

A Novel Theoretical Study of Elastic and Electronic Properties of M_2CdC ($M = Zr, Hf,$ and Ta) MAX Phases

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In this study, we have investigated the structural, electronic, and elastic properties of the M_2CdC ($M = Ta, Zr,$ and Hf) MAX phases, using the first-principle methods based on the density functional theory. The calculated formation energies revealed that these compounds are thermodynamically stable in the hexagonal MAX phase. The stability is confirmed by the elastic constants and the conditions of mechanical stability criterion. Also, we have determined the bulk and shear modules of the Young modulus and the Poisson coefficient. The band structures indicate that the three materials are electrically conductive. The chemical bond in M_2CdC is covalent-ionic in nature with the presence of metallic character. For the density of states the hybridization peak between $M d$ and $C p$ occurs in the lower energy range. We have found that there is no gap for these materials due to the existence of a maximum peak of DOS around Fermi level.

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1. Introduction

For fifty years, the carbides and nitrides materials have been known for their interest in research. In the 1960s the searchers discovered more than 100 carbides and nitrides. The so-called nanolaminates or MAX phases since their discovery by Nowotny et al. [1] have attracted a lot of interest among the research community due to their remarkable properties having attributes of both ceramic and metal [1, 2]. Their general formula can be written as $M_{n+1}AX_n$ where M is a transition metal, A is a group element and X is carbon and/or nitrogen, and $n = 1-3$ [2, 3]. Most of the MAX phases have M_2AX stoichiometry.

The coordination of the A element is trigonal prismatic, whereas for X it is octahedral [4]. For this crystal structure, the height of the M atoms above the X sheets is determined by a free internal parameter designated by Z_M . Then, the dimensionless crystallographic coordinate is defined by $z_M = Z_M/c$, where the planes M and A are evenly spaced for the ideal value of $z_M = 1/12 = 0.0833$ [4]. Generally, the MAX phases have interesting properties; they are good electrical and thermal conductors [5] resistant to oxidation, tolerant damage and relatively low, low thermal expansion, elastically rigid [6] high elastic modulus machinable [7] excellent thermal resistance and corrosion resistance [79]. Besides,

the MAX phases are used as trainers for health care products, as well as hot pressing tools and resistance heating elements [10, 11]. Bortolozzo et al. [12] computed the magnetic measurements and the resistivity of Ti_2InC by X-ray diffraction. Scabarozzi et al. [13] report on correlations of specific measurements of heat and transport in the MAX phase family. In addition, the electronic properties of these materials have been studied theoretically and experimentally [14]. Recently, the physical properties of thin films MAX phases have been reported [10], where the anisotropy of their conductivity is of great interest, but it is difficult to solve this problem experimentally [10].

The two-dimensional (2D) or MXenes materials with M a transition metal and X are C or N have attracted much attention because of their unique mechanical and electronic properties and their many potential applications [15]. Recently, the family of 2D materials was synthesized by the exfoliation of the layered ternary transition metal carbides, which are known as MAX phase [16, 17]. The layered structure does the exfoliation of the MAX phases which are feasible by suppression of the group "A" ($Al, Si, Ga, In,$ and Sn) from the bulk MAX phases, 2D MXenes which share the structural similarities with graphene can be obtained [18]. The extraordinary properties of 2D MXenes have been studied invasive since its experimental synthesis [19]. High conductivities and high elastic moduli are found in MXenes [15]. The study of the carbide properties of transition metals of the general formulae M_2C or M is a transition metal of column V or VI of the periodic table ($M = Zr, Hf, Ta$) are

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already studied in [15, 18, 20–25], can be concluded in the following points.

1) All the looked MXenes are metallic in the strain free state and the metallic characteristics are not influenced even with a large applied strains [15].

2) The formation energy decreases with the increase in the number of valence electrons. This can be attributed to the filling of the anti-bound states [21].

3) The type of bonding in these materials is a mixture of a metallic character with a mixture of the covalent bonds of ionic character [21].

4) The bonding nature is rather covalent than metallic with, however, an ionic aspect. The ionic character of the M–C bond is determined by a large transfer of charge from the M atoms to the C atoms which are more electronegative [21].

5) Among the MXenes studied, the magnetic moment of Hf_2C exhibits a large variation which makes it magnetic with a magnetic moment of $1.5 \mu_B/\text{unit}$ at a strain of 1.80%. The analysis shows that the magnetism originates from the shift of the Hf bands ($5d$) [15].

