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First-principles study of the physical properties of Ti_2SnX (X: C, N) based 211-MAX phases

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ABSTRACT

In this article, we report the physical behavior of Ti_2SnX (X: C, N) compounds that belong to the family 211-MAX phases and provide a detailed analysis of their structural parameters, electronic structures, and optical spectra in comparison with available literature. The calculations carried out to perform this study are based on the full-potential linearized augmented-plane-wave (FP-LAPW) method within the Density functional theory (DFT). Like other MAX phases, the electronic structure calculations show the Ti_2SnX (X: C, N) compounds as metallic with a considerable density of states (DOS) over the Fermi level. In addition, these compounds exhibited symmetrical electronic structures for up and down spin states and a negligible magnetic moment of 0.00036 μ_β and 0.00153 μ_β for Ti_2SnC and Ti_2SnN, respectively. Our detailed predictions of the structural and electronic properties are well-matched to the available literature. These compounds exhibited the static refractive indices in the *x*- and *z*- directions, respectively, as 8.17 and 6.95 for Ti_2SnC and 10.07 and 9.73 for Ti_2SnN. Moreover, we comprehensively discussed the reflection and absorption of light by these 211-MAX phases, which may benefit researchers in the relevant field.

1. Introduction

MAX phases are a class of ternary carbides/nitrides that adopt hexagonal structures and are represented by the general chemical formula $M_{n+1}AX_n$ ($n = 1$–3). In the MAX phase formula, n is an integer that plays a vital role in classifying MAX phases into different categories, such as 211, 312, 413, and 514. The symbols M, A, and X are the transition metals, Group-IIIA/Group-IV elements, and carbon/nitrogen, respectively [1]. Although the MAX phases of the 514 categories are rarely available [2], the 413 and 312 phases exist in relatively higher numbers. Whereas the 211 MAX (M_2AX) phase has been reported to have the highest numbers, up to 60 candidates of the mentioned family have already been synthesized [3]. Furthermore, nearly 150 MAX phases of M_2AX have been reported in recent literature [2,4,5].

Within the hexagonal structure of the MAX phases, the M and X atoms are covalently bonded to each other in the form of an $M_{n+1}X_n$ octahedron. The edge-shared $M_{n+1}X_n$ octahedra are sandwiched between layers of A-atoms along the *c*-axis. These materials' simultaneous ceramic and metallic behavior has made them attractive to researchers in recent years. Their nano-laminate structure has evolved interesting features within these materials, such as excellent thermal shock resistance, superior machinability, and good electrical and thermal conductivities [6–9]. They have been reported as potential materials for applications such as concrete's dry drilling, high-temperature foil bearings, tribological components, and gas burner nozzles, as well as an alternative to graphite for high-temperature applications [10,11]. In addition, they have been used in cutting-edge technologies such as high-temperature ceramics, electrical contacts for catalysis, sensors, and protective coatings [2]. Due to their abundant availability and reliable applicability and metals like electronic conductivity at room

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temperature, the M_2AX type of MAX phases have attracted more attention in recent years [1–5,7–22]. Among them, the Ti_2SnC MAX Phase has been experimentally realized by Kang et al. [22] by Sn-melt infiltration into the sub-stoichiometric titanium carbide in the porous preform.

Following their investigations, we studied the electronic structures, structural parameters, and optical spectra of Ti_2SnC using the FP-LAPW approach in DFT. In the present work, we performed similar investigations for additional MAX phases such as Ti2SnN and Ti2SnC. Our results show these 211-MAX phases as nonmagnetic and metallic behavior. These comprehensive investigations of the optical spectra and electronic properties of these new MAX phases will likely provide information for these materials in futuristic technological applications.

2. Computational details

We used the WIEN2k code [23] to perform calculations of the physical properties of these 211-MAX phases using the FP-LAPW approach. We use the generalized gradient approximations by Perdew et al. (GGA-PBE) [24] for exchange–correlation potential. A dense k-mesh grid of 12 × 12 × 1 has been used for high-quality calculations. The radii of muffin tin spheres (RMT) have been chosen as Ti = 2.24 a.u., Sn = 2.50 a.u., C = 1.83 a.u., N = 1.76 a.u. The core and valence electrons are separated by providing the energy of −81.634 eV. The electrons residing in the T-3*s*, 3*p*, 3*d*, 4*s*, Sn-4*d*, 5*s*, 5*p*, C-2*s*, 2*p* and N-2*s*, 2*p* orbital's are treated as the valence electrons. The wave-functions expansion and Fourier-expanded charge density truncation have been set to $l_{max} = 10$ and $G_{max} = 16$ au^{-1}, respectively. The energy cutoff $K_{max} = 8.0/R_{MT}$ (Ry)$^{1/2}$ has been used to realize highly accurate results. The total energy of the Ti_2SnX compounds is converged to 10^{-5}Ry/unit cell. The phonon dispersions have been determined for the dynamical stability of these MAX phases using the PHONOPY code [25]. Our previous studies show that the methodology adopted in the present study delivers accurate results for the electronic and optical properties of crystalline materials [26–39].

