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## Research Article

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# Ab initio Study of the Structure, Elastic, and Electronic Properties of $Ti_3(Al_{1-n}Si_n)C_2$ Layered Ternary Compounds

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## Abstract

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## Introduction

The MAX phase materials such as layered ternary carbides that simultaneously exhibit characteristics of metallic and ceramic materials have received substantial interest in recent years. Here, we present a systematic investigation of the electronic, structural stabilities, and elastic properties of  $Ti_3(Al_{1-n}Si_n)C_2$  ( $n = 0,1$ ) MAX phase materials using the ab initio method via a plane-wave pseudopotential approach within generalized-gradient-approximations. The computed electronic band structures and projected density of states show that both  $Ti_3SiC_2$  and  $Ti_3AlC_2$  are metallic materials with a high density of states at the Fermi level emanating mainly from Ti-3d. Using the calculated elastic constants, the mechanical stability of the compounds was confirmed following the Born stability criteria for hexagonal structures. The Cauchy pressure and the Pugh's ratio values establish the brittle nature of the  $Ti_3SiC_2$  and  $Ti_3AlC_2$  MAX phase materials. Due to their intriguing physical properties, these materials are expected to be suitable for applications such as thermal shock refractories and electrical contact coatings.

Researchers have paid special attention over the last 30 years to MAX compounds owing to their essential characteristics and applications<sup>1-3</sup>. MAX phases are a family of more than fifty ternary nitrides and carbides of general formula  $M_{n+1}AX_n$  where n is for 1, 2, or 3, M denotes the early transition metal (TM), A represents the A- group element (typically IIIA or IVA) and X is used for nitrogen or carbon<sup>4</sup>. Most MAX phases were discovered experimentally by Nowotny et al about 40 years back<sup>5</sup>. In 1996, Barsoum and El-Raghy's<sup>6</sup> reported the synthesis of bulk  $Ti_3SiC_2$  material and its unique properties and applications. Thereafter, research on the ternaries increased rapidly. Based on WOS<sup>7</sup>, to date, there are around 4,168 published papers on MAX compound alone, with  $Ti_3SiC_2$  having roughly half of the published

works in the past six years. The space group of these phases is commonly reported hexagonal, P63/mmc, and contain at least two forms of ionic, covalent, or metallic chemical bonds. Specific forms of MAX phases called 211, 312, or 413 (and higher orders such as 514, 615, and 716) are known in the literature. These numbers denote the stoichiometry of MAX phase materials, for example,  $Ti_2SiC$  and  $Ti_2AlC$  represent 211 MAX phases,  $Ti_3SiC_2$  and  $Ti_3AlC_2$  denote 312-MAX phase while 413-type are the  $Ti_4SiC_3$  and  $Ti_4AlC_3$ , indicating that the individual phases differ by the number of M layers parting the A-layers, that is there are two in the 211-type, three in the 312-type, and four M-layers in the 413 MAX phase-type<sup>1-3,8</sup>.

MAX phases are useful in numerous applications due to their unique, hybrid ceramic/metal properties, that result from their structure as well as their atomic arrangements<sup>1,8,9</sup>. More categorically, these materials are considered for purposes in extreme environments as they exhibit outstanding oxidation resistance and thermal stability. These compounds combine some characteristics of metals like strong compressive strength, high fracturing strength, low hardness, ductile behaviour, good thermal conductivity with high stiffness, damage tolerance, relatively low thermal expansion coefficient, good electrical conductivity, outstanding thermal and chemical tolerance typical of ceramics. Furthermore, these compounds are considered as one of the best classes of materials for coating on steel surfaces in heavy liquid metal and as pump impellers. However,  $Ti_3SiC_2$  and  $Ti_3AlC_2$  are among the best-accepted representatives of the MAX phase compounds and are known as the best thermal conductors than titanium metal<sup>10-14</sup>.

First-principles approaches are widely employed to study MAX phases, for example,  $M_2GaN$  ( $M=Ti, V$  and  $Cr$ )<sup>15</sup>,  $Ti_2TiC$ ,  $Zr_2TiC$  and  $Hf_2TiC$ <sup>8,11</sup>,  $Ti_3AlC_2$  and  $Ti_2SiC_2$ <sup>3</sup>. Zhou et al<sup>16</sup> reported the distribution of charge density on the (1120) plane of  $Ti_3AlC_2$ , where robust directional Ti-C-Ti-C-Ti covalent bond chains were observed that linked to fairly weaker Ti-Al covalent bindings. In a similar study of electronic structure and bonding properties of  $Ti_3AlC_2$ , Wang and Zhou<sup>17</sup> reported that electrical conductivity of  $Ti_3AlC_2$  decreases with increasing pressure, and over the whole pressure range, the material was found to exhibit elastic anisotropy. Furthermore many other studies were, more recently reported on the mechanical properties, and structural stabilities of  $Ti_3SiC_2$  and  $Ti_3AlC_2$ <sup>18-23</sup> since both materials exhibit excellent structural properties that are suitable for many practical applications. Synchrotron x-ray diffraction measurements indicate that the  $Ti_3SiC_2$  and  $Ti_3AlC_2$  materials as stable materials under pressure from 0 to 61 GPa at room temperature<sup>24</sup>.

