

**Research Article**

Harnessing the Potential of 2D Ti₃C₂ MXene: A First-Principles Study on Structural, Electronic, Optical, and Mechanical Properties

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Abstract

In this study, we employ first-principles density functional theory (DFT) calculations using the CASTEP framework to investigate the structural, electronic, mechanical, and optical properties of the two-dimensional (2D) Ti₃C₂ MXene material. The optimized structure reveals a hexagonal P6₃/mmc (194) symmetry, confirming its stability. As a promising 2D nanomaterial, MXene is widely explored for energy storage applications. Our computed lattice parameters at zero pressure show strong agreement with previous experimental and theoretical findings. The negative cohesive energy further validates the thermodynamic stability and experimental feasibility of Ti₃C₂ MXene. Electronic structure analysis, including band structure and density of states (DOS), confirms its metallic nature. The optical properties, particularly the reflectivity spectrum, reveal a maximum reflectivity at 0.49 eV, further supporting its metallic behavior. Additionally, mechanical property calculations suggest that Ti₃C₂ MXene exhibits ductile behavior depending on specific mechanical indicators. These findings provide valuable insights into the potential applications of Ti₃C₂ in electronic and optoelectronic devices.

Keywords: Ti₃C₂ MXene, DFT study, Titanium Carbide, 2- Dimensional, TDOS, PDOS

1. Introduction

Two-dimensional (2D) materials have attracted substantial research interest for their exceptional properties, including tunable band gaps, high surface area, and superior electrical conductivity [1]. These characteristics make them promising candidates for applications, such as sensors, electronics, energy storage, and catalysis. Additionally, their ability to integrate with other materials also provides a versatile platform for developing next-generation technologies. Since the discovery of graphene in 2004, interest in 2D materials has grown significantly because their reduced dimensionality imparts unique properties absent in their bulk counterparts [2]. This has opened new avenues for applications in electrochemical catalysis, electronic devices, and optoelectronic technologies [3].

Recent advances in synthesis techniques have enabled the successful fabrication of various 2D materials beyond graphene [4]. Among these, MXenes, a newly discovered family of early transition metal carbides and nitrides, have emerged as promising candidates due to their remarkable electronic and mechanical properties [5]. The general formula for MXene is M_{n+1}AX_n, where M represents a transition metal, A is an element from groups IIIA or IVA, X denotes either carbon (C) or nitrogen (N), and n takes values of 1, 2,

or 3 [6]. MXenes are derived from their parent MAX phases by selectively etching the A element, typically using chemical etching methods [7]. MAX phases possess a layered hexagonal structure, with alternating stacks of A layers and M_{n+1}X_n units observed [8]. Because M-X bonds are stronger than M-A bonds, the A layer can be selectively removed without disrupting the M-X connections. This yields weakly bonded M_{n+1}X_n layers that can be easily separated via sonication [9]. These exfoliated 2D materials are named MXenes for their structural and layered morphological similarity to graphene [10].

During etching, surface functional groups such as hydroxyl (-OH), oxygen (O), and fluorine (F) are typically introduced onto MXene layers, thereby influencing their surface chemistry and electronic properties [11]. The resulting formula is often expressed as M_{n+1}X_nT_x, where T_x denotes these functional groups. The presence and composition of these surface terminations depend on the synthesis conditions, which can be tailored for specific applications [12]. The excellent mechanical flexibility, layered structure, and high conductivity of MXenes make them ideal for hybrid material integration, enabling enhanced functionality [13]. Their exceptional electrical conductivity and electrochemical



activity have spurred extensive research in energy storage applications, particularly as electrode materials for lithium-sulfur batteries, sodium-ion batteries, and supercapacitors [14].

Among the various MXenes, Titanium Carbide (Ti_3C_2) has been the most extensively studied. Since its discovery, research on Ti_3C_2 has grown exponentially [15]. In 2012, only four research papers on MXenes were published, two of which focused on Ti_3C_2 . By 2020, the number had surged to 1313 publications on MXenes and 828 specifically on Ti_3C_2 , demonstrating its increasing significance in materials science [16]. The unique 2D morphology of Ti_3C_2 makes it an excellent host material for various applications [17]. Due to its optical properties in the visible and infrared spectra, it has potential use in transparent heat mirrors and solar energy absorbers. These properties, combined with its structural flexibility, make it suitable for diverse applications in optoelectronics and energy storage [18].