3. Results and discussion

Crystal structures of the Ti_2SnX compounds of the 211-MAX phase family are presented in Fig. 1(a). Their unit cell is composed of two formula units that exhibit a hexagonal structure of space group $P6_3/mmc$ (No 194). Within the unit cell, the Wyckoff positions (1/3, 2/3, z), (1/3, 2/3, 3/4), and (0, 0, 0) are occupied by the Ti, Sn, and X elements. The unit cell is defined by the vertically stacked atomic layers of the Ti_6X octahedron and Sn layers such that the Ti_6X octahedron layer is sandwiched between two Sn layers and vice versa. These 211-MAX phases exhibited the optimized lattice parameters as $a = b = 3.154$ Å and $c = 13.726$ Å for Ti_2SnC and $a = b = 3.152$ Å and $c = 13.781$ Å for Ti_2SnN. Our results for the lattice parameters of the Ti_2SnX compounds are nearly similar to the lattice parameters reported for Ti_2SnC as $a = b =$ 3.136 Å [21], 3.163 Å [40], 3.171 Å [41], 3.096 Å [42], and $c = 13.641$ Å [21], 13.679 Å [40], 13.857 Å [41], 13.404 Å [42].

Although Ti_2SnC has already been synthesized and reported as stable [43], we determined the phonon dispersions for these compounds, as shown in Fig. 1 (b,c), to confirm the stability of Ti_2SnN in particular. Evidently, the phonon dispersions appear at positive frequencies, and no phonon modes are found at negative frequencies, which indicates adequate stability of the Ti_2SnX compounds. Additionally, we calculated the cohesive energies of Ti_2SnX compounds to recognize the nature of the ground-state magnetization following the literature [44–47]. In this regard, we calculated the total energy of the Ti_2SnX compounds ($E_{Ti2SnX}^{211-MAX}$) (in the ferromagnetic and antiferromagnetic states) and Ti, Sn, and X elements ($E_{Ti} + E_{Sn} + E_X$) and incorporated them in Eq. (1).

$$E_{Coh} = \left(E_{Ti2SnX}^{211-MAX}\right) - (xE_{Ti} + yE_{Sn} + zE_X)/(x + y + z) \quad (1)$$

Using Eq. (1), the E_{Coh} has been recorded as −6.712 eV and −6.248 eV in the ferromagnetic state, respectively, for Ti_2SnC and Ti_2SnN. In the antiferromagnetic state, the cohesive energies have been recorded as −6.709 eV and −6.247 eV for Ti_2SnC and Ti_2SnN, respectively. Evidently, the ferromagnetic state of these materials is slightly lower in energy than the antiferromagnetic state, and therefore, both Ti_2SnC and Ti_2SnN can be inferred as ferromagnetic in the ground state. Our results for the cohesive energies show a good resemblance with stable MAX phases reported as 6.29 eV [48] for Ti_2AlC, 7.183 for Ti_2CdC [49], and 6.09 for Ti_2AlN [48], respectively.

The electronic structure of the Ti_2SnX compounds determined for the up and down spin cases is shown in Fig. 2. Like other MAX phases, the Ti_2SnX compounds also showed metallic behavior due to their gapless electronic structure. The metallic nature of Ti_2SnC has also been reported by Kanoun *et al.* in a First-principles study based electronic structure study [21]. The metallic nature of the Ti_2SnX compounds is due to the occurrence of states over the Fermi-level with significant density. Fig. 3 shows that the energy bands appearing over the Fermi level mainly originated from the Ti-*d* states. A similar trend has earlier been reported for a number of Tantalum- and hafnium-bearing carbides and/or nitrides [50–52]. The Ti-*d* states demonstrate the highest density in the energy range of ∼−2 eV in the valence band to 4 eV in the conduction band. This indicates that electronic transitions between the valence and conduction bands in the vicinity of the Fermi level are mainly between the Ti-*d* states. However, the Sn-*p* and X-*p* states have also been seen in the lower valence band (below −2 eV) and upper conduction band (above 2 eV). Fig. 3 further indicates that the up-spin states are symmetrical to the down-spin states. This kind of arrangement is unwanted in the case of magnetic materials, as the down-spin