Hence, In this study,  $Ti_3SiC_2$  and  $Ti_3AlC_2$  are investigated as potential structural materials to expose their further potential for technological and industrial applications as they are considered promising candidates for applications where materials are subjected to extreme

environments, like nuclear reactors <sup>1,3,13,14,20</sup>. Therefore, comprehensive knowledge of their electronic, structural stabilities and elastic properties is crucial so that our results will resolve some inconsistency where they exist in the reported properties of these materials.

## Result and Discussion

### Structural Properties

The layered ternary  $Ti_3(Al_{1-n}Si_n)C_2$  compounds are based on the layers of hexagonally close-packed Si/Al and Ti layers with C occupying octahedral centres between the Ti layers. The end phases could also be characterized as alternating stacking of two layers of a planar close-packed Si/Al and  $Ti_6C$  octahedral layers. The Ti atom is found to be located at 4f (0.33, 0.67, z), Al/Si atoms are positioned at 2b (0, 0, 0.25) whereas the atom of C is in 4f (0.33, 0.67, z) Wyckoff positions. Figure 1 illustrates the crystal symmetries of the studied compounds and their computed structural parameters whereas the experimental results from literature and our computed results in this study are summarized in Table 1. The results of the equilibrium lattice constants, bulk modulus, and its pressure derivative are computed by fitting the obtained data of the equilibrium energy as well as volume to the 2<sup>nd</sup> order Murnaghan's equation of state (EOS) <sup>25</sup>. The obtained results show the reasonability of our calculations.

$$E(V) = E_o \frac{9}{16} B_o \left[ (4 - B'_o) \frac{V_o^3}{V^2} - (14 - 3B'_o) \frac{V_o^{7/3}}{V^{4/3}} + (16 - 3B'_o) \frac{V_o^{5/3}}{V^{2/3}} \right] \quad (1)$$

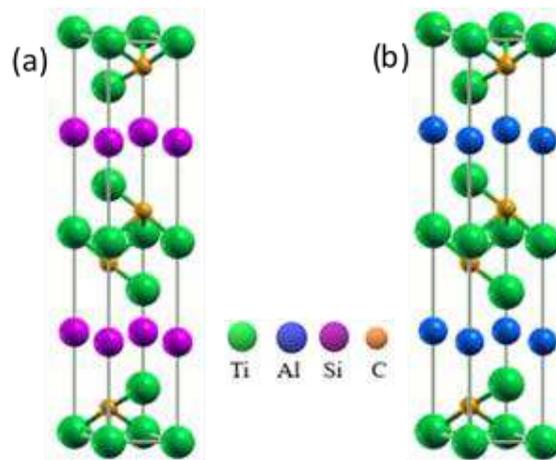


Figure 1. Crystal structure of (a)  $Ti_3AlC_2$  (b)  $Ti_3SiC_2$  MAX phase compounds.

One can easily note that the difference between our obtained results and experimental data of equilibrium lattice parameters is lesser than 1%, showing that our results obtained at the level

of the PBE functional are sufficiently reliable. However, the bulk modulus of  $\text{Ti}_3\text{SiC}_2$  is higher than that of  $\text{Ti}_3\text{AlC}_2$ , showing that  $\text{Ti}_3\text{SiC}_2$  is harder than  $\text{Ti}_3\text{AlC}_2$ .

Compound	Reference	$a$ (Å)	$c$ (Å)	$c/a$	$V$ (Å <sup>3</sup> )	$B_0$ (GPa)	$B'$
$\text{Ti}_3\text{AlC}_2$	This work	3.0781	18.7681	6.0973	153.93	145	2.81
	Exp. <sup>26</sup>	3.082	18.642	6.0487			
	Calc. <sup>23</sup>	3.083	18.652	6.040		163.35	
$\text{Ti}_3\text{SiC}_2$	This work	3.0697	17.6864	5.7000	145.60	180.5	4.14
	Exp. <sup>26</sup>	3.075	17.734	5.7672			
	Calc. <sup>23</sup>	3.077	17.715	5.7572		192.61	

Table 1. Calculated equilibrium lattice parameters  $a$ ,  $c$ ,  $c/a$  ratio, volume,  $V$ , bulk modulus  $B_0$ , and its pressure derivative,  $B'$  and values from the literature.

### Electronic properties

Figure 2 exhibits computed band structures and total density of states (TDOS) computed at equilibrium constants, along with high symmetry points in the BZ. It is seen that both valence bands and conduction bands overlap significantly resulting in no energy gap at the Fermi level, thus, the studied compounds demonstrate metallic character which is a common feature of the MAX phase materials. However, there are more valence electrons in the  $\text{Ti}_3\text{SiC}_2$  unit cell than in  $\text{Ti}_3\text{AlC}_2$ . This gives rise to the further occupation of the bonding states near Fermi. It is also shown that the originally empty valence band near the gamma ( $\Gamma$ ) point shifts downward and is positioned below the Fermi in  $\text{Ti}_3\text{AlC}_2$ . The substitution of Si by Al in  $\text{Ti}_3\text{AlC}_2$  presents additional valence electrons per atom, and consequently, the Fermi level is moved to a higher energy level. This suggests that the increased extra valence electrons fill in the Si/Al-Ti pd hybridized bonding states as well as the metal to metal dd consequential bonding.