Ongoing research continues to explore the influence of film thickness and nano-structuring on the electrical and optical behavior of 2D materials, leading to the development of novel nano-based devices such as light emitters, luminescent diodes, and photovoltaic solar cells. Both theoretical and experimental studies have investigated Ti_3C_2 -based layers for various applications. Notably, Naguib et al. demonstrated a method to synthesize Ti_3C_2 by etching MAX phases with hydrofluoric acid [19]. Furthermore, density functional theory (DFT) calculations have provided insights into the structural, mechanical, and electronic properties of monolayer Ti_3C_2 , revealing graphene-like characteristics [20]. Additionally, Xie et al. employed first-principles calculations to investigate the relationship between surface composition and lithium-ion storage capacity in MXene [21]. Given the promising features of Ti_3C_2 MXene, this study aims to conduct a first-principles investigation into its structural, electronic, mechanical, and optical properties. Through density functional theory (DFT) calculations, we explore its stability, electronic structure, and potential for technological applications.

2. Computational methodology

The CASTEP simulation was utilized to compute the electronic properties, band structure, optical properties, and elastic properties of Ti_3C_2 MXene [22]. The calculations were performed using Density Functional Theory (DFT) within the generalized gradient approximation (GGA) approach. Vanderbilt-type ultrasoft pseudopotentials were used to demonstrate ion-electron interactions. For Ti and C, the valence-electron configurations were $3s^23p^6 3d^24s^2$ and $2s^22p^2$, respectively. The CASTEP module was applied as an efficient and reliable method to determine the minimum-energy crystalline structure of the material. The Brillouin Zone (BZ) k-point sampling was carried out using an $8 \times 8 \times 1$ Monkhorst-Pack grid, ensuring accurate convergence in electronic structure calculations. The kinetic energy cutoff and BZ sampling were tested for convergence, confirming the reliability of these parameters. The geometry optimization was performed using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) minimization approach, which allowed the structure to attain a stable and well-relaxed configuration [23]. The

plane-wave expansion was set to a 600 eV cutoff energy to ensure computational accuracy. The energy resistance criterion for optimization was maintained at 5×10^{-6} eV/atom, while the convergence thresholds were set as follows: energy tolerance of 2×10^{-5} eV/atom, maximum force of 5×10^{-2} eV/Å, maximum stress of 0.1 GPa, and maximum atomic displacement of 2×10^{-3} Å. These computational parameters ensured self-consistent field (SCF) convergence, stabilizing the internal forces and optimizing the overall crystal structure [24].

3. Results and discussion

3.1. Structural properties

In recent years, Ti_3C_2 MXene has gained significant attention in both computational and experimental research due to its promising structural and electronic properties. The unit cell of Ti_3C_2 consists of ten atoms and crystallizes in a hexagonal structure belonging to the P63/mmc (194) space group [25]. To determine the optimized structural parameters, we performed geometry optimization by minimizing the total energy of the crystal using the Murnaghan equation of state. This approach ensures that the structure achieves its most stable configuration with minimal lattice energy. The computed lattice parameters for hexagonal Ti_3C_2 are $a = b = 3.07$ Å and $c = 15.13$ Å, which agree well with previously reported computational and experimental values. These numbers are consistent with the previously reported theoretical values $a = b = 3.101$ Å, 3.110 Å, and 3.048 Å; the corresponding c values are 15.39 Å, 15.346 Å, and 15.006 Å, respectively. The difference in the results may be due to different studies using different calculation methods and parameters. The optimized crystal structure of Ti_3C_2 is presented in figure 1, while the calculated lattice parameters are summarized in Table 1. To further assess the structural stability of Ti_3C_2 MXene, we evaluated its cohesive energy, which quantifies the binding strength of atoms within the crystal. The cohesive energy of Ti_3C_2 was calculated using the equation (1) [26]:

$$E_{coh} = \frac{E_{total} - \sum E_{atomic}}{N} \quad (1)$$

Where E_{total} is the total energy of the system, E_{atomic} is the energy of individual atoms, and N is the number of atoms in the unit cell. The computed cohesive energy is -15.3 eV/atom; this negative value confirms the thermodynamic stability of Ti_3C_2 and reinforces its feasibility for experimental synthesis. The calculated structural parameters and stability metrics strongly support the reliability of our DFT-based approach and further validate the structural robustness of Ti_3C_2 MXene for potential applications in electronic and energy storage devices.

3.2. Electronic properties

The electronic properties of a material are fundamental in determining its potential for energy-related applications. To accurately assess a material's efficiency in these fields, a comprehensive analysis of its energy band gap, total density of states (TDOS), and partial density of states (PDOS) is

essential. These parameters provide valuable insights into the electronic band structure, charge carrier dynamics, and optical absorption characteristics, which significantly impact its performance in solar energy conversion and optoelectronic

devices. To investigate the electronic properties of hexagonal Ti_3C_2 MXene, we performed electronic band structure (EBS), total density of states (TDOS), and partial density of states (PDOS) calculations.

Table 1. Calculated lattice constants and unit-cell volumes of Ti_3C_2 .

Compound	Lattice constants ($\text{\AA}$)	Volume ($\text{\AA}^3$)
Ti_3C_2 (Present work)	$a=b = 3.07, c = 15.13$	152.54
Ti_3C_2 (Previous study) [27]	$a=b = 3.101, c = 15.39$	148.741
Ti_3C_2 (Previous study) [28]	$a=b = 3.110, c=15.346$	128.5723
Ti_3C_2 (Previous study) [29]	$a=b = 3.048, c=15.006$	139.410

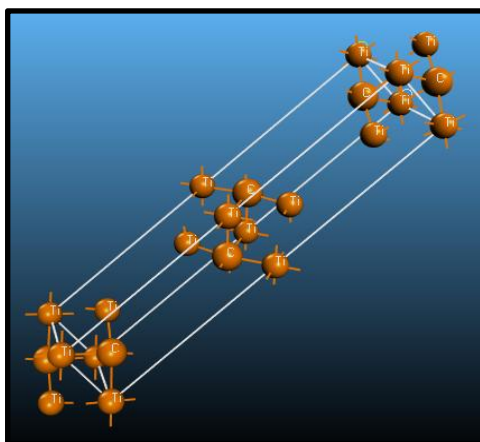


Figure 1. The electronic crystal structures of Ti_3C_2 .

