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Bi₂Se₂Te and related tetradymites: SOC-induced optoelectronic tunability and multifaceted physical behavior

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Abstract

Bi₂Se₂Te, a ternary tetradymite topological insulator, has been widely studied for its protected surface states, yet its bulk physical properties remain comparatively underexplored. We present a comprehensive first-principles investigation of its structural, elastic, vibrational, electronic, and optical characteristics, benchmarked against Bi₂Te₂Se and Bi₂Te₃. Optimized lattice parameters show excellent agreement with experiment, validating the computational framework. Elastic constants satisfy mechanical stability criteria, while phonon dispersion confirms dynamical robustness. Mechanical analysis reveals pronounced elastic anisotropy, with Poisson's ratio, Pugh's ratio, and Cauchy pressure collectively indicating a predominantly brittle character governed by ionic bonding. The estimated Vickers hardness of 4.6 GPa and low lattice thermal conductivity ($0.302 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$) underscore its potential for thermoelectric functionality. Electronic band structure calculations reveal a direct band gap at the Γ point, strongly reshaped by spin-orbit coupling (SOC). Comparative SOC analysis demonstrates that Bi₂Se₂Te undergoes the most pronounced SOC-driven band gap reduction, Bi₂Te₂Se exhibits moderate effects, and Bi₂Te₃ displays the archetypal SOC-induced band inversion. Density of states analysis confirms Se $4p$ orbitals dominate the valence band and Bi $6p$ states the conduction band, with SOC enhancing orbital hybridization across the family. Optical spectra reveal strong absorption in the visible-UV range, high reflectivity, and favorable dielectric response. Bi₂Se₂Te shows the most versatile SOC-induced tunability and pronounced anisotropy, with clear optical differences between [100] and [001] directions. Together, these insights establish Bi₂Se₂Te as a structurally robust and electronically adaptable material, highlighting its promise for photovoltaic, thermoelectric, spintronic, optoelectronic, and quantum technologies.

Keywords: Bi₂Se₂Te topological insulator; Tetradymites; Spin-orbit coupling (SOC); Elastic anisotropy; Mechanical and dynamical stability; Band-gap modulation; Optoelectronic properties

1. Introduction

The continuous demand for faster information processing, energy-efficient electronics, and quantum technologies has accelerated the search for materials exhibiting unconventional electronic states and multifunctional physical properties. In this context, topological insulators (TIs) have emerged as one of the most intriguing classes of quantum materials owing to their unique coexistence of an insulating bulk and metallic surface states protected by time-reversal symmetry [1,2]. Unlike conventional materials, the surface states of topological insulators are protected against non-magnetic perturbations by time-reversal symmetry and are governed by strong spin-orbit coupling (SOC), giving rise to exotic quantum phenomena and unprecedented opportunities for technological applications [2,3]. Furthermore, TIs have been predicted to host a variety of remarkable physical phenomena, including Majorana bound states, topological superconductivity, and the quantum anomalous Hall effect [4–6]. These properties have stimulated extensive research efforts aimed at identifying new topological materials with improved stability, tunable electronic structures, and enhanced functionality.

Among the various families of topological insulators (TIs), Bi-based chalcogenides have attracted considerable attention owing to their relatively large bulk band gaps and simple single-Dirac-cone surface states. Binary compounds such as Bi_2Se_3 and Bi_2Te_3 are regarded as prototype three-dimensional topological insulators and have been extensively studied both theoretically and experimentally [7,8]. However, their practical applications are often limited by residual bulk conductivity arising from intrinsic defects, such as vacancies and antisite disorders, which shift the Fermi level away from the bulk band gap [2]. To mitigate these issues, ternary tetradymite compounds, including $\text{Bi}_2\text{Te}_2\text{S}$, $\text{Bi}_2\text{Te}_2\text{Se}$, and $\text{Bi}_2\text{Se}_2\text{Te}$, have been proposed as promising alternatives [9]. The additional compositional flexibility provided by the mixed chalcogen sublattice enables improved control over defect formation and carrier concentration, thereby suppressing bulk conduction and enhancing the contribution of topological surface states. Consequently, these ternary compounds offer a viable route toward realizing intrinsic topological insulating behavior and are considered attractive candidates for future spintronic, quantum-information, and low-power electronic applications.

Within the family of ternary tetradymite topological insulators, $\text{Bi}_2\text{Se}_2\text{Te}$ has attracted considerable interest because it combines the favorable characteristics of both Bi_2Se_3 and Bi_2Te_3 [9]. The partial substitution of Te within the chalcogen layers modifies the spin-orbit coupling (SOC) strength and electronic band structure, resulting in a well-isolated Dirac cone located within the bulk band gap [9,10]. Experimental investigations, including angle-resolved photoemission spectroscopy (ARPES) and magneto-transport measurements, have confirmed its topological insulating nature and demonstrated its potential for spintronic and quantum-device applications [11–14]. Despite these advances, research on $\text{Bi}_2\text{Se}_2\text{Te}$ has largely focused on its topological surface states, while its bulk physical properties remain comparatively unexplored.

This lack of comprehensive knowledge is significant because the practical deployment of topological materials depends not only on their surface-state characteristics but also on their bulk mechanical stability, thermal transport behavior, optical response, and electronic performance. In particular, understanding these properties is essential for evaluating the suitability of $\text{Bi}_2\text{Se}_2\text{Te}$ for optoelectronic, photovoltaic, thermoelectric, and multifunctional device applications. Moreover, the interplay between strong SOC, lattice dynamics, and optical transitions in this material remains insufficiently understood.

Motivated by these considerations, the work addresses the gap by providing the first comprehensive first-principles analysis of its structural, mechanical, vibrational, electronic, and optical behavior. By establishing the interplay between spin-orbit coupling, lattice dynamics, and optical response, our study not only deepens the fundamental understanding of $\text{Bi}_2\text{Se}_2\text{Te}$ but also highlights its potential as a multifunctional material for optoelectronic, photovoltaic, thermoelectric, and quantum technologies.

2. Computational Details

The present investigation of $\text{Bi}_2\text{Se}_2\text{Te}$ was carried out using first-principles calculations within the framework of density functional theory (DFT) under periodic boundary conditions. Ground-state properties were obtained by solving the Kohn–Sham equations [15]. Structural, elastic, and vibrational properties were computed using the CASTEP (Cambridge Serial Total Energy Package) code [16], while electronic and optical properties were investigated with the WIEN2k package based on the full-potential linearized augmented plane-wave (FP-LAPW) method [17].

In CASTEP, the exchange-correlation interaction was treated within the generalized gradient approximation (GGA) using the Perdew–Burke–Ernzerhof revised for solids (PBEsol) functional [18]. Electron-ion interactions were described with ultrasoft pseudopotentials, and the valence electronic configurations considered were Bi [$6s^26p^3$], Te [$5s^25p^4$], and Se [$4s^24p^4$]. Periodic boundary conditions were applied throughout.

To ensure reliable convergence, both the plane-wave energy cut-off and the Monkhorst-Pack [19] k-point mesh were carefully optimized. A cut-off energy of 650 eV was adopted, and the Brillouin zone was sampled using a $17 \times 17 \times 3$ Monkhorst-Pack grid. The ground-state crystal structure was optimized using the Broyden–Fletcher–Goldfarb–Shanno (BFGS) minimization algorithm [20], with

convergence thresholds of 1.05×10^{-5} eV atom⁻¹ for total energy, 0.03 eV Å⁻¹ for maximum force, 0.05 GPa for maximum stress, and 0.001 Å for maximum atomic displacement. All computational parameters were thoroughly tested and found to yield well-converged total energies and reliable structural properties.