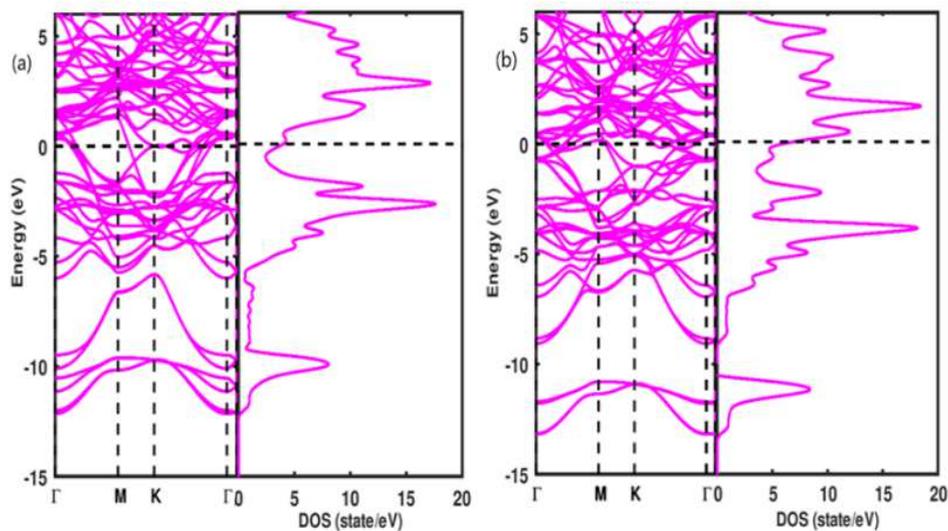


Figure 2. Band structures and TDOS of (a)  $\text{Ti}_3\text{SiC}_2$  (b)  $\text{Ti}_3\text{AlC}_2$  MAX phase compounds.

Accordingly, the filling of the bonding orbitals rises the strength of the bond and thereby increasing the bulk moduli. The energy band also exhibits a highly anisotropic character along with lesser *c*-axis energy dispersion. The anisotropy of the band structure near and below the Fermi implies that, for single crystals, both  $\text{Ti}_3\text{SiC}_2$  and  $\text{Ti}_3\text{AlC}_2$  are conductors and anisotropic, and electrical conductivity is lowered along *c* direction than the *ab* plane similar to the observed trend in the literature <sup>16</sup>.

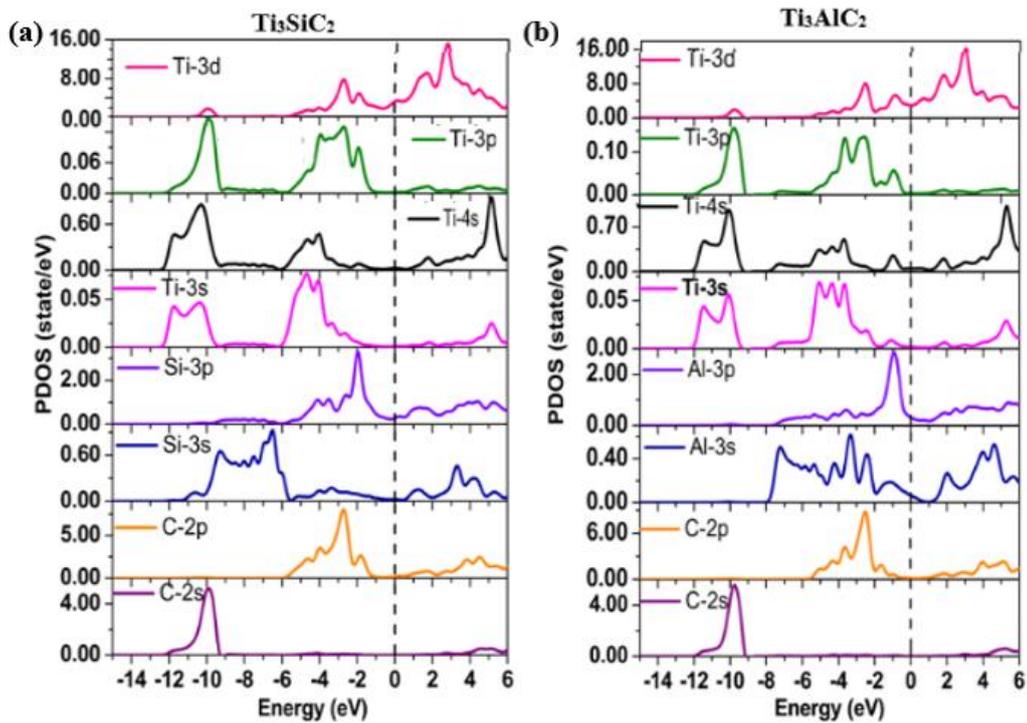


Figure 3. Calculated PDOS of (a)  $\text{Ti}_3\text{SiC}_2$  and (b)  $\text{Ti}_3\text{AlC}_2$  MAX phases.