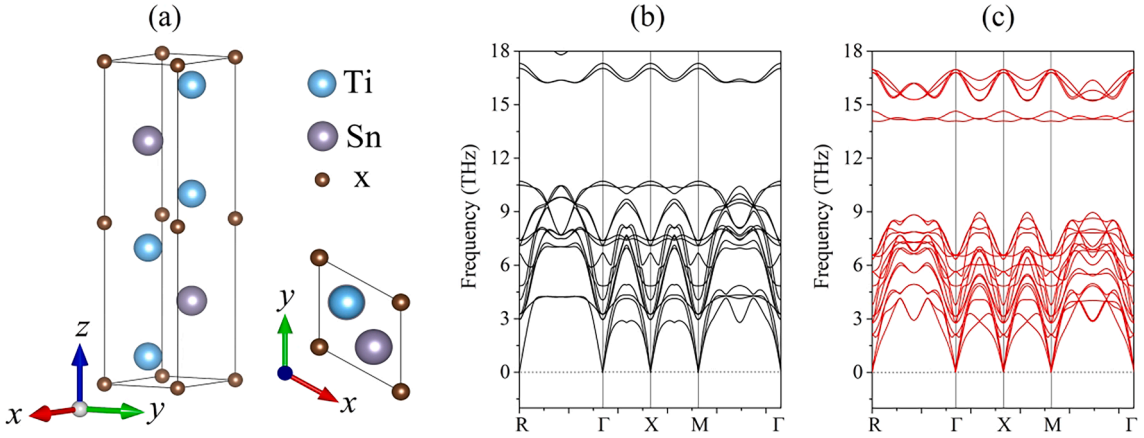

Fig. 1. (a) Crystal structure of the Ti_2SnX based 211-MAX phases. The phonon dispersions of Ti_2SnC (b) and Ti_2SnN (c) determined using the PHONOPY code.

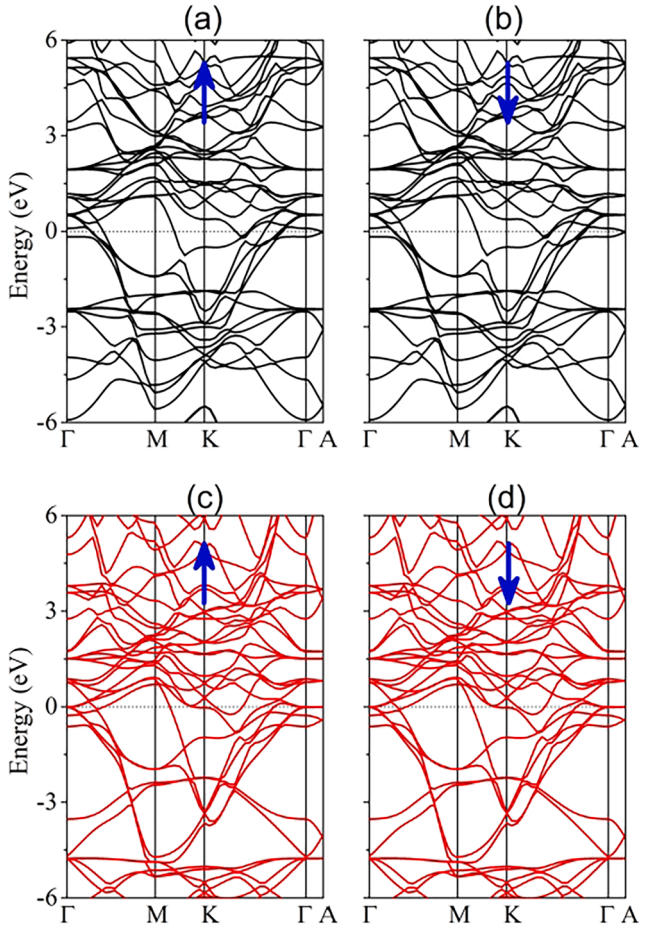

Fig. 2. Electronic structures of Ti_2SnX based 211-MAX phases (Ti_2SnC (a,b), Ti_2SnN (c,d)) determined for up spin state (represented by upward arrowhead) and down spin state (represented by downward arrowhead).

states cancel the magnetic effect of the up-spin states. We accordingly recorded a minute magnetic moment of magnitude 0.00036 μ_β and 0.00153 μ_β respectively, for Ti_2SnC and Ti_2SnN. Therefore, the Ti_2SnX MAX phases can be considered ferromagnetic metallic materials with a marginal magnetic moment. However, no literature relevant to the magnetic moment of the Ti_2SnX MAX phases is available to our knowledge to compare or results for the magnetic properties of these materials.

