteristics in the energy range of 0 eV to 13.5 eV indicates that both compounds are transparent to visible photons and optically active in the UV region, suggesting applications such as anti-reflection coatings, lenses, and scintillators. This combination of properties is not a drawback but rather a fingerprint for specialized applications. Specifically, the sharp UV absorption edges and high absorption coefficients (up to $1.7 \times 10^6 \text{ cm}^{-1}$) for InBaCl₃ and TlBaCl₃ as strong candidates for solar-blind UV photodetectors and high-performance scintillation detectors, where wide bandgaps reduce thermal noise. The low visible-range refractive index ($n_o = 1.4\text{--}1.5$) and low reflectivity ($R_o = 0.03$ to 0.04) suggest utility as anti-reflective coatings, while the high deep-UV reflectivity ($R > 0.45$) supports applications in UV optics and lithography mirrors. Furthermore, the low static dielectric constant ($\epsilon_i(0) = 2.0$ to 2.3) and mechanical stability (satisfying Born–Huang criteria) make them potentially useful as interlayer dielectric materials in microelectronics. This comprehensive and systematic calculation of XBaCl₃ (X = In, Tl) offers worthwhile insights into the potential of “Ba”-based chloro-perovskites, motivating experimental synthesis and device prototyping for these UV-centric optoelectronic applications.

Ethical Statement

This study does not contain any studies with human or animal subjects performed by any of the authors.

Conflicts of Interest

The authors declare that they have no conflicts of interest to this work.

Data Availability Statement

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

Author Contribution Statement

Shujaat Ali Khan: Conceptualization, Methodology, Software, Validation, Investigation, Writing – original draft, Writing – review & editing, Visualization. **Nasir Rahman:** Software, Validation, Resources, Writing – original draft, Writing – review & editing, Supervision. **Shah Zeb Ullah:** Conceptualization, Writing – original draft, Writing – review & editing, Visualization. **Muhammad Sajjad:** Validation, Resources, Supervision, Project

administration. **Junaid Rehman:** Validation, Formal analysis, Writing – review & editing, Visualization.

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