The investigated total densities of states (TDOS) plot for  $\text{Ti}_3\text{SiC}_2$  and  $\text{Ti}_3\text{AlC}_2$  presented in Figure 2 points out that, the peak structures and corresponding heights of the peaks are equivalent, signifying resemblance in chemical bonding. The DOS per unit cell at the Fermi for  $\text{Ti}_3\text{SiC}_2$  and  $\text{Ti}_3\text{AlC}_2$  is 4.029 and 6.855 states/eV, respectively. Therefore, there is an increasing trend in the DOS at the Fermi level with an increasing number of valence electrons of the transition metal showing that the transition metal bands play a dominant role in the TDOS and their electrical transport properties. Analysis of bonding properties is obtained from the PDOS of each contributing element in Figure 3. Here, the width of Al-3s and Si-3s states are wider for each one than that of the C-2s state. With several less contributing peaks in the Al/Si- are due to 3s states. The Al/Si-3s energy states show that there are s-p interactions in Al/Si, i.e. close-packed layer of Al/Si atoms are bonded through s-p interactions. For the energy range -12 eV to 9.4 eV in the valence bands of both  $\text{Ti}_3\text{SiC}_2$  and  $\text{Ti}_3\text{AlC}_2$ , there is a high-level degree

of hybridization of C-2p with Ti-3d energy states, which suggests a covalent interaction. Hence the stabilization is because of pd hybridization or p-d bondings. Thus, the Ti-3d and C-2p hybridization is a driving bonding force in  $\text{Ti}_3\text{SiC}_2$  and  $\text{Ti}_3\text{AlC}_2$ , similar to bonding properties in some 312 MAX phases like  $\text{Ti}_3\text{SnC}_2$  and  $\text{Ti}_3\text{GeC}_2$ <sup>27,28</sup>.

### Elastic Properties

Investigations of elastic constants are vital for applications related to the mechanical properties of solids. They provide information on stability, bonding, ductility, brittleness, anisotropy, compressibility, Vicker's hardness, and stiffness of solids<sup>29,30</sup>. For hexagonal crystals structures, five independent elastic constants ( $C_{11}$ ,  $C_{12}$ ,  $C_{13}$ ,  $C_{33}$ ,  $C_{44}$ ) are required. Table 2 summarizes our computed results of the five independent elastic constants of  $\text{Ti}_3\text{SiC}_2$  and  $\text{Ti}_3\text{AlC}_2$  alongside available experimental and theoretical data.

For stability, a hexagonal crystal must satisfy the Born-Huang stability criteria<sup>31</sup>;

$$C_{11} > 0; C_{11} - C_{12} > 0; C_{44} > 0; (C_{11} + C_{12})C_{33} - 2C_{13}^2 > 0 \quad (2)$$

As presented in Table 2, the computed results of the independent elastic constants for  $\text{Ti}_3\text{SiC}_2$  and  $\text{Ti}_3\text{AlC}_2$  MAX phase compounds satisfy the mechanical stability criteria which signify that all the compounds are mechanically stable. It is also well known that elastic constants  $C_{11}$ , and  $C_{33}$  shows linear compression resistances along  $a$  and  $c$  directions, respectively, whereas  $C_{12}$ ,  $C_{13}$ , and  $C_{44}$  are related to the shape elasticity. Consistent with Table 2, the value of  $C_{11}$  is higher than  $C_{33}$  for both  $\text{Ti}_3\text{SiC}_2$  and  $\text{Ti}_3\text{AlC}_2$  compounds which indicate that these materials are more easily compressible along  $c$ -axis than along the  $a$ -axes and also agree well with that of (43).

Comp.	XC	$C_{11}$	$C_{12}$	$C_{13}$	$C_{33}$	$C_{44}$	Ref.
$\text{Ti}_3\text{AlC}_2$	PBE	277	93	70	242	114	This work
	Exp.	361	75	70	299	124	<sup>32</sup>
	Others	353	75	69	296	119	<sup>32</sup>
$\text{Ti}_3\text{SiC}_2$	PBE	326	98.3	115	317	143	This work
	Exp.	365	125	120	375	122	<sup>32</sup>
	Others	366	94	100	352	153	<sup>32</sup>

Table 2. Computed elastic constants  $C_{ij}$  (GPa) alongside experimental and theoretical results.

From the computed elastic constants, several polycrystalline elastic moduli comprising, bulk, shear, Young moduli, and Poisson's ratio were evaluated using Voigt<sup>33</sup>, Reuss<sup>34</sup>, and Hill<sup>35</sup> approximations. It is assumed that, in the Voigt scheme, the strain is uniform all along the polycrystalline materials aggregating to external strain. By following this approach, for the hexagonal lattices, the Voigt shear modulus ( $G_V$ ) and Reuss shear modulus ( $G_R$ ) are expressed as:

$$G_V = \frac{1}{15} \{2C_{11} - C_{12} + C_{33} - 2C_{13}\} + \frac{1}{5} \left\{ 2C_{44} + \frac{1}{2}(C_{11} - C_{12}) \right\} \quad (3)$$

$$G_R = \frac{5}{2} \left\{ \frac{[(C_{11} + C_{12})C_{33} - 2C_{13}^2]C_{44}C_{66}}{3B_V C_{44} C_{66} + [(C_{11} + C_{12})C_{33} - 2C_{13}^2](C_{44} + C_{66})} \right\} \quad (4)$$