6) 2D sheets of transition metal carbides are fairly inflexible when drawn along the basal plane. They should also be admirable conductors of electricity. This new family of solids, which we label MXenes, present much more possibilities of the composition of properties compared to graphene [23].

Our work supports the idea of the existence of a new class of superconducting materials. Despite all the efforts, it is obvious that the Zr_2CdC , Hf_2CdC , and Ta_2CdC MAX phases compounds have not been subjected to theoretical and experimental studies. The aim of our work is to calculate and investigate the structural, electronic, and elastic properties of these three MAX phases, using first-principle calculations of density functional theory (DFT) within the full-potential linearized augmented plane-wave (FP-LAPW) approach.

2. Method of calculation

We have computed the structural, electronic, elastic properties of the M_2CdC compounds, with $\text{M} = \text{Ta}$, Zr , and Hf , using the first-principle calculations of density functional theory (DFT) based on the full-potential linearized augmented plane-wave (FP-LAPW) method as implemented in WIEN2k code [26, 27] which is better approach to calculate many proprieties for several materials. In our calculations, we have treated the exchange and correlation potential by the use of local density approximation (LDA) defined by Perdew and Wang [28].

The M_2CdC ($\text{M} = \text{Ta}$, Zr , Hf) three materials belong to the MAX phases, which have a hexagonal structure with a space group $P6_3/mmc$, No. 194 (see Fig. 1). The electronic configurations of the sets of the system studied are: $\text{Ta}((\text{Xe})5d^36s^2)$, $\text{Zr}((\text{Kr})5s^24d^2)$, $\text{Hf}((\text{Xe})6s^24f^{14}5d^2)$, $\text{Cd}((\text{Kr})4d^{10}5s^2)$, and $\text{C}((\text{He})2s^22p^2)$. We have chosen muffin-tin radii R_{MT} as 2.6, 1.9, 2.8, 2.65, and 1.4 for the Ta, Zr, Hf, Cd, and C atoms, respectively, in such a way that the muffin-tin spheres do not overlap. The number of k points used

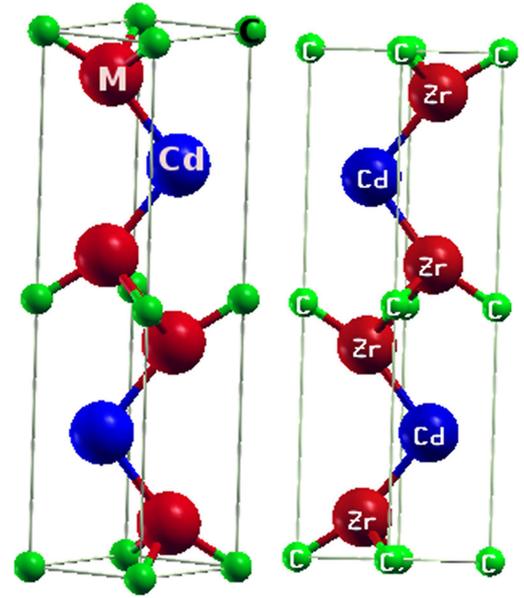


Fig. 1. The crystal structure of M_2CdC , $\text{M} = \text{Zr}$, Hf , Ta (space group $P6_3/mmc$).

in the integration of the first Brillouin zone is 1500 for the three compounds. The $R_{\text{MT}}K_{\text{max}}$ is taken equal to 7 (where R_{MT} represents the smallest radius of muffin-tin and K_{max} is the cut-off of plane waves), and inside the spheres the wave functions of the valence region extend to $l_{\text{max}} = 10$.