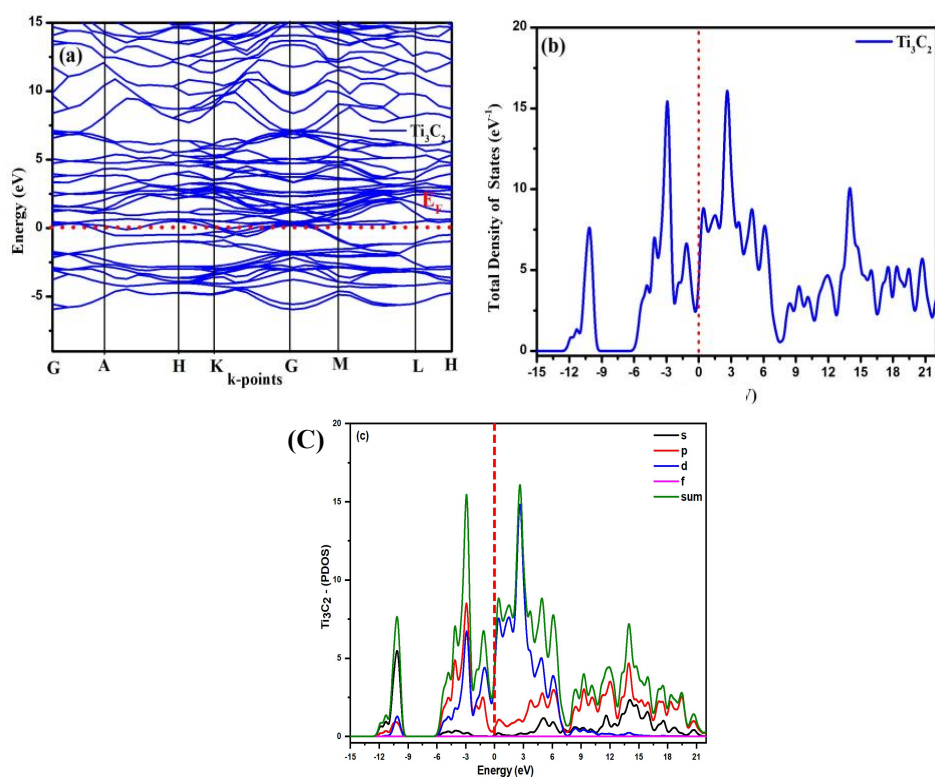


Figure 2. (a) Electronic band structure of Ti_3C_2 , (b) Total density of states of Ti_3C_2 and (c) Partial density of states of Ti_3C_2 .

These analyses provide insights into the material's electronic behavior and its potential applications in electronic and optoelectronic devices. The electronic band structure (EBS) of Ti_3C_2 , computed using the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional under the generalized gradient approximation (GGA), is presented in [figure 2\(a\)](#). A dashed line indicates the Fermi energy (E_F). The high-symmetry k-points G, A, H, K, G M, L, and H were selected to analyze the band dispersion of Ti_3C_2 over the energy range -10 eV to 15 eV. The results indicate that the valence band (VB) and conduction band (CB) overlap at the Fermi level (E_F), confirming the metallic nature of Ti_3C_2 MXene. This finding is consistent with previous theoretical and experimental studies.

Total and Partial Density of States Analysis. To further confirm the metallic behavior of Ti_3C_2 , we computed the total density of states (TDOS) and partial density of states (PDOS), as shown in [figure 2\(b\)](#) and [figure 2\(c\)](#), respectively. The TDOS spectrum is calculated over the -15 eV to 20 eV energy range, with the Fermi level (E_F) marked by a vertical dashed line in [figure 2\(b\)](#). The TDOS pattern indicates values of 16.12 states/eV above the Fermi level and 15.4 states/eV below the Fermi level, and these values define how many electronic states are available in those energy ranges. At the Fermi level (E_F), there are electronic states present; this means electrons can easily move through the material. The material behaves like a metal.

The absence of a zero-density region at E_F further confirms the metallic nature of Ti_3C_2 MXene. Additional information about the orbital contribution to the electronic arrangement of Ti_3C_2 is given by the PDOS study in [figure 2\(c\)](#). Ti-d orbitals provide many electronic states, which are larger than C-p orbitals near the Fermi energy level. It displays that Ti-d orbitals play a vital role in the electronic states near the Fermi level and are also responsible for metallic behavior. Whereas the d-orbital states exhibit major roles at higher energy levels, the s-orbital states mostly participate in the low-energy area. The consistency between the EBS, TDOS, and PDOS results confirms the intrinsic metallic nature of Ti_3C_2 MXene, making it a promising material for applications in electronic transport, optoelectronics, and energy storage.

3.3. Optical properties

The optical properties of Ti_3C_2 MXene were investigated using density functional theory (DFT) with the generalized gradient approximation (GGA). The study focused on key optical parameters, including the absorption coefficient ($\alpha(\omega)$), optical conductivity ($\delta(\omega)$), reflectivity ($R(\omega)$), dielectric function ($\epsilon(\omega)$), energy loss function ($L(\omega)$), and refractive index ($n(\omega)$). These properties provide crucial insights into the interaction of Ti_3C_2 with electromagnetic radiation, which is essential for its potential applications in photonic and optoelectronic devices. The dielectric function ($\epsilon(\omega)$), comprising its real ($\epsilon_1(\omega)$) and imaginary ($\epsilon_2(\omega)$) components, plays a fundamental role in describing the optical response of Ti_3C_2 MXene. The complex dielectric function, as stated below, was used to compute the optical properties of Ti_3C_2

MXene. The complex dielectric function, as given in Eq. (2), was used to calculate the optical properties of Ti_3C_2 MXene.

$$\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega) \quad (2)$$

where ω is the angular frequency of incoming electromagnetic radiation and $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$ are the real and imaginary components of the dielectric function, respectively.