In the following, we discuss the optical behavior of these MAX phases. Figs. 4, 5, and 6 show the reflection, refraction, and absorption coefficients of Ti_2SnC and Ti_2SnN obtained from the dielectric functions (shown in Figs. 7 and 8). Fig. 4 indicates that Ti_2SnX compounds demonstrate a significant reflection of the incident light. These MAX phases' optical reflection can be associated with their metallic behavior. The reflection of the infrared and UV light (of energy less than 8 eV) is higher than the visible light. The average reflection of visible light has been estimated at around 40 %, whereas the reflection of infrared and UV light is more than 60%. The rest of the light is either refracted or absorbed by these compounds. Fig. 5 shows the optical refraction of incident light by these compounds. One can see that these materials exhibited the highest optical refraction for infrared light; however, it has rapidly declined for visible and UV light. These compounds showed the static refractive indices in the *x*- and *z*- directions, respectively, as 8.17 and 6.95 for Ti_2SnC and 10.07 and 9.73 for Ti_2SnN. The refraction spectra indicate the transparent behavior of these compounds for incident light of energy less than 8 eV as their refractive indices remain larger than 1.

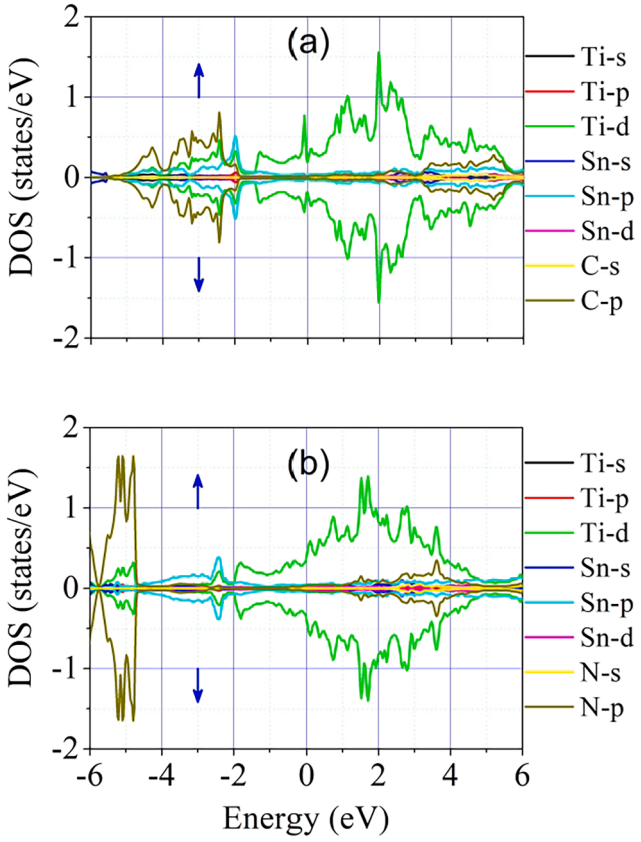

Fig. 3. DOS of Ti_2SnX-based 211-MAX phases (Ti_2SnC (a), Ti_2SnN (b)) determined for the up spin state (represented by upward arrowhead) and down spin state (represented by downward arrowhead).

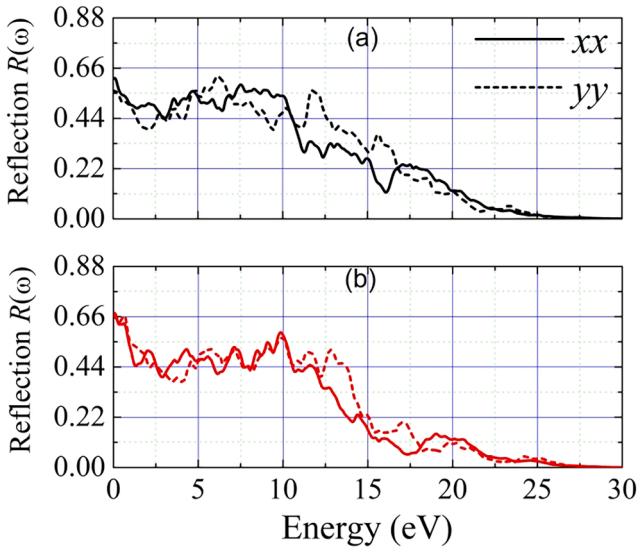

Fig. 4. The reflection of light by Ti_2SnC (a) and Ti_2SnN (b) based 211-MAX phases.