Elastic constants were obtained by linearly fitting stress–strain curves from first-principles calculations. For trigonal Bi₂Se₂Te, the elastic stiffness matrix reduces to six independent constants: C_{11} , C_{12} , C_{13} , C_{14} , C_{33} , and C_{44} [21].

For electronic and optical properties, the Tran-Blaha modified Becke-Johnson (TB-mBJ) exchange correlation potential [22] was employed, as it provides significantly improved band-gap predictions compared to conventional GGA functionals. Calculations were performed both with and without spin-orbit coupling (SOC) [23] to assess its influence on the band structure and density of states. Optical properties were also evaluated with and without SOC explicitly included, given its strong effect on states near the Fermi level.

Accurate optical spectra were ensured by employing a dense k-point mesh of ~2700 points together with Gaussian broadening of 0.2 eV [24]. Optical parameters were derived from the complex dielectric function, $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$. The real part $\varepsilon_1(\omega)$ was obtained from $\varepsilon_2(\omega)$ using the Kramers-Kronig relations [25], while $\varepsilon_2(\omega)$ was calculated following Ref.[26]. Other optical quantities- including refractive index $n(\omega)$, extinction coefficient $k(\omega)$, and reflectivity $R(\omega)$ were determined using the relations in Ref.[27]. Furthermore, the absorption coefficient $\alpha(\omega)$, optical conductivity $\sigma(\omega)$, and energy-loss function $L(\omega)$ were evaluated following Ref.[28].

3. Results and discussion

3.1. Structural properties

The crystal structure of the Bi₂Se₂Te compound is shown in Fig. 1. It is a ternary tetradymite compound crystallizing in a trigonal structure with the $R\bar{3}m$ (No. 166) space group. The unit cell comprises 15 atoms in total, including 6 Bi, 6 Se, and 3 Te atoms. The atomic positions are given as Bi at the 6c site (0, 0, 0.4054), Se at the 6c site (0, 0, 0.2096), and Te at the 3a site (0, 0, 0) [29]

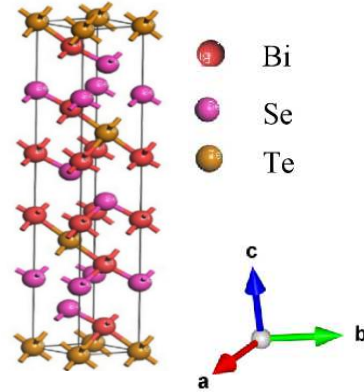


Fig. 1. The crystal structure of Bi₂Se₂Te.

To obtain the fully relaxed and stable structure of Bi₂Se₂Te, the lattice geometry was optimized. The optimized structural parameters were calculated using different exchange–correlation functionals and compared with the available experimental data [29]. The optimized lattice parameters, together with the corresponding reference values, are listed in Table 1.

Table 1: Calculated lattice parameters, a and c , unit cell volume V , deviation from the experimental values and cohesive energy, E_{coh} of Bi₂Se₂Te obtained using different exchange–correlation functionals.

$a(\text{\AA})$	$\Delta a(\text{\AA})$	$c(\text{\AA})$	$\Delta c(\text{\AA})$	$V(\text{\AA}^3)$	E_{coh} (eV/atom)	Functional	Pseudo- potential	Ref.
4.183	0.001	29.137	0.003	441.5	-	-	-	[29]
4.190	0.007	29.094	0.043	442.5	-4.40	GGA-PBEsol	Ultrasoft	This work
4.218	0.035	30.932	1.794	476.5	-4.08	GGA-PBE	Ultrasoft	This work

4.231	0.048	28.955	0.182	448.9	-4.46	GGA-PBEsol	OTFG Ultrasoft	This work
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Table 1 shows that the results obtained using the ultrasoft pseudopotential within the GGA-PBEsol scheme are in very good agreement with the experimental values [29]. Therefore, the GGA-PBEsol functional is considered reliable and was employed for all subsequent calculations. To assess the thermodynamic stability of $\text{Bi}_2\text{Se}_2\text{Te}$, the cohesive energy E_{coh} was calculated using the following formula [28]:

$$E_{\text{coh}}(\text{Bi}_2\text{Se}_2\text{Te})_{\text{fu}} = \frac{E_{\text{tot}}(\text{Bi}_2\text{Se}_2\text{Te})_{\text{fu}} - 2E_{\text{s}}(\text{Bi}) - 2E_{\text{s}}(\text{Se}) - E_{\text{s}}(\text{Te})}{5} \quad (1)$$

where $E_{\text{tot}}(\text{Bi}_2\text{Se}_2\text{Te})_{\text{fu}}$ represents the total energy of $\text{Bi}_2\text{Se}_2\text{Te}$ per formula unit, while $E_{\text{s}}(\text{Bi})$, $E_{\text{s}}(\text{Se})$ and $E_{\text{s}}(\text{Te})$ denote the total energies of isolated Bi, Se and Te atoms, respectively. The negative value of the cohesive energy confirms the thermodynamic stability of $\text{Bi}_2\text{Se}_2\text{Te}$.

3.2. Elastic properties, anisotropy, and mechanical behavior

$\text{Bi}_2\text{Se}_2\text{Te}$ crystallizes in a trigonal structure characterized by six independent elastic constants: C_{11} , C_{12} , C_{13} , C_{14} , C_{33} , and C_{44} . These parameters provide fundamental insight into the crystal's mechanical response under applied stress and its resilience to external perturbations. The calculated values are presented in Table 2, alongside those of $\text{Bi}_2\text{Te}_2\text{Se}$ and Bi_2Te_3 for direct comparison.

Table 2: Calculated elastic constants, C_{ij} (GPa) of $\text{Bi}_2\text{Se}_2\text{Te}$, $\text{Bi}_2\text{Te}_2\text{Se}$ and Bi_2Te_3 .

Compound	C_{11}	C_{33}	C_{44}	C_{12}	C_{13}	C_{14}	Ref.
$\text{Bi}_2\text{Se}_2\text{Te}$	90.1	65.3	41.0	24.1	33.8	-21.2	This work
$\text{Bi}_2\text{Te}_2\text{Se}$	74.2	23.7	24.9	16.2	17.2	-10.1	[30]
Bi_2Te_3	88.3	53.3	37.7	18.2	29.3	-23.8	[31]

$\text{Bi}_2\text{Se}_2\text{Te}$ exhibits substantially larger axial constants than $\text{Bi}_2\text{Te}_2\text{Se}$, particularly C_{33} , indicating stronger bonding and reduced compressibility along the c-axis. Similarly, the shear constant C_{44} is nearly twice as large, reflecting enhanced resistance to shear deformation. The substitution of Te by the smaller, more electronegative Se atom shortens bond lengths and strengthens covalent interactions, thereby increasing rigidity. Mechanical stability of both compounds was verified using the Born-Huang criteria, confirming their stability.