3. Results and discussion

3.1. Structural properties

To determine the elastic constants and electronic structures, we have firstly calculated the ground state properties of our compounds such as the total energies, the lattice constants (a and c), internal factor (Z), bulk modulus (B) and their pressure derivatives (B'). We have calculated these parameters by the fitting the total energy as a function of volume, using the Murnaghan equation [29]. Our results and other theoretical calculations are summarized in Table I. As in the case of other *ab initio* calculations for different compounds M_2AX (M : Ti, Zr, and Hf), [10, 30, 31], the bulk modulus values of the three compounds studied are compared to those of the MAX phases [32, 33]. The bulk moduli B of Zr_2CdC , Hf_2CdC , and Ta_2CdC were found to be 146.82, 165.46, and 211.78 GPa, respectively, and are the same as M_2SCM ($\text{M} = \text{Ti}$, Zr , Hf) [33], and that of Sun et al. [34]. We note that when we go on increasing Zr–Hf–Ta and fixing $\text{A} = \text{Cd}$ and $\text{X} = \text{C}$ the mass modulus of M_2AC increases. On the basis of the comparison between the bulk moduli of the M_2AlC phase ($\text{M} = \text{Ti}$, Zr , Hf ...) and the bulk modulus of the corresponding binary carbide MC. Sun et al. have shown that the M_2AC phases MAX can be divided into two groups. A group with transition metals V–B and VI–B where the bulk modulus of M_2AC is approximately the same as MC and the second group with transition metals IV–B where the M_2AC

mass modulus is significantly less than MC. Our calculations show that the three MAX phases studied in this ratio belong to the second group with their bulk moduli significantly lower than their binary carbides [3334]. Another remark is that the internal equilibrium coordinates Z_M increases as the atomic number of the transition metal (Zr→Hf→Ta) decreases. It is reported that Ta₂CdC is more difficult than Zr₂CdC and Hf₂CdC.

TABLE I

The equilibrium lattice parameters a , c [Å] and c/a , internal parameter Z , bulk modulus B and its pressure derivative B' for M₂CdC with M = Zr, Hf, and Ta.

	a	c	c/a	B_0	B'	Z
Ta ₂ CdC	3.145	13.997	4.44	211.78	4.4	0.073
Hf ₂ CdC	3.176	14.453	4.55	165.46	4.02	0.084
Zr ₂ CdC	3.226	14.839	4.59	146.82	4.03	0.081

3.2. The formation energies and cohesive energies

To study the relative stabilities of the hexagonal phases, it is necessary to calculate the energy of formation (E_{form}) per atom using the Eq. (1) [35]:

$$E_{\text{form}}^{\text{M}_2\text{CdC}} = \frac{E_{\text{tot}}^{\text{M}_2\text{CdC}} - [xE_{\text{at}}^{\text{M}} + yE_{\text{at}}^{\text{Cd}} + zE_{\text{at}}^{\text{C}}]}{x + y + z}. \quad (1)$$

Whither x, y, z indicate a number of M, Cd, and C atoms in a unit cell of in the cell, respectively $E_{\text{form}}^{\text{M}_2\text{CdC}}$, $E_{\text{form}}^{\text{M}}$, $E_{\text{form}}^{\text{Cd}}$, and $E_{\text{form}}^{\text{C}}$ are the calculated energies. M denotes a metal and Zr, Hf and Cd crystallizing in the hexagonal structure ($P63/mmc$, Mg prototype [3638], Ta crystallizes in the centered cubic structure of space $Im - 3m$, prototype W), C crystallizes in the diamond structure (spatial group $Fd3 - m$), [39]. There are two atoms in the unit cell for each metal. The formation energy calculation gives the following value. Values -0.81 , -0.55 , and -0.47 eV/atom for Zr₂CdC, Hf₂CdC and Ta₂CdC respectively are listed in Table II. All values are negative. It assures the stability of the compound since we have energetically favorable systems.

TABLE II

The calculated values of the formation energy E_{form} [eV/at.], bulk modulus B [Gpa], cohesive energy E_{coh} [eV/at.] and the valence electron concentration (val-el) for M₂CdC, with M = Zr, Hf, and Ta.

	Ta ₂ CdC	Hf ₂ CdC	Zr ₂ CdC
E_{eq}	-147450.66897	-143226.11555	-51278.10579
E_{form}	-0.47	-0.55	-0.81
E_{coh}	8.9	8.5	7.8
val-el	152	148	92
B	211.78	165.46	146.82
E_{F}	0.7	0.93	0.65