Similarly, the absorption of the incident light by these compounds has been comprehended by calculating the spectrum of the absorption coefficient against photon energy (Fig. 6). Fig. 6 shows these compounds as a strong absorbent of the incident light of energy less than 15 eV. The optical absorption has been found to be relatively marginal for infrared light. This is because these compounds either reflect or refract a significant part of the incident light. However, the increase in the energy of

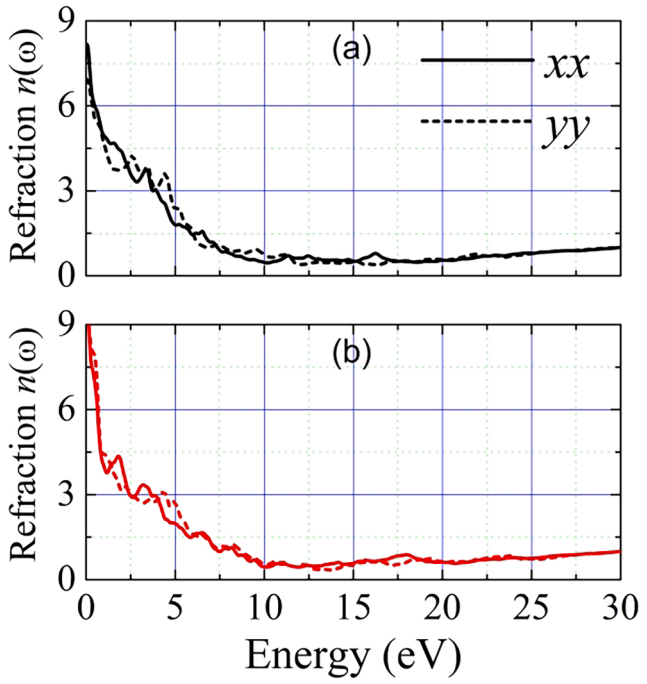

Fig. 5. The refraction of light by Ti_2SnC (a) and Ti_2SnN (b) based 211-MAX phases.

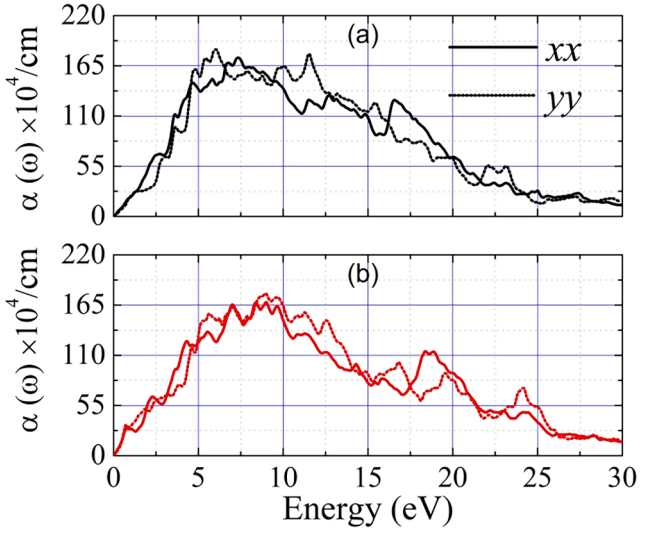

Fig. 6. The absorption coefficient of Ti_2SnC (a) and Ti_2SnN (b) based 211-MAX phases.