Polycrystalline elastic moduli, evaluated using Voigt-Reuss-Hill averaging [(32–34)] (Table 3), further highlight the differences. As shown in Table 3, $\text{Bi}_2\text{Se}_2\text{Te}$ exhibits a comparatively stronger and stiffer elastic response than $\text{Bi}_2\text{Te}_2\text{Se}$, as reflected by its higher bulk, shear, and Young's moduli. Bi_2Te_3 displays an intermediate bulk response, while its shear and Young's moduli are comparable to those of $\text{Bi}_2\text{Se}_2\text{Te}$. The differences in the B/G and Poisson's ratio values further indicate distinct elastic deformation characteristics among the three compounds. Overall, the tabulated results demonstrate appreciable variations in mechanical stiffness and elastic response within these bismuth-based chalcogenides. The smaller discrepancy between Voigt and Reuss bounds for $\text{Bi}_2\text{Se}_2\text{Te}$ suggests a more homogeneous elastic response.

*These indices were not explicitly reported in the cited works but derived from available elastic constants and moduli following Voigt-Reuss-Hill averaging schemes ([32-34]).

It is evident that $\text{Bi}_2\text{Se}_2\text{Te}$ combines moderate anisotropy with practical machinability and balanced hardness, making it a promising candidate for applications requiring both mechanical stability and ease of processing. In contrast, $\text{Bi}_2\text{Te}_2\text{Se}$, with its pronounced directional stiffness, may be less favorable for machining despite its higher hardness, while Bi_2Te_3 , though softer and more easily deformed, lacks the mechanical robustness of the other two compounds. Such distinctions underscore the importance of anisotropy indices in guiding the selection of materials for thermoelectric and related functional applications.

3.3. Dynamical stability

Understanding phonon dispersion is essential for evaluating a material's dynamic stability, detecting possible phase transitions, and elucidating how vibrational properties govern key thermal behaviors such as thermal conductivity, expansion, and heat capacity [37]. The phonon dispersion curves (PDC) and phonon density of states (PDOS) of $\text{Bi}_2\text{Se}_2\text{Te}$, calculated using the CASTEP code, are presented in Fig. 2 along the high-symmetry paths of the Brillouin zone. At 0 K, a material is regarded as dynamically stable when its phonon spectrum exhibits no soft modes along the high-symmetry directions of the Brillouin zone. Conversely, the occurrence of soft modes or imaginary (negative) frequencies signifies lattice instability and may initiate a structural phase transition through atomic displacements or distortions [38].

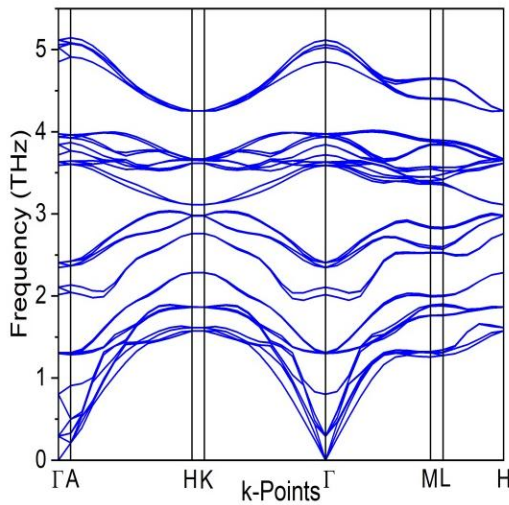


Fig. 2. Phonon dispersion curves confirming lattice stability.

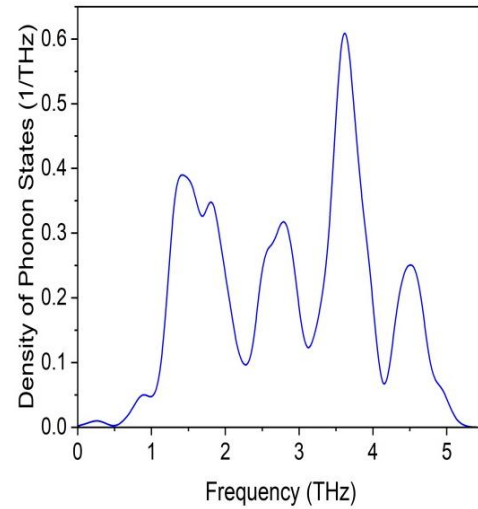


Fig. 3. Phonon density of states illustrating vibrational contributions up to 5 THz.

The PDC of $\text{Bi}_2\text{Se}_2\text{Te}$ (Fig. 3) reveals that all phonon branches remain positive throughout the Brillouin zone, with acoustic branches smoothly approaching zero frequency at the Γ -point. The PDOS spans from 0 to ~ 5.2 THz, displaying pronounced peaks near ~ 3.5 THz arising from optical phonon modes. The absence of negative frequencies in both dispersion and density of states confirms the robustness of the lattice against distortions.

Comparative analysis across the tetradymite family highlights subtle distinctions. $\text{Bi}_2\text{Te}_2\text{Se}$ exhibits similar dynamical resilience, though with moderately softened optical branches relative to $\text{Bi}_2\text{Se}_2\text{Te}$. Bi_2Te_3 , enriched in Te content, shows slightly softer optical modes, reflecting weaker bonding strength. Importantly, while spin-orbit coupling (SOC) is primarily electronic in origin, its

indirect influence on vibrational spectra emerges through modified orbital hybridization and bonding. In $\text{Bi}_2\text{Se}_2\text{Te}$, SOC enhances phonon stability by reinforcing Bi–Se/Te orbital coherence, yielding a more balanced vibrational spectrum compared to Bi_2Te_3 .

This comparative SOC-driven perspective underscores $\text{Bi}_2\text{Se}_2\text{Te}$ as the most favorable system, combining strong dynamical stability with electronic tunability. The tetradymite family as a whole demonstrates resilience suitable for device applications, but $\text{Bi}_2\text{Se}_2\text{Te}$ offers the optimal interplay of vibrational robustness and SOC-mediated electronic flexibility.

3.4. Thermo-physical properties

The thermo-physical characteristics of $\text{Bi}_2\text{Se}_2\text{Te}$ were evaluated through its Debye temperature, melting temperature, and minimum thermal conductivity, parameters that are intimately linked to lattice stiffness, bonding strength, and heat transport.

The Debye temperature (θ_D) was estimated using the elastic constants and the mean sound velocity (v_m) [39]:

$$\theta_D = \frac{h}{k_B} \left(\frac{3n}{4\pi N_A \rho M} \right)^{1/3} v_m \quad (2)$$

where h is Planck's constant, k_B the Boltzmann constant, N_A Avogadro's number, ρ the mass density, M the molecular mass, and n the number of atoms per formula unit. The mean sound velocity was obtained with longitudinal (v_l) and transverse (v_t) sound velocities derived from the bulk and shear moduli.

The melting temperature (T_m) was estimated empirically from the elastic constants [40]:

$$T_m = 354 + 1.5(2C_{11} + C_{33}) \quad (3)$$

while the minimum thermal conductivity (κ_{min}) was determined from [41]:

$$\kappa_{min} = k_B v_m \left(\frac{n N_A \rho}{M} \right)^{2/3} \quad (4)$$

The calculated Debye temperature (θ_D), melting temperature (T_m), and minimum thermal conductivity (κ_{min}) of $\text{Bi}_2\text{Se}_2\text{Te}$ are listed in Table 6. $\text{Bi}_2\text{Se}_2\text{Te}$ exhibits a Debye temperature of 201.6 K, significantly higher than $\text{Bi}_2\text{Te}_2\text{Se}$ (168.4 K) and Bi_2Te_3 (~165 K). This indicates stronger interatomic bonding and enhanced lattice stiffness. Its melting temperature (722.4 K) lies above $\text{Bi}_2\text{Te}_2\text{Se}$ (612.1 K) but below Bi_2Te_3 (853 K), suggesting intermediate thermal stability- superior to $\text{Bi}_2\text{Te}_2\text{Se}$ yet not as robust as Bi_2Te_3 .