The dielectric function can be used to calculate the refractive index and extinction coefficient as expressed in Eqs. (3) and (4), respectively.

$$n(\omega) = \left[\frac{\sqrt{\epsilon_1^2(\omega) + \epsilon_2^2(\omega)} + \epsilon_1(\omega)}{2} \right]^{1/2} \quad (3)$$

$$k(\omega) = \left[\frac{\sqrt{\epsilon_1^2(\omega) + \epsilon_2^2(\omega)} - \epsilon_1(\omega)}{2} \right]^{1/2} \quad (4)$$

The lost energy function can be identified according to Eq. (5):

$$L(\omega) = \frac{\epsilon_2(\omega)}{\epsilon_1^2(\omega) + \epsilon_2^2(\omega)} \quad (5)$$

The reflectivity, $R(\omega)$, can be calculated using the refractive index and extinction coefficient according to Eq. (6):

$$R(\omega) = \frac{[n(\omega) - 1]^2 + k^2(\omega)}{[n(\omega) + 1]^2 + k^2(\omega)} \quad (6)$$

where n is the refractive index, k is the extinction coefficient, R is the reflectivity, L is the loss of energy function, and ϵ_1 and ϵ_2 represent the dielectric function's real and imaginary components, respectively. [30]

The Ti_3C_2 optical graphs are presented in depth together with the predicted optical characteristics of Ti_3C_2 for photon energies between 0 and 60 eV. When light travels through anything, its intensity decreases. This is described by the absorption coefficient $\alpha(\omega)$ over a fixed distance in a substance.

As the photon energy changes, [figure 3](#) displays the absorption coefficient spectrum of Ti_3C_2 . It shows which solar energy conversion rate is the highest, as well as the maximum distance that a specific light frequency (energy) may travel through a material before being absorbed [31]. Anything that exhibits metallic characteristics will have good electrical conductivity. This is the material's maximum light-absorbing point. The material abruptly reduces its absorption to 40.93 eV after absorbing a significant amount of light. Thus, the amount of sunlight that these materials can absorb is limited, but they are rather effective at capturing it for energy, particularly at 36.3 eV. The reflective spectra of Ti_3C_2 in [figure 3\(b\)](#) show the properties of the energy of light. Eq. 5 is used to compute the reflectivity $R(\omega)$ of the materials under study. The highest reflectivity of Ti_3C_2 is approximately 0.64, and its photon energy is 0.49 eV.