And Voigt bulk modulus ( $B_V$ ), Reuss bulk modulus ( $B_R$ ) by:

$$B_V = \frac{1}{9} \{2(C_{11} + C_{12}) + C_{33} + 4C_{13}\} \quad (5)$$

$$B_R = \frac{(C_{11} + C_{12})C_{13} - 2C_{13}^2}{C_{11} + C_{12} + 2C_{33} + 4C_{13}} \quad (6)$$

Hill showed that Voigt/Reuss averages gives upper and lower bounds, and therefore, proposed that real effective moduli can be approximated by the arithmetic mean of the two bounds<sup>36</sup>. Thus, using Hill's approximations

$$B = \frac{1}{2}(B_R + B_V), \quad G = \frac{1}{2}(G_R + G_V) \quad (7)$$

We have also computed  $Y$ , and  $\eta$ , which are commonly evaluated for polycrystalline materials to study their hardness. Both  $Y$  and  $\eta$  are defined by the following expressions as;

$$Y = \frac{9BG}{3B + G}, \quad \eta = \frac{3B - 2G}{2(3B + G)} \quad (8)$$

The computed bulk modulus, Young's modulus, shear moduli, and Poisson's ratio of both  $Ti_3SiC_2$  and  $Ti_3AlC_2$  as defined in Equations (3-8) are listed in Table 3. The calculated values for the bulk modulus of  $Ti_3SiC_2$  and  $Ti_3AlC_2$  are 139 GPa and 182 GPa respectively. These values agree well with the reported value by<sup>32</sup>, with less than 13% and 7% deviation respectively for  $Ti_3AlC_2$  and  $Ti_3SiC_2$ . Moreover, our results for shear modulus of 87 GPa for  $Ti_3AlC_2$  although are lower than the reported experimental value in Table 3, the results of

Ti<sub>3</sub>SiC<sub>2</sub> of 121 GPa are in good agreement with the reported value. Comparing Tables 3 and 1, it can be seen that the calculated value of  $B$  obtained from the single crystal elastic constants summarized in Table 3 has approximately the same value as the one obtained from the data fitting in the Murnaghan's equation of state (Table 1). This clearly indicates the accuracy and reliability of our computed elastic constants for both Ti<sub>3</sub>SiC<sub>2</sub> and Ti<sub>3</sub>AlC<sub>2</sub> MAX phase compounds.

Comp.	$B$	$Y$	$G$	$\eta$	$B^{-1}$	$B/G$	$C_c$	$A$	$H_V$	Ref.
Ti <sub>3</sub> AlC <sub>2</sub>	139	215	87	0.24	0.007	1.60	-44	1.203	40.28	This work
	161.2	321	132	0.178	0.006	1.22	-50	0.971	36,88	<sup>1,32</sup>
Ti <sub>3</sub> SiC <sub>2</sub>	189	297	121	0.23	0.005	1.56	-28	1.398	46.75	This work
	203.9	307	123	0.248	0.005	1.66	-53	1.202	25,53	<sup>1,32</sup>

Table 3. Computed bulk modulus  $B$  (GPa), Young modulus  $Y$ (GPa), shear modulus  $G$  (GPa), Poisson's ratio  $\eta$ , compressibility  $B^{-1}$  (GPa)<sup>-1</sup>, Pugh's ratio ( $B/G$ ), Cauchy pressure ( $C_c$  in GPa), anisotropic factor- $A$  and Vicker's hardness  $H_V$ .

Following the Pugh ratio,  $B/G$  shows the brittle or ductile character of materials. Pugh's critical value is 1.75. The calculated ratio  $B/G$  for Ti<sub>3</sub>AlC<sub>2</sub> and Ti<sub>3</sub>SiC<sub>2</sub> are 1.60 and 1.56, respectively, which are less than Pugh's critical value. As such, these compounds have a brittle feature which agreed well with the result given in Table 3<sup>37</sup>. Cauchy relation which is defined as:  $C_c = C_{13} - C_{44}$  is another parameter signifying ductility or brittleness of a material. Positive values of  $C_c$  shows ductility otherwise the material is brittle<sup>38</sup>. The evaluated  $C_c$  of the ternaries are -44 and -28 GPa respectively. From these values, one can conclude that the studied materials are brittle in nature which confirmed the Pugh's result. Consequently, the brittle nature of Ti<sub>3</sub>AlC<sub>2</sub> and Ti<sub>3</sub>SiC<sub>2</sub> can be related to their ceramic character.