Table 6: Calculated mass density (ρ in gm cm^{-3}), longitudinal, transverse and average sound velocities (v_l , v_t , and v_m , all in km s^{-1}) Debye temperature (θ_D in K), melting temperature (T_m in K) and minimum thermal conductivity (κ_{min} in $\text{W m}^{-1} \text{K}^{-1}$) of $\text{Bi}_2\text{Se}_2\text{Te}$. The available values $\text{Bi}_2\text{Te}_2\text{Se}$ and Bi_2Te_3 are taken from literature [30,42] for comparison.

Compound	ρ	v_l	v_t	v_m	θ_D	T_m	κ_{min}	Ref.
$\text{Bi}_2\text{Se}_2\text{Te}$	7.919	3.28	1.88	2.09	201.6	722.4	0.302	This work
$\text{Bi}_2\text{Te}_2\text{Se}$	7.39	2.694	1.667	1.832	168.4	612.1	0.2415	[30]
Bi_2Te_3	7.74	-	-	-	~165	853	~0.24	[42]

In terms of heat transport, $\text{Bi}_2\text{Se}_2\text{Te}$ shows a minimum thermal conductivity of $0.302 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$, slightly higher than $\text{Bi}_2\text{Te}_2\text{Se}$ ($0.2415 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$) and Bi_2Te_3 ($\sim 0.24 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$). Despite this modest increase, all three compounds exhibit very low values, confirming poor lattice heat

conduction. Such suppression of thermal transport is highly beneficial for thermoelectric and thermal-insulation applications.

Taken together, $\text{Bi}_2\text{Se}_2\text{Te}$ combines stronger bonding and higher lattice stiffness than $\text{Bi}_2\text{Te}_2\text{Se}$, intermediate melting stability between $\text{Bi}_2\text{Te}_2\text{Se}$ and Bi_2Te_3 , and comparably low thermal conductivity across the family. These attributes underscore its promise as a structurally stable and thermally efficient candidate for next-generation energy-conversion technologies.

3.5. Electronic band structure and density of states

A comprehensive understanding of the electronic band structure and density of states (DOS) is essential for evaluating the suitability of layered Bi-chalcogenides in optoelectronic and thermoelectric applications. In this work, the electronic properties of $\text{Bi}_2\text{Se}_2\text{Te}$ were calculated using the WIEN2k package with GGA-PBE and Tran-Blaha modified Becke-Johnson (TB-mBJ) potential approximation [22] involving spin orbital coupling (SOC) and without SOC. The inclusion of SOC is crucial, as it strongly influences band-gap values, band dispersion, and effective masses, thereby shaping the fundamental electronic behavior of these compounds. The band-gap values calculated from the band structure are tabulated in Table 8.

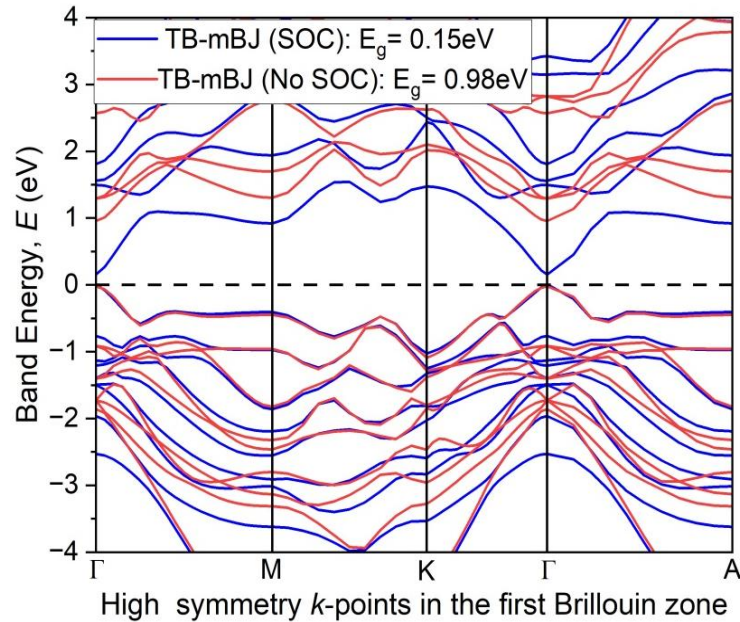


Fig. 4. Electronic band structure of $\text{Bi}_2\text{Se}_2\text{Te}$ compound using TB-mBJ approach with SOC and without SOC

However, it is noted that the TB-mBJ potential is designed to improve electronic-structure calculations, particularly the accuracy of band-gap predictions. So, despite performing band structure calculations using both the GGA-PBE and TB-mBJ approaches, we have plotted only the results obtained using the TB-mBJ potential to achieve a more accurate description. It is well recognized for its improved prediction of semiconductor band gaps compared to the systematic underestimation typical of GGA-based functionals. The electronic band structure of $\text{Bi}_2\text{Se}_2\text{Te}$ using TB-mBJ approach with SOC and without SOC along high symmetry directions is presented in Fig. 4.

As shown in Fig. 4, the TB-mBJ functional yields a direct band gap of 0.98 eV in the absence of SOC, which narrows significantly to 0.15 eV when SOC is incorporated, corresponding to a ~84% reduction. This pronounced narrowing reflects the strong relativistic influence of Bi and Te atoms and is accompanied by band splitting along high-symmetry directions.

Carrier mobility is strongly influenced by the effective mass, which is directly related to the curvature of the electronic bands near the conduction-band minimum (CBM) and valence-band maximum (VBM) [43]. Effective masses were calculated using a second-order finite-difference approach applying a parabolic fit to the energy dispersion $E(k)$ near the Γ point using the conventional formula [44].

$$m^* = \hbar^2 \left(\frac{d^2 E}{dk^2} \right)^{-1} \quad (5)$$

where m^* , $\hbar$, E and k are the effective mass, reduced Planck constant, energy and the wave vector respectively. This calculation was conducted using WIEN2k code with TB-mBJ potential taking SOC in account.

Table 7 shows that the calculated electron and hole effective masses of $0.104 m_0$ and $0.117 m_0$, respectively, confirm the high carrier mobility in $\text{Bi}_2\text{Se}_2\text{Te}$, with electrons being slightly more mobile than holes. This behavior arises from the SOC-induced dispersion, which lifts the degeneracy of electronic states, modifies the band curvature near the Fermi level, and thereby reduces the electron effective mass relative to the hole effective mass.

Table 7: Calculated electron (m_e^*) and hole (m_h^*) effective masses of $\text{Bi}_2\text{Se}_2\text{Te}$ compared with related Bi-chalcogenides.