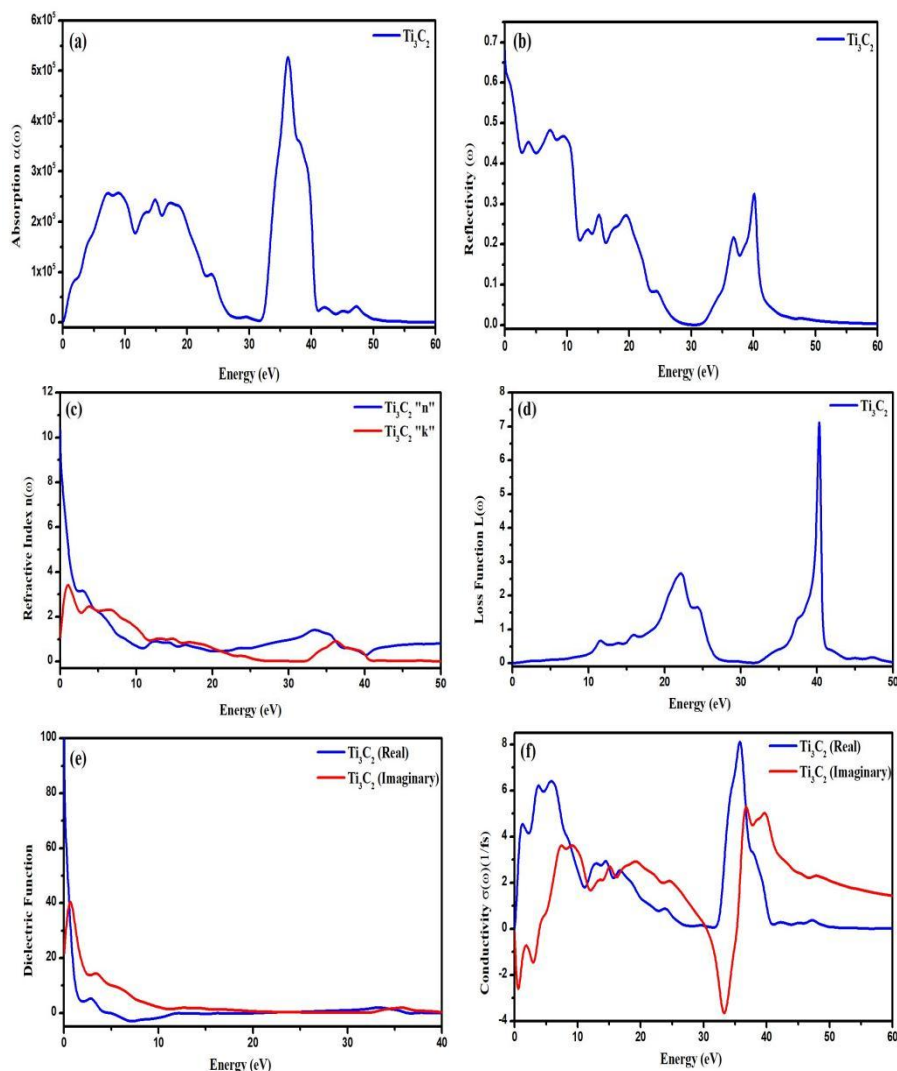


Figure 3. Optical properties of Ti_3C_2 : (a) Absorption, (b) Reflectivity, (c) Refractive index, (d) Loss Function, (e) Dielectric Function and (f) Conductivity.

The energy of a photon that corresponds to the greatest reflectivity is 0.49 eV, although the reflectivity itself is a dimensionless quantity. When photon energy increases, the reflectivity decreases and starts showing fluctuations.

Extremely high light energy causes materials to lose some of their reflective properties due to internal transitions. The degree to which light is twisted or refracted when it enters a material is determined by its refractive index, a fundamental optical feature. Ti_3C_2 refractive index is shown in [figure 3\(c\)](#). Eq. 2 can be used to determine the value of $n(\omega)$. This is comparable to a measurement of the amount of light bending that occurs within a substance. It is 10.3 for Ti_3C_2 . This indicates the amount of light bending that these materials do under typical circumstances. The substance bends light more when it has less energy. The loss function is an essential optical property that explains the decrease in power caused by a fast electron passing through a substance. Eq. 4 can be used to get the result for the loss function $L(\omega)$. [Figure 3\(d\)](#) displays it as an expression of the energy of

photons. Rapid electron motion causes some energy loss when electrons pass through a substance. The "loss function," which quantifies this loss, is an essential component in understanding how materials behave around electrons. There are peaks in the resulting loss function that indicate the highest energy loss points. The highest peak for Ti_3C_2 is located at 40.21 eV. There is a connection between these peaks and "plasma resonance." It's a unique phenomenon in which the material's electrons move collectively at a particular frequency, resembling a wave [32].