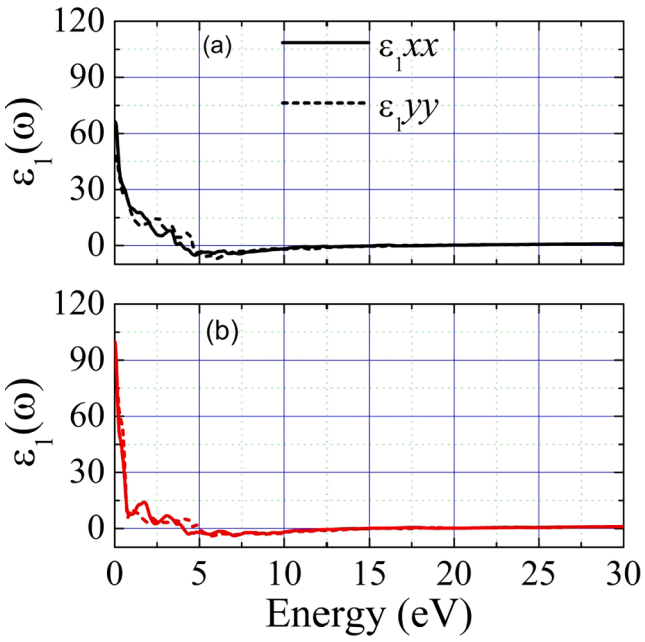

Fig. 7. The real part of the dielectric function of Ti_2SnX-based 211-MAX phases.

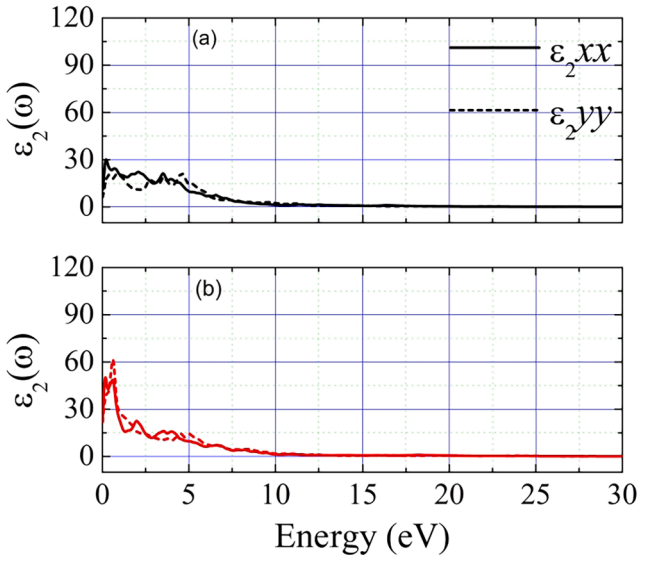

Fig. 8. The imaginary part of the dielectric function of Ti_2SnC (a) and Ti_2SnN (b) based 211-MAX phases.

light photons has caused a rapid enhancement in optical absorption, as the high-energy photons can trigger the hopping of electrons from low-energy to high-energy states within the electronic structures.

Moreover, light's reflection (shown in Fig. 4) and refraction (shown in Fig. 5) are relatively lower for higher energy photons. This indicates that these compounds mostly absorb high-energy photons within the UV range of the electromagnetic spectrum. Therefore, they can be considered as potential materials for applications in energy harvesting devices.

4. Conclusion

This is a DFT-based study of the structural, electronic, magnetic, and optical properties of the Ti_2SnX (X: C, N) compounds of the MAX family. The comparison of our results of structural and electronic properties reveals the high accuracy of the adopted FP-LAPW approach in DFT. The phonon dispersion calculations showed no phonon modes at negative frequencies, which implies adequate stability of the Ti_2SnX compounds. Our results showed that the considered MAX phases are metallic that exhibit a marginal magnetic moment due to considerably symmetrical states over the Fermi level. The ferromagnetic state of these materials is found to be slightly lower in energy than the antiferromagnetic state. Therefore both Ti_2SnC and Ti_2SnN can be inferred as ferromagnetic in the ground state. Furthermore, these MAX phases showed prominent optical behaviors in terms of high optical reflection, static refractive indices, and optical absorption. Calculations of the refractive indices indicated these materials as transparent for a broad range of incident electromagnetic light. Our results may provide valuable information regarding the physical properties of these materials for futuristic studies

and applications.

CRediT authorship contribution statement

Bakhtiar Ul Haq: Conceptualization, Methodology, Software, Data curation, Writing – original draft. **M.M. Alsardia:** Visualization, Methodology, Investigation, Validation. **I.B. Khadka:** Visualization, Validation. **R. Ahmed:** Methodology, Software. **S. AlFaify:** Methodology, Software. **Faheem K. Butt:** Validation. **Zulfiqar Ali Shah:** Methodology, Software, Data curation. **Se-Hun Kim:** Supervision, Project administration, Investigation, Writing – review & editing.

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.

Data availability

Data will be made available on request.

Acknowledgment

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