Compound	$m_e^* (m_0)$	$m_h^* (m_0)$	References
$\text{Bi}_2\text{Se}_2\text{Te}$	0.104	0.117	This work
Bi_2Se_3	0.124	-	[44]
Bi_2Te_3	0.06	-	[45]

The direct band-gap nature of $\text{Bi}_2\text{Se}_2\text{Te}$ is confirmed, with both CBM and VBM located at the Γ point. A comparison of the calculated band-gap values in Table 8 reveals that $\text{Bi}_2\text{Se}_2\text{Te}$ exhibits intermediate band-gap values between $\text{Bi}_2\text{Te}_2\text{Se}$ and Bi_2Te_3 , reflecting its balanced electronic character. Specifically, $\text{Bi}_2\text{Te}_2\text{Se}$ shows a GGA-PBE band gap of 0.61 eV, while Bi_2Te_3 exhibits much smaller gaps (0.23 eV without SOC and 0.15 eV with SOC), consistent with its well-known narrow-gap semiconducting nature.

Table 8: Comparison of calculated electronic band gaps of $\text{Bi}_2\text{Se}_2\text{Te}$, $\text{Bi}_2\text{Te}_2\text{Se}$, and Bi_2Te_3 with and without SOC, using different exchange-correlation functionals.

Compound	Code used	Approach	Present work		Other works	
			Band gap (eV)		Band gap (eV)	
			Without SOC	With SOC	Without SOC	With SOC
$\text{Bi}_2\text{Se}_2\text{Te}$	WIEN2k	GGA-PBE	0.483	0.393	0.702 [46]	
					0.52 [47]	0.22 [47]
$\text{Bi}_2\text{Se}_2\text{Te}$	WIEN2k	TB-mBJ	0.98	0.15	0.782 [46]	-
$\text{Bi}_2\text{Te}_2\text{Se}$	CASTEP	GGA-PBE	-	-	0.61 [30]	-
Bi_2Te_3	WIEN2k	LDA	-	-	0.23 [48]	0.15 [48]

These results indicate that the electronic structure of $\text{Bi}_2\text{Se}_2\text{Te}$ cannot be accurately described without considering SOC effects. Although SOC substantially alters the band dispersion and narrows the band gap, the observed changes alone do not constitute direct evidence of a topological phase transition. Confirmation of the topological nature would require further orbital-projected band structure analysis to identify possible band inversion. Nevertheless, the combination of a direct band gap,

favorable effective masses, and SOC-driven tunability underscores $\text{Bi}_2\text{Se}_2\text{Te}$'s potential as a multifunctional candidate for optoelectronic and thermoelectric applications.

When viewed alongside related Bi-chalcogenides, $\text{Bi}_2\text{Se}_2\text{Te}$ occupies an intermediate position that balances band-gap magnitude with carrier mobility. $\text{Bi}_2\text{Te}_2\text{Se}$, with a GGA-PBE band gap of 0.61 eV, exhibits a wider gap but suffers from stronger anisotropy and reduced mechanical resilience. Bi_2Te_3 , in contrast, is characterized by its narrow band gap (0.23 eV without SOC, 0.15 eV with SOC) and very light electron effective mass ($\approx 0.06 m_0$), making it highly conductive but less stable for multifunctional applications. $\text{Bi}_2\text{Se}_2\text{Te}$, with its SOC-tuned direct band gap 0.15 eV, favorable effective masses, and balanced dispersion, thus emerges as a compound that unites electronic tunability with mechanical and optical adaptability. This comparative positioning underscores its promise as a versatile candidate for next-generation optoelectronic and thermoelectric technologies.

The calculated total density of states (TDOS) and partial density of states (PDOS) of $\text{Bi}_2\text{Se}_2\text{Te}$, including the effects of SOC and without SOC effects, are presented in Fig. 5 over the energy range from -4.5 eV to 4.5 eV. In the valence-band region, the states at lower energies are primarily composed of Bi-6*p*, Se-4*p*, and Te-5*p* orbitals, with the Se-4*p* states providing the dominant contribution. Near the Fermi level, a small contribution from Bi-6*s* states is also observed.

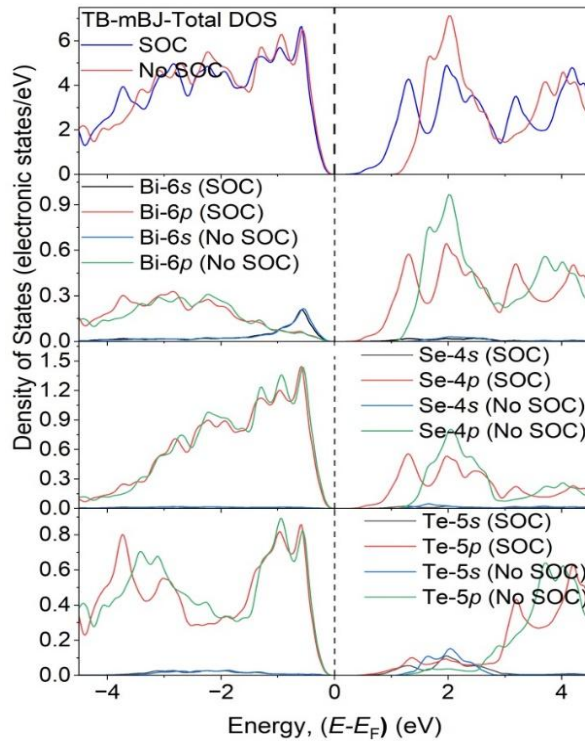


Fig. 5. TDOS and PDOS of $\text{Bi}_2\text{Se}_2\text{Te}$ with and without SOC. The vertical line shows the position of the Fermi level.

In the conduction-band region, extending up to approximately 2 eV, the electronic states are mainly derived from Bi-6*p* and Se-4*p* orbitals, while the contribution from Te-5*s* states is relatively minor. Among these, the Bi-6*p* states constitute the dominant contribution. At higher energies, above 2 eV, the conduction band is primarily formed by Bi-6*p*, Te-5*p*, and Se-4*p* states. In this energy range, the contributions from Bi-6*p* and Te-5*p* orbitals are nearly equal, whereas the contribution from Se-4*p* states is comparatively small.

The strong hybridization among Bi-6*p*, Se-4*p*, and Te-5*p* orbitals near the band edges indicates that these states play a crucial role in determining the electronic properties of $\text{Bi}_2\text{Se}_2\text{Te}$.

Building upon the electronic insights, it is essential to investigate the optical properties of Bi-chalcogenides, since their SOC-driven band dispersion, effective masses, and direct band-gap nature

directly govern photon absorption, reflectivity, and overall suitability for optoelectronic and energy-conversion applications.

3.6. Optical Properties

The interaction of tetradymite compounds with electromagnetic radiation is fundamentally governed by their electronic and optical characteristics, which dictate absorption, reflection, and energy dissipation processes. These parameters are indispensable for evaluating band structures, excitonic behavior, impurity states, and defect-related transitions, thereby informing potential optoelectronic applications across the visible, ultraviolet, and infrared regimes [43,44,46,49,50]. Recent studies have further highlighted the role of heterojunction architectures in enhancing photocurrent response, particularly in $\text{Bi}_2\text{Se}_3/\text{Bi}_2\text{Te}_2\text{Se}$ systems, underscoring the technological relevance of these materials in optoelectronic device design [51].