Young's modulus ( $Y$ ) measures the stiffness in materials, the higher the  $Y$ , the stiffer a material is. Our result presented in Table 3 shows that there is good agreement with the reported values of 215 GPa and 297 GPa for Ti<sub>3</sub>AlC<sub>2</sub> and Ti<sub>3</sub>SiC<sub>2</sub>, respectively. Information about the bonding forces can be obtained via Poisson's ratio ( $\eta$ ). The  $\eta$  for Ti<sub>3</sub>AlC<sub>2</sub> and Ti<sub>3</sub>SiC<sub>2</sub> are 0.24 and 0.23 respectively, which shows the interatomic forces within studied materials are central since upper and lower limits of the Poisson's ratio is 0.5 and 0.25 respectively and the calculated values fall within the two limits. Our results are closer to the experimental value of 0.178 for Ti<sub>3</sub>AlC<sub>2</sub> and 0.248 for Ti<sub>3</sub>SiC<sub>2</sub><sup>37</sup>. We have further calculated the Vickers' hardness  $H_V$ <sup>39</sup> of studied compounds. Vickers's hardness is another key mechanical property of solids that

explains stability, which is predicted using Equation (9). It is reported that solids with Vickers hardness  $H_V > 40$  GPa<sup>40</sup> are graded as super hard solids. The calculated  $H_V$  of  $\text{Ti}_3\text{AlC}_2$  and  $\text{Ti}_3\text{SiC}_2$  MAX phase compounds are 40.2831 GPa, and 46.7458 GPa respectively (Table 2). Therefore, these crystals, have an excellent ability to withstand dents or scratches.

$$H_V = 0.92 \left( \frac{B}{G} \right)^{1.3137} G^{0.708} \quad (9)$$

## Method

Ab initio calculations were used to investigate the elastic, and electronic properties of  $\text{Ti}_3\text{SiC}_2$  and  $\text{Ti}_3\text{AlC}_2$  using plane-wave pseudopotentials (PW-PP), as implemented in Quantum Espresso<sup>41</sup>. Generalized gradient approximation (GGA) parametrized by Perdew-Burke-Ernzerhof (PBE) is used to treat exchange, and correlation (XC) functional<sup>42</sup>. The core ion and valence electrons interactions were described using ultrasoft-pseudopotentials (UPP). A 600 Ry kinetic energy cut-off of the plane wave is used in the calculations. The electronic configurations:  $3s^2, 4s^2, 3p^6, 3d^2$  for Ti,  $3s^2, 3p^2$  for Si,  $3p^1, 3s^2$  for Al and  $2s^2, 2p^2$  for C were considered for the valence electrons. For the Brillouin zone (BZ) integration,  $12 \times 12 \times 12$  k-points mesh was generated using the Monkhorst-Pack scheme<sup>43</sup>. These parameters were found to be adequate to converge total energies up to  $10^{-8}$  eV. Both studied materials were fully relaxed relating to the cell parameters and atomic positions. Analysis of independent elastic constant ( $C_{ij}$ ) were performed using thermo\_pw<sup>30</sup>.  $C_{ij}$  delineates response of materials to macroscopic stress. In computing elastic constants, a small strain,  $e$  is applied to a material and the variation of total energy per volume,  $U$  of the material is obtained<sup>44</sup>:

$$U = \frac{\Delta E}{V_0} = \frac{1}{2} \sum_i^n \sum_j^m C_{ij} e_i e_j \quad (10)$$

where  $V_0$  and  $\Delta E$  represent the equilibrium volume and the difference between the initial and deformed total energy of the system respectively. The hexagonal  $\text{Ti}_3\text{SiC}_2$  and  $\text{Ti}_3\text{AlC}_2$  MAX phase compounds are characterized by five independent elastic constants which include  $C_{11}$ ,  $C_{12}$ ,  $C_{13}$ ,  $C_{33}$  and  $C_{44}$ . Therefore, the elastic matrix of the hexagonal system is written as<sup>45,46</sup>;

$$C_{ij} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & \cdot & \cdot & \cdot \\ \cdot & C_{11} & C_{13} & \cdot & \cdot & \cdot \\ \cdot & \cdot & C_{33} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & C_{44} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & C_{44} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} \quad (11)$$

## Conclusion

In this work, structural stability, electronic, and mechanical properties, independent micro elastic parameters were investigated using first-principles calculations. The complete set of independent elastic constants  $C_{ij}$ , shear modulus, bulk modulus, Poisson's ratio, and Young's modulus were calculated. Results of independent elastic constants showed the studied ternaries are mechanically stable. The investigated electronic band structures, TDOS, and PDOS showed the metallic behavior of these compounds. In  $Ti_3SiC_2$ , the top of the VB and bottom of the CB were found to be dominated by the Si-3p, C-2p, and Ti-3d energy states while for the  $Ti_3AlC_2$  the top and bottom of VB and CB were respectively were found to be shaped by Al-3p, C-2p, and Ti-3d orbitals. We expect that our findings will inspire additional experimental and theoretical studies on these interesting MAX phases.

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## Author contributions

**S. T A.** Performed calculations, analysis, interpretation, and preparation of original draft. **A. S.:** Supervision, validation, and approval of final draft. **R. A. :** Proofreading and validation of results. **I. M. C** and **N. F A. :** Analysis, and interpretation of the result. **B. U. H. :** Review and proofreading.