An optical constant called the dielectric function describes how a material responds to an electric field. [Figure 3\(e\)](#) displays the dielectric functions of Ti_3C_2 . The actual portion illustrates how an electric field works using a dielectric coefficient, which causes a substance to become polarized or organized. The amount of light that the substance absorbs is referred to as the imaginary part because of the electric field. For Ti_3C_2 , 10.8 eV represents the dielectric constant's imaginary part. This figure shows the amount of

light absorption by these substances. Ti_3C_2 exhibits a zero imaginary part of the dielectric constant at about 18.6 eV. According to this, the materials begin to become transparent above these energy levels. Stated differently, they stop absorbing light as much and instead start to let it through more readily. Fig. 3(f) shows the conductivity spectrum of Ti_3C_2 composites as a function of photon energy. There may be multiple peaks and valleys in a conductance plot, which illustrates how readily a substance conducts electricity at various energy levels. It displays a material's ease of conductivity at various energy levels; Ti_3C_2 exhibits higher conductivity of 8.1 (1/fs) at a photon energy of 35.7 eV. The examined materials appear to be metallic and exhibit conducting behavior based on these conductivity values. A similar peak is observed in the electrical conductivity plot within the studied energy range. Conversely, the electrical conductivity grows as a consequence of photon absorption [33].

Table 2. The evaluated values of the elastic constants of Ti_3C_2 .

Parameter	Ti_3C_2
C_{11} (GPa)	335.93
C_{12} (GPa)	76.08
C_{13} (GPa)	37.90
C_{33} (GPa)	296.92
C_{44} (GPa)	9.78
G_V (GPa)	57.84
G_R (GPa)	15.53
B (GPa)	162.70
Y (GPa)	102.36
G (GPa)	36.68
ν	0.39
A	0.07
B/G	4.43
$C_{12} - C_{44}$ (GPa)	66.30

3.4. Elastic properties

The elastic constants are fundamental parameters that describe the response of a material to external stress, providing insights into its mechanical stability, anisotropy, strength, ductility, and brittleness. In hexagonal crystals, the elastic behavior is governed by five independent elastic constants: C_{11} , C_{12} , C_{13} , C_{33} , and C_{44} [34]. These elastic parameters are crucial for determining a material's mechanical strength, Debye temperature, melting point, longitudinal (V_l) and transverse (V_t) sound velocities, and specific heat capacity.

The elastic constants of Ti_3C_2 MXene were computed using the finite strain method as implemented in the CASTEP package. Since mechanical stability is a prerequisite for any material's structural integrity, the mechanical stability of a hexagonal crystal can be evaluated using the following standards, according to Eq. (7) [35]:

$$C_{11} > |C_{12}|, 2C_{13}^2 < C_{33}(C_{11} + C_{12}), C_{44} > 0 \quad (7)$$

The computed elastic constants for the Ti_3C_2 compound are found to be mechanically stable, as they satisfy the conditions given in Eq.6, as displayed in Table 2. The Voigt-Reuss-Hill (VRH) method can be used to find the shear modulus (G), bulk modulus (B), Young's modulus (E), Pugh's ratio B/G , & Poisson's ratio of polycrystalline materials based on the defined variables C_{ij} of one individual crystal [36]. The bulk and shear moduli of the hexagonal form in the VRH estimate are given by the following equations (8) and (9):

$$B = \frac{B_V + B_R}{2} \quad (8)$$

$$G = \frac{G_V + G_R}{2} \quad (9)$$

While B_V and G_V are used to represent the Voigt bulk & shear moduli, B_R and G_R are used to represent those of Reuss and shear moduli (Eqs. 10–12). Pugh's ratio indicates that brittleness and ductility are connected with greater and smaller B/G ratio values, respectively [37]. The Cauchy pressure ($C_{12} - C_{44}$) indicates whether a material exhibits brittle or ductile behavior. If the $C_{12} - C_{44}$ value is negative, the material is considered brittle; if it is positive, the material is considered ductile. According to the calculated results, the Ti_3C_2 MXene material exhibits ductile behavior. Pugh's ratio (B/G) is an important parameter for evaluating the brittle or ductile behavior of a material (Eq. 13). The material will behave in a ductile manner if B/G is greater than 1.75 and brittle if B/G is less than 1.75.