In what follows, we first present our calculated results for the optical response of $\text{Bi}_2\text{Se}_2\text{Te}$ in subsection 3.6.1. Subsequently, in subsection 3.6.2, we provide a comparative analysis using published data for $\text{Bi}_2\text{Te}_2\text{Se}$ and Bi_2Te_3 [30,51], thereby situating our findings within the broader tetradymite family. This comparative framework draws upon both spin-orbit coupling (SOC) and non-SOC datasets, including polarization-dependent optical responses along the [100] and [001] directions [30].

3.6.1. Optical response of $\text{Bi}_2\text{Se}_2\text{Te}$

Optical properties provide a direct probe of how a material responds to incident electromagnetic waves. They reveal information about the electronic band structure, excitons, impurity levels, and localized defect states, while also guiding the identification of suitable spectral ranges for device applications. The response is quantified through frequency-dependent optical constants, including the absorption coefficient $\alpha(\omega)$, reflectivity $R(\omega)$, energy-loss function $L(\omega) = \text{Im}[-1/\epsilon(\omega)]$, optical conductivity $\sigma(\omega)$, refractive index $n(\omega)$, extinction coefficient $k(\omega)$, and the real and imaginary parts of the dielectric function $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$.

Since spin-orbit coupling (SOC) exerts a pronounced influence on these parameters, we calculated the optical properties of $\text{Bi}_2\text{Se}_2\text{Te}$ with SOC included, employing the WIEN2k code. The resulting spectra - covering incident energies up to 14 eV along the [100] and [001] directions- are presented in Fig. 7(a–h), highlighting both anisotropy and SOC-induced modifications across the optical constants.

It is instructive to note that such SOC-driven variations, together with directional anisotropy, are not unique to $\text{Bi}_2\text{Se}_2\text{Te}$ but recur across the tetradymite family. In order to place our findings in context, we next turn to $\text{Bi}_2\text{Te}_2\text{Se}$ and Bi_2Te_3 , compounds for which both SOC and non-SOC datasets are available. Their comparative optical responses- particularly in terms of absorption edges, dielectric dispersion, and conductivity spectra- provide a valuable benchmark against which the distinct features of $\text{Bi}_2\text{Se}_2\text{Te}$ can be assessed. This comparative analysis is presented in subsection 3.6.2.

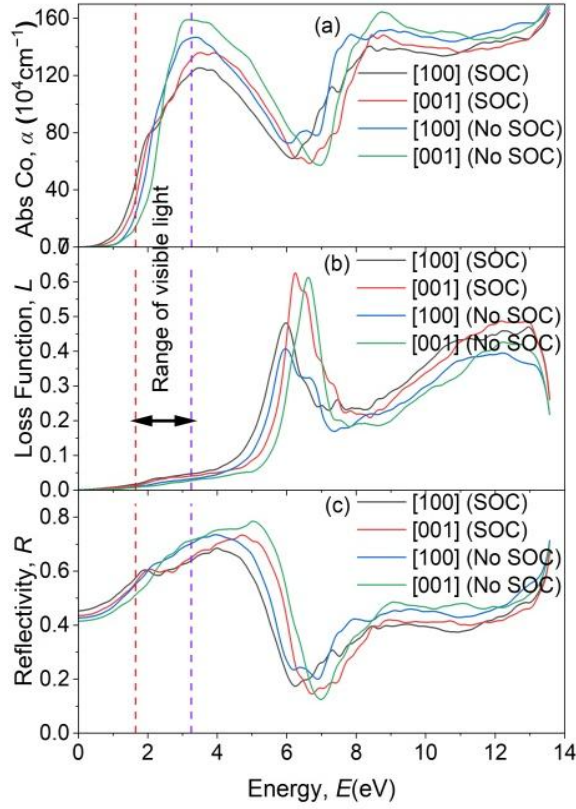


Fig. 7 (a–c). Absorption coefficient, loss function, and reflectivity of Bi₂Se₂Te with and without SOC along [100] and [001].

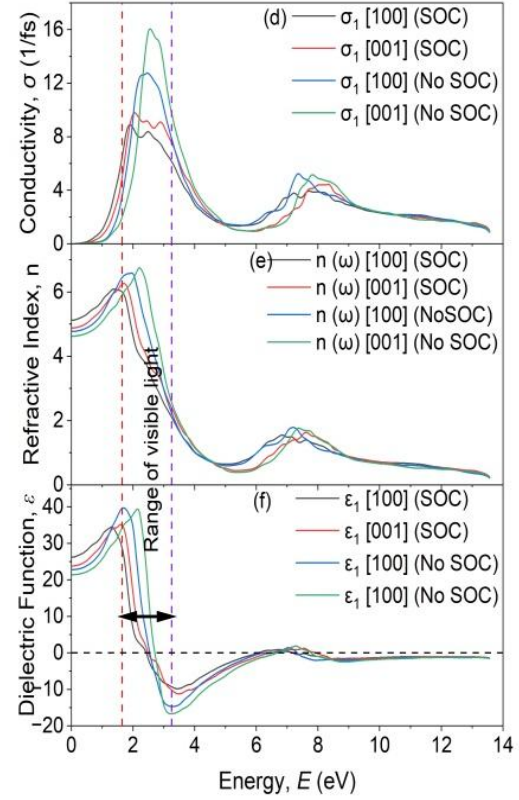


Fig. 7(d–f). Optical conductivity, refractive index, and dielectric function (ϵ_1) showing SOC-induced anisotropy.

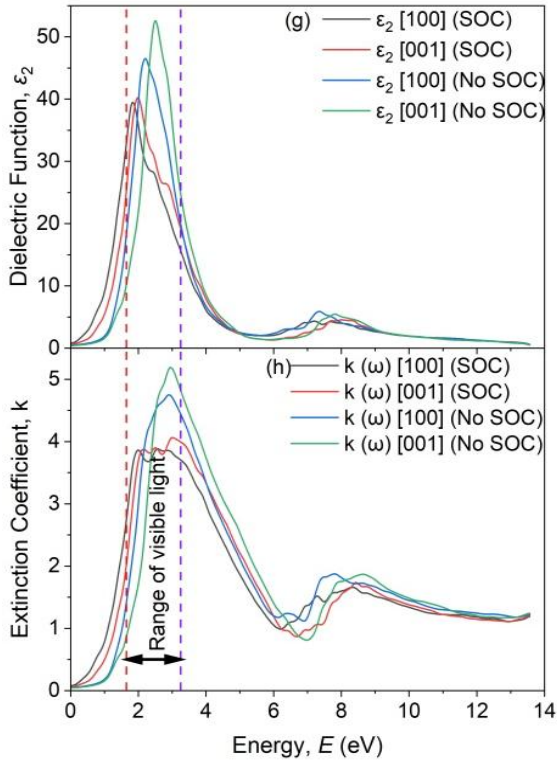


Fig. 7 (g–h). Dielectric function (ϵ_2) and Extinction coefficient highlighting SOC effects in the visible range.

The absorption coefficient, $\alpha(\omega)$, describes the extent to which incident light of a given energy is absorbed as it propagates through a material. Fig. 7(a) presents the calculated absorption spectra of $\text{Bi}_2\text{Se}_2\text{Te}$ with and without SOC along the [100] and [001] crystallographic directions. The onset of absorption occurs at slightly lower photon energies when SOC is included, indicating a small SOC-induced reduction of the band gap. For both crystallographic directions, the overall spectral shape remains similar with and without SOC. However, SOC causes a slight red-shift of the major absorption peaks and modifies their intensities. The [001] direction exhibits somewhat higher absorption than the [100] direction in the (2–6 eV) energy range, indicating optical anisotropy. The maximum absorption coefficient reaches approximately $(1.6 \times 10^6 \text{ cm}^{-1})$, demonstrating excellent light-harvesting capability in the visible and ultraviolet regions. Overall, the high absorption coefficient over a broad energy range demonstrates strong light–matter interaction and highlights the potential of $\text{Bi}_2\text{Se}_2\text{Te}$ for optoelectronic and photovoltaic applications.