The importance of cohesive energy is the fact that it represents the ground state of the solid, its sign such measures that the solid is stable or not. The isolated atomic energies are calculated with the same WIEN2K

code using the base of the augmented plane wave. We calculated the energies of the individual atoms by increasing the unit cell of a face-centered cubic structure up to 30 Bor (about 16 Å), [40] for the three materials. The cohesive energy $E_{\text{coh}}^{\text{M}_2\text{CdC}}$ of M₂CdC is known as the total energy of the constituent atoms minus the total energy of the compound [35] is given by:

$$E_{\text{coh}}^{\text{M}_2\text{CdC}} = \frac{[xE_{\text{at}}^{\text{M}} + yE_{\text{at}}^{\text{Cd}} + zE_{\text{at}}^{\text{C}}] - E_{\text{tot}}^{\text{M}_2\text{CdC}}}{x + y + z}, \quad (2)$$

where $E_{\text{coh}}^{\text{M}_2\text{CdC}}$ is the total energy of the unit cell used in the present calculation, x, y, z are the atom numbers of M, Cd, C atoms in the unit cell, respectively, $E_{\text{coh}}^{\text{M}_2\text{CdC}}$ refers to the total energy of type M₂CdC in the equilibrium configuration $E_{\text{coh}}^{\text{M}}$, $E_{\text{coh}}^{\text{Cd}}$, $E_{\text{coh}}^{\text{C}}$ are the atomic energies isolated from the pure constituents. The calculated cohesive energies are shown in Table II. The calculated cohesive energies are respectively 7.8 eV / atom, 8.5 eV / atom and 8.9 eV / atom for Zr₂CdC, Hf₂CdC and Ta₂CdC. Therefore, The larger the absolute value, the more stable the crystal structure, From this result, it can be concluded that the Ta₂CdC configuration has the most structural stability. Because of the uppermost absolute value of the cohesive energy. and the Hf₂CdC configuration has relatively low structural stability, whereas the structural stability of the Zr₂CdC configuration is the worst because of the lowest absolute value of cohesive energy [41].

3.3. The electronic properties

The importance of the electronic properties of a material lies in the fact that they inform us about the electronic and thermal conductivity, they also make it possible to analyze and to understand the nature of the bonds which form between the different elements of this material; these properties include band structures, state densities and charge densities.

3.3.1. The electronic band structure

Figure 2 shows the band structure of the study systems calculated from the optimal values. Noting the overlap of the valence and conduction bands at Fermi level and the absence of a band. The valence bands are shifted to the conduction bands for these compounds. the states of lower energies of below Fermi level come from the C-2s states, these states are separated from the upper part of the valence band, the upper part of Valence consists mainly of states (M = Ta, Hf, Zr)- d , C- p , and Cd-5s, 5p. The states near the Fermi level are the (M = Ta, Hf, Zr)- d , states which offer birth to magnetic properties of this compounds [42]. This result confirms the metallicity of these materials. The band structures also exhibit strong anisotropic characteristics with smaller energy dispersion along the c axis. The electrical conductivity is anisotropic for this material, i.e. the electrical conductivity along the c axis is much lower than that of the basal plane [10]. The three materials are characterized by the existence of pseudo-gaps, between bond states and unbound. A similar pseudo deviation is also found in many other MAX phases [3143].

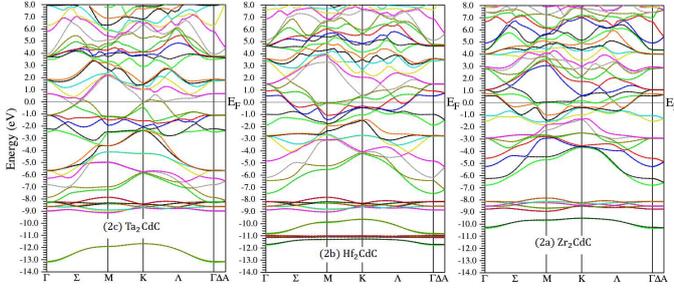


Fig. 2. Calculated band structure of M_2CdC : $M = Zr, Hf, Ta$.

3.3.2. The density of states

The projected total (DOST) and partial (DOSP) state densities between -14 and 8 are illustrated in figures. (3a, 3b, 3c, 3d), respectively, and the Fermi level is taken as the origin of the energies. The analysis of the total and partial densities of the Zr_2CdC , Hf_2CdC , Ta_2CdC indicates a non-zero density at Fermi level and the absence of the forbidden band E_g allows us to deduce that these materials have a metallic nature. Thus, the wide values of the Fermi energies (E_F) (see Table II) confirms this result. On the other hand, an important characteristic is the existence of a pseudo gap in the DOS in the vicinity of the Fermi level, which is an indication of stability [43]. At the level of Fermi, the DOS is 2.44, 2.04 and 1.77 states per unit cell per eV, for Zr_2CdC , Hf_2CdC and Ta_2CdC respectively. Therefore there is a provision, to the decrease of E_F with increasing atomic numbers of the transition metal M. It can be concluded that Ta_2CdC is more conductive than Hf_2CdC and Zr_2CdC . On the other hand, the carbon and cadmium do not imply in the DOST at Fermi level which means they do not involve