# Figures

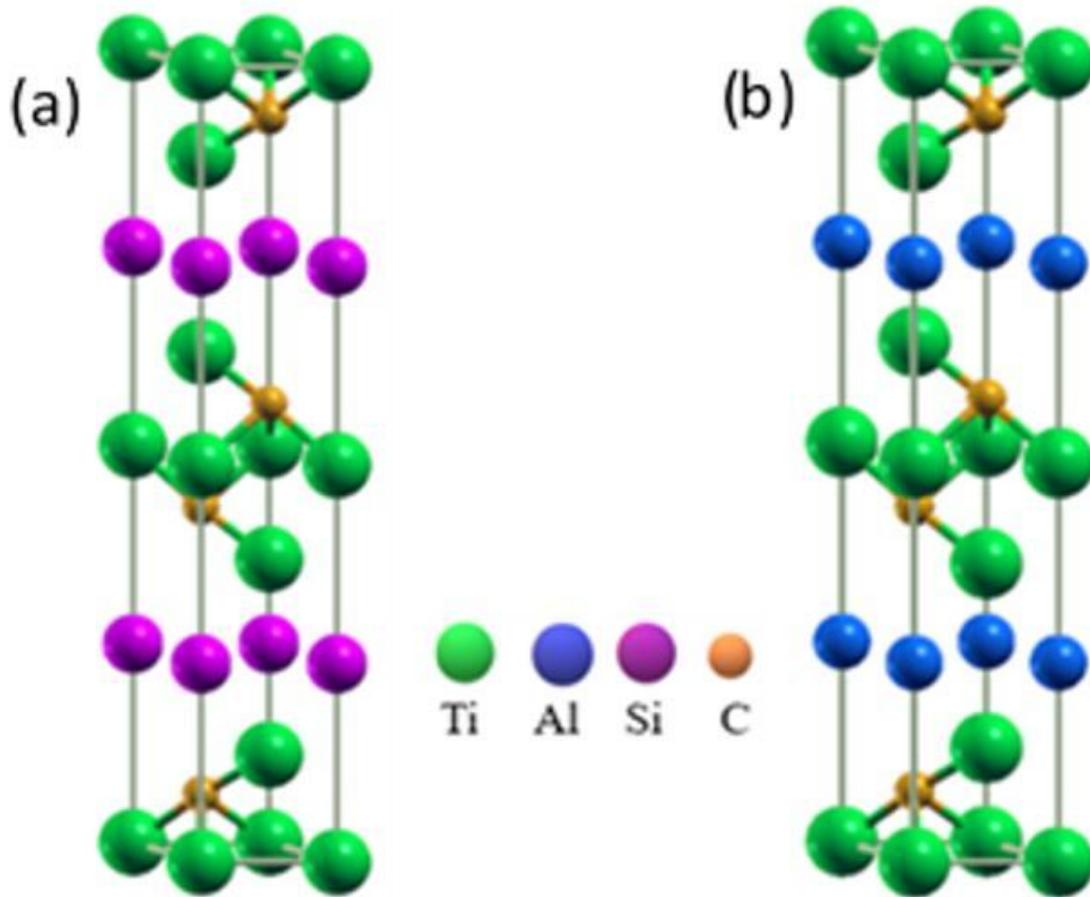


Figure 1

Crystal structure of (a)  $Ti_3AlC_2$  (b)  $Ti_3SiC_2$  MAX phase compounds.

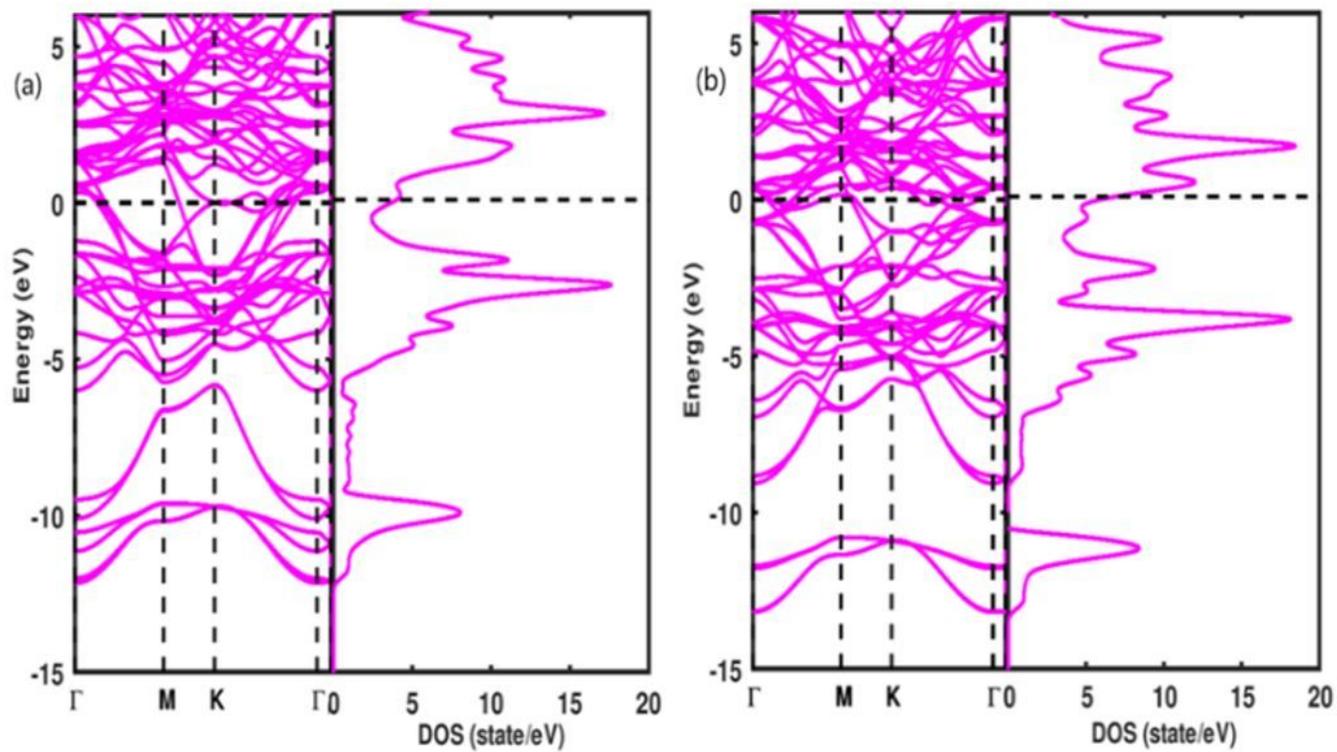


Figure 2

Band structures and TDOS of (a)  $\text{Ti}_3\text{SiC}_2$  (b)  $\text{Ti}_3\text{AlC}_2$  MAX phase compounds.

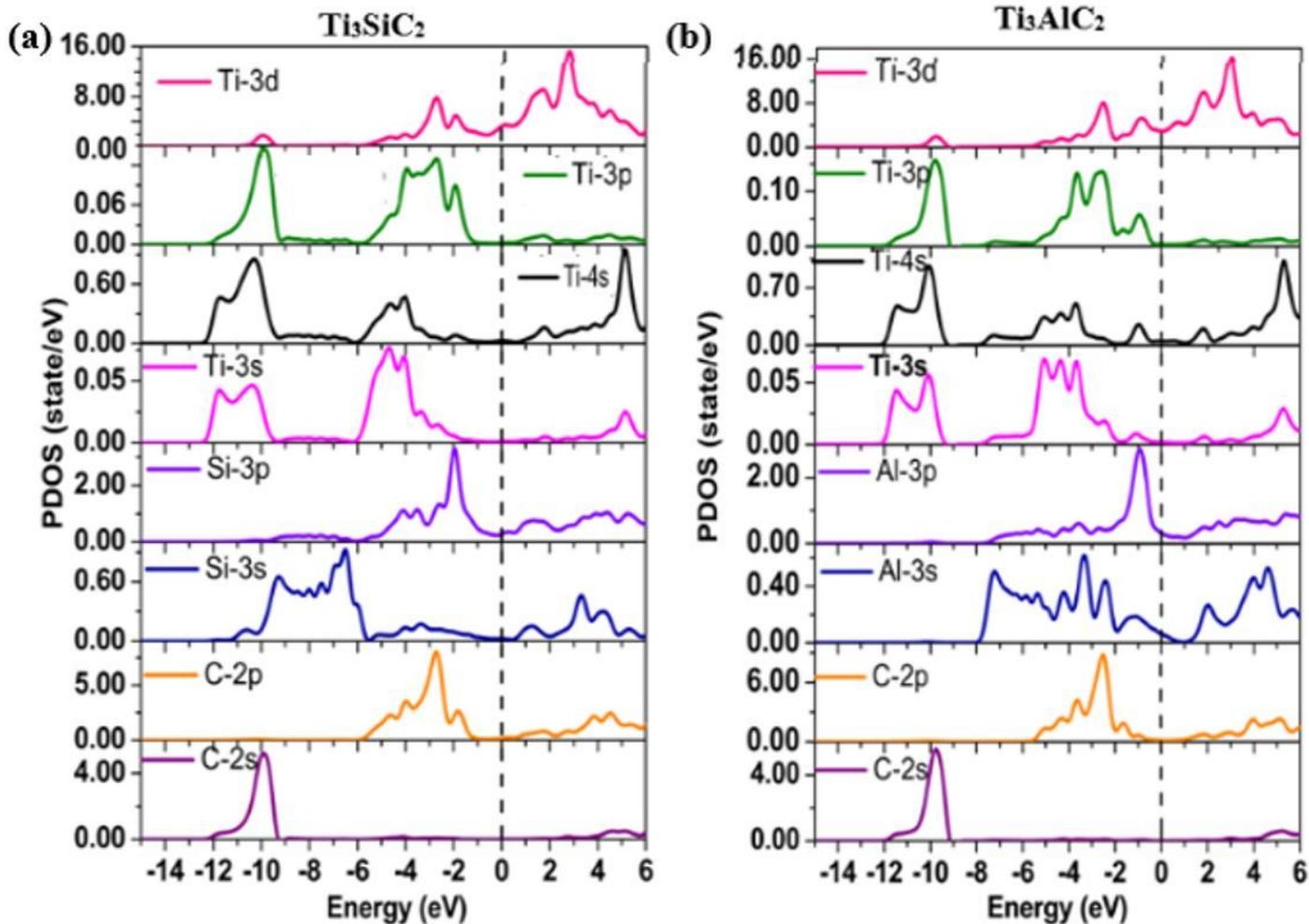


Figure 3

Calculated PDOS of (a)  $\text{Ti}_3\text{SiC}_2$  and (b)  $\text{Ti}_3\text{AlC}_2$  MAX phases.

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