Fig. 7(b) shows the energy loss function, $L(\omega)$, of $\text{Bi}_2\text{Se}_2\text{Te}$ along the [100] and [001] polarization directions. The dominant loss peaks appear around 5.5–7.0 eV for all cases. Inclusion of SOC slightly shifts the principal loss peaks toward lower energies and alters their amplitudes. In particular, the maximum loss peak for the [001] direction decreases and broadens in the presence of SOC, while the [100] direction exhibits a moderate reduction in peak intensity. These variations indicate that SOC modifies the collective electronic excitations and plasmon-related behavior of the material.

Fig. 7(c) presents the reflectivity spectrum, $R(\omega)$, of $\text{Bi}_2\text{Se}_2\text{Te}$ along the [100] and [001] polarization directions. At low photon energies, the reflectivity ranges from approximately 0.42 to 0.45 and increases gradually before reaching a maximum near 4.5–5.5 eV. Beyond this energy, a pronounced minimum appears around 6–7 eV, corresponding closely to the strong peaks observed in the energy-loss spectra. Inclusion of SOC generally reduces the reflectivity in this energy region and shifts the reflectivity minima slightly toward lower energies. The differences between the [100] and [001] spectra further confirm the anisotropic optical response of the material.

Therefore, the optical response of the system as regards optical conductivity, refractive index, and dielectric function exhibits pronounced anisotropy, with clear distinctions between the [100] and [001] crystallographic directions as well as between the spin-orbit coupled (SOC) and non-SOC cases.

Fig. 7(d) shows the real part of the optical conductivity, $\sigma(\omega)$, of $\text{Bi}_2\text{Se}_2\text{Te}$ along the [100] and [001] polarization directions. The optical conductivity shows a strong peak in the visible range. Without SOC, the [100] direction reaches a maximum conductivity of ~ 0.045 (1/fs) near 1.8–2.0 eV, while the [001] direction remains slightly lower. Upon inclusion of SOC, the peak red-shifts to ~ 1.6 –1.8 eV and the magnitude increases to ~ 0.052 (1/fs) along [100], with a corresponding enhancement along [001]. This indicates that SOC strengthens carrier excitation and enhances absorption in the visible regime.

In Fig. 7(e), the refractive index $n(\omega)$ attains its highest values in the low-energy region. For the non-SOC case, maxima of ~ 6.8 ([100]) and ~ 6.5 ([001]) are observed around 1–2 eV. With SOC, the maxima are reduced to ~ 6.2 and ~ 6.0 , respectively, while maintaining directional anisotropy. The reduction in n reflects the SOC-induced modification of electronic band dispersion, which lowers the effective optical response.

In Fig. 7(f), the real part of the dielectric function $\epsilon_1(\omega)$ exhibits strong positive peaks near ~ 2 eV, with values of ~ 42 ([100]) and ~ 39 ([001]) in the absence of SOC. With SOC, these peaks decrease to ~ 38 and ~ 35 , respectively, and the zero-crossing shifts slightly toward lower energies (~ 11 eV). The diminished ϵ_1 magnitude and altered zero-crossing highlight the reduced polarization strength and modified screening effects arising from SOC.

The imaginary part of the dielectric function, $\epsilon_2(\omega)$, shown in Fig. 7(g), highlights the SOC-induced modifications in interband transitions. In the non-SOC case, ϵ_2 exhibits pronounced maxima in the visible range, reaching ~ 52 for the [100] orientation and ~ 48 for the [001] orientation near 2.0–2.2 eV. With SOC, these peaks undergo a slight red-shift (~ 1.8 –2.0 eV) and are reduced in magnitude to ~ 45 ([100]) and ~ 42 ([001]). This attenuation reflects the SOC-driven redistribution of optical transition strength, consistent with the modified joint density of states at critical points.

In Fig. 7(h), the extinction coefficient $k(\omega)$ further highlights the SOC effect on absorption. Without SOC, k reaches ~ 3.5 ([100]) and ~ 3.2 ([001]) in the visible region. With SOC, the maxima rise

to ~ 4.0 and ~ 3.6 , respectively, accompanied by a slight red-shift in peak positions. The elevated k values confirm that SOC enhances attenuation of electromagnetic waves within the material, thereby increasing absorption efficiency.

The anisotropic behavior of $k(\omega)$, together with its SOC dependence, confirms that the electromagnetic-wave attenuation in the material is strongly influenced by both crystallographic direction and spin-orbit interaction.

Taken together, ϵ_2 and k reveal that spin-orbit coupling (SOC) significantly amplifies absorption in the visible range while preserving anisotropy between the [100] and [001] directions. The [100] orientation consistently exhibits stronger responses, underscoring the directional dependence of the optical properties of $\text{Bi}_2\text{Se}_2\text{Te}$. These findings complement the results of Fig. 7(d–f), where SOC was shown to enhance optical conductivity while simultaneously reducing the refractive index and dielectric function maxima. Overall, the inclusion of SOC reshapes the photonic response of $\text{Bi}_2\text{Se}_2\text{Te}$ by strengthening absorption and conductivity in the visible region, lowering refractive and dielectric peaks, and maintaining persistent anisotropy across all parameters, with the [100] orientation emerging as the dominant axis of optical activity.

3.6.2 Comparative optical analysis

The comparative evaluation of the optical response of $\text{Bi}_2\text{Se}_2\text{Te}$ vis-à-vis its sister tetradymites, $\text{Bi}_2\text{Te}_2\text{Se}$ and Bi_2Te_3 [30,51] reveals how subtle compositional variations within this family orchestrate distinct modes of optoelectronic tunability. This analysis highlights both the decisive influence of spin-orbit coupling (SOC) and the pronounced anisotropy of optical constants along the [100] and [001] crystallographic axes, thereby underscoring the intricate interplay between composition, electronic structure, and directional optical behavior.

$\text{Bi}_2\text{Se}_2\text{Te}$ is distinguished by strong absorption across the visible and ultraviolet regimes, accompanied by pronounced spin-orbit coupling (SOC)-induced anisotropy. In contrast, $\text{Bi}_2\text{Te}_2\text{Se}$ and Bi_2Te_3 exhibit distinct optical signatures that reflect their electronic structures and the decisive role of SOC in shaping their responses.

For $\text{Bi}_2\text{Te}_2\text{Se}$, density functional theory (DFT) studies report a direct band gap of approximately 0.61 eV, coupled with strong ultraviolet absorption and relatively high refractive indices in the infrared-visible region. Reflectivity remains low in the ultraviolet, reinforcing its potential for optoelectronic applications. SOC exerts only a modest influence on bulk optical constants, though the surface states remain SOC-protected, thereby preserving their topological character. The frequency-dependent parameters of $\text{Bi}_2\text{Te}_2\text{Se}$, namely absorption coefficient, energy loss function, reflectivity, optical conductivity, refractive index, and dielectric constant, are illustrated in Fig. 8, highlighting the directional dependence of its optical response and reinforcing the comparative framework for evaluating tetradymite compounds.