in the conduction properties. We have noted that the electrons of the d state of metal M ($M = Zr, Hf, Ta$) are predominantly involved in DOST due to the peak plus near-Fermi level instance, which shows that the metallic character of these compounds comes from the d -state of the transition metal. The PDOS (Fig. 3b,c,d) shows another interesting feature: the Zrd and Cp hybridization peak is lower in energy than that of Zrd and Cdp . This suggests that the M ($M = Zr, Hf, Cd$) and C are more rigid than the Md , Cdp bonds. These results are in agreement with other results calculated on some MAX phases [44].

3.3.3. The charge density

The calculation of the electronic charge density which is generally in a plane or in a direction, the latter informs us of the transfer of charge and therefore of the nature of the connections. Thus, in order to visualize the nature of the character of the Zr_2CdC bonds, Hf_2CdC , Ta_2CdC we calculated the charge densities as the contour in the basal plane (112). To better understand it is important to call the electronegativity of the atom, the electronegativity of an atom is a concept that covers two properties: Its ability to attract electrons from its established bonds

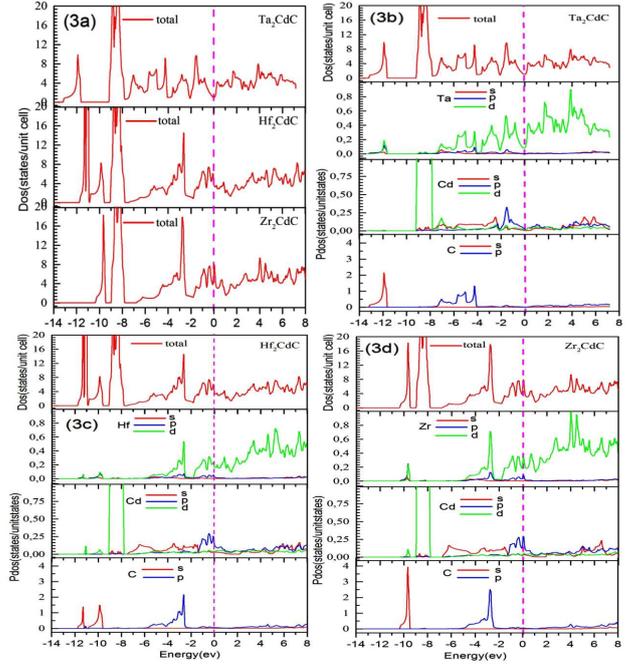


Fig. 3. Total and partial density of states of M_2CdC , $M = Zr, Hf, Ta$. The Fermi level is set to zero energy and marked by a vertical dashed line.

with other atoms and its ability to keep them. Actually speaking of electronegativity of an isolated atom has no meaning since this property only manifests itself when links are established. However for a given element the behavior is substantially constant and an average numerical value representative of the electronegativity character of this atom can be given. The analysis of the charge density in figure 4(4a, 4b, 4c) allows us to deduce that the interaction between the atom ($M = Zr, Hf, Ta$) and the carbon is covalent in nature and very hard. Thus, the more electronegative nature of the C atom (electronegativity of C = 2.55) [45] compared to the M atom ($M = Zr, Hf$ and Ta) (electronegativity of Zr, Hf and Ta is 1.33, 1.3, 1.5, respectively) [45] confirms the presence of an ionic bond between M and C. Whereas the more electronegative nature of Cd (electronegativity of Cd = 1.69) [45] confirms the presence of the ionic bond between Cd and M. The chemical bond of these compounds is metallic covalent-ionic. The covalent bond is due to the local interactions of the hybridization M ($M=Zr, Hf, Ta$)- d and C- p , and the ionic bond is relative to the local interactions of the hybridization $M = Zr, Hf, Ta$ - d and C- p .

3.4. Elastic properties

The elastic properties have an important role by giving useful knowledge on the nature of the bonding between the neighboring atomic planes, the elastic constants are used to define the mechanical stability of the deformation of the crystal face. as the elastic constants for the M_2CdC compound is evaluated for the first time, and no experimental or theoretical study exists, we can not to liken them with other results. For a hexagonal crystal