The compound Ti_3C_2 has consistent mechanical properties.

$$B = B_V = B_R = \frac{C_{11} + 2C_{12}}{3} \quad (10)$$

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

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

So,

$$G_R \leq G \leq G_V \quad (13)$$

Young's modulus (γ), Anisotropy factor (A), and Poisson's ratio (ν) can be described as in the following equations (14), (15), and (16):

$$Y = \frac{9BG}{3B + G} \quad (14)$$

$$A = \frac{2C_{44}}{(C_{11} - C_{12})} \quad (15)$$

$$\nu = \frac{3B - Y}{6B} \quad (16)$$

Using the Cauchy pressure (C_p equation $C_{12} - C_{44}$), one can report that the atomic interaction of alloys and related substances is rotational [38]. A material is considered non-metallic with a straight bond if the Cauchy pressure (C_p) is negative; an alloy of metals is anticipated if the C_p is positive [39]. Cauchy pressure is positive in the Ti_3C_2 instance, indicating that the material is metallic. Table 2 above shows that for Ti_3C_2 compounds, $C_{11} > C_{33}$, indicating that the

nearest-neighbor bonds in the (100) and (001) planes are not the same.

There are multiple methods to represent the degree of anisotropy in the elasticity of crystalline substances, one of which is the use of computed C_{ij} constants. Thus, one can use shear-anisotropic parameters to determine the extent to which atomic bonds are asymmetrical in various surfaces [40]. The shear anisotropic coefficient A for the {100} shear planes that lie in the $\langle 011 \rangle$ and $\langle 010 \rangle$ orientations are given by $A = 4C_{44} / (C_{11} + C_{33} - 2C_{13})$. The degree of elastic anisotropy is determined by $A = 1$ for a crystal with isotropic elastic properties; values less than or greater than 1 indicate the level of elastic anisotropy [41]. However, in this instance, A is less than 1. The value is equal to 0.07. Anisotropy for linear compression along the a and c axes is evident for Ti_3C_2 compounds, as Table 2 shows. Using the f variable is an additional choice that is described in the following equation (17):

$$f = \frac{C_{11} + C_{12} - 2C_{13}}{C_{33} - C_{13}} \quad (17)$$

For hexagonal crystals. It establishes the ratios of hexagonal crystalline linear-compressible materials; isotropic compressibility is represented by $f = 1$, while anisotropy in linear compression along the c -axis is represented by a departure from 1 [42]. In this instance, $f=1.2$. Table 2 shows that for Ti_3C_2 compounds, there is anisotropic linear compression along the c and a axes.

4. Conclusion

In conclusion, the structural, electronic, elastic, and optical properties of Ti_3C_2 have been studied using density functional theory and CASTEP. The calculated results and improved Ti_3C_2 lattice parameters agree well. The conductivity research indicates that the Ti_3C_2 structure has optical conductivity that begins at zero photon energy, meaning that the substance under study has zero band gap. Thus, each of these compounds' band structures and density of states demonstrated that they possessed a metallic nature of Ti_3C_2 . The optical calculations show that Ti_3C_2 has a strong optical response. For Ti_3C_2 , the maximum reflectivity value occurs at a photon energy of 0.49 eV. When Ti_3C_2 is at 35.7 eV, the maximum conductivity value is 8.1 (1/fs). The investigated materials appear to be metallic based on these conductivity values. Based on our data on mechanical properties, we can observe that Ti_3C_2 is mechanically stable according to the Born stability criteria. Ti_3C_2 materials have ductile behavior, as indicated by Pugh's ratio (B/G), which is a crucial metric. A value greater than 1.75 is the value of B/G . Thus, the behavior of Ti_3C_2 is ductile. Overall, the calculated electronic, optical, structural, and elastic properties indicate the Ti_3C_2 MXene has potential for use in modern energy and electronic components.

Author contributions

Conceptualization, Muhammad Aqib; methodology, Muhammad Irfan and Hadia Khalil; software, Muhammad Mubashir Khan; formal analysis, Muhammad Aqib,

Muhammad Irfan, and Hadia Khalil; writing—original draft preparation, Muhammad Aqib, Muhammad Irfan, and Hadia Khalil; writing—review and editing, Mazhar Khan and Zeeshan Akmal. All authors have read and agreed to the published version of the manuscript.

Ethical approval

Not applicable.

Conflicts of Interest

The authors report no conflicts of interest.

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Data availability statement

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

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