In contrast, Bi_2Te_3 is distinguished by its ultrahigh refractive index and narrow band gap (~ 0.15 – 0.3 eV), as highlighted in recent reports [51]. Its absorption coefficients exceed 10^5 cm^{-1} , and thin films display pronounced optical anisotropy. Here, SOC plays a decisive role: without SOC, Bi_2Te_3 behaves as a conventional semiconductor, whereas inclusion of SOC transforms it into a topological insulator with modified band dispersion and enhanced optical transition probabilities.

We have seen in section 3.6.1 that for $\text{Bi}_2\text{Se}_2\text{Te}$, the calculated spectra reveal clear anisotropy between the [100] and [001] directions, particularly in the dielectric function and optical conductivity. This directional dependence suggests tunability in device architectures where polarization control is critical. $\text{Bi}_2\text{Te}_2\text{Se}$ [30] displays similar anisotropy, though less pronounced, consistent with its intermediate SOC effects. Bi_2Te_3 [51] is reported to show relatively isotropic behavior in the low-energy regime but develops stronger anisotropy at higher photon energies, reflecting its layered crystal structure and SOC-driven band inversion.

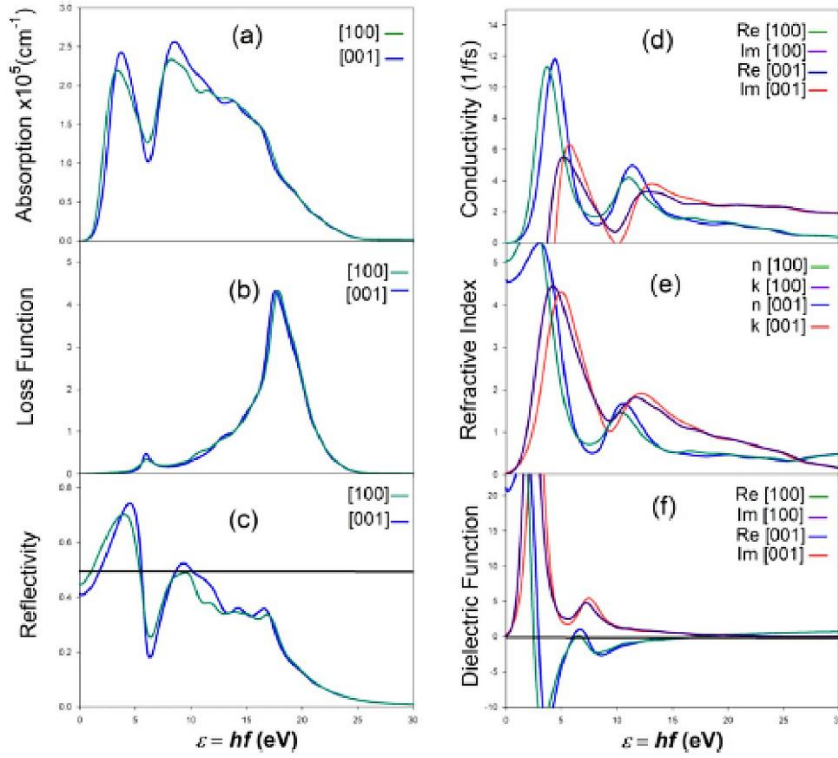


Fig. 8. Frequency-dependent optical parameters of $\text{Bi}_2\text{Te}_2\text{Se}$ [30] calculated using CASTEP: (a) absorption coefficient, (b) energy loss function, (c) reflectivity, (d) optical conductivity, (e) refractive index, and (f) dielectric constant, with electric-field polarization vectors oriented along the [100] and [001] crystallographic directions.

By comparison, $\text{Bi}_2\text{Se}_2\text{Te}$ bridges these behaviors. Its absorption onset shifts slightly under SOC, accompanied by red-shifts in peak intensities and enhanced conductivity maxima. The refractive index reaches values as high as ~ 7.0 with SOC, while dielectric constants and extinction coefficients also increase significantly. These SOC-induced modifications strengthen polarization response and optical anisotropy, positioning $\text{Bi}_2\text{Se}_2\text{Te}$ as an intermediate compound whose tunability arises directly from Se/Te substitution.

Taken together, the optical investigations of $\text{Bi}_2\text{Se}_2\text{Te}$, $\text{Bi}_2\text{Te}_2\text{Se}$, and Bi_2Te_3 illuminate the delicate interplay between composition, spin–orbit coupling, and crystallographic orientation in shaping the electromagnetic response of tetradymite compounds. Substitution of Se and Te systematically modulates absorption thresholds, dielectric dispersion, and conductivity spectra, thereby offering a rational pathway to tailor spectral selectivity for targeted applications. Within this comparative framework, $\text{Bi}_2\text{Se}_2\text{Te}$ emerges as a particularly compelling candidate: its SOC-driven anisotropy, red-shifted absorption features, and enhanced conductivity maxima position it as an intermediate yet distinctive compound whose tunability arises directly from Se/Te substitution. These findings reinforce the broader conclusion that tetradymite materials, through compositional engineering, constitute a versatile platform for advancing both fundamental optical science and applied photonic technologies, spanning domains from photodetection and energy harvesting to next-generation topological optoelectronics.

4. Conclusion

In this study, we have systematically explored the multifaceted physical properties of $\text{Bi}_2\text{Se}_2\text{Te}$ and related tetradymites, with particular emphasis on the role of spin-orbit coupling (SOC) in driving optoelectronic tunability. The combined analysis of structural stability, elastic anisotropy,

thermophysical behavior, and electronic-optical characteristics reveals that SOC not only governs the band topology but also modulates the broader physical response of these layered compounds.

Comparative evaluation with $\text{Bi}_2\text{Te}_2\text{Se}$ and Bi_2Te_3 underscores the delicate interplay between chemical composition, lattice dynamics, and relativistic effects, thereby establishing $\text{Bi}_2\text{Se}_2\text{Te}$ as a promising candidate for next-generation topological and optoelectronic applications. The observed tunability highlights the potential of compositional engineering within the tetradymite family to optimize performance across diverse functional domains.

Overall, this work advances the fundamental understanding of SOC-induced phenomena in tetradymites and provides a coherent framework for correlating structural, elastic, and optoelectronic properties. The insights gained here not only enrich the physics of layered topological materials but also pave the way for designing tailored compounds with enhanced stability and multifunctional capabilities for multifunctional applications in photovoltaic, thermoelectric, spintronic, optoelectronic, and quantum technologies.

Ethical approval

This is a pure computational study with zero health hazards, and it is approved by review committee board of Unisa.

CRedit authorship contribution statement

Islam A.K.M.A.: Conceptualization, Supervision, Methodology, Validation, Writing review & editing. **Parvin F:** Conceptualization, Supervision, Methodology, Validation, Project administration. Review & editing. **Hossain M A:** Methodology, Validation. **Rahman M M:** Methodology, Investigation, Writing original draft.

Declaration of Generative AI

We confirm that AI was not used to generate scientific ideas, design methodology, analyze data, interpret results, create or alter citations. Copilot was used to polish language in several sections of the manuscript. The authors reviewed and edited the content as required and take full responsibility for the content of the publication.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

The data supporting the findings of this study are available from the corresponding author upon reasonable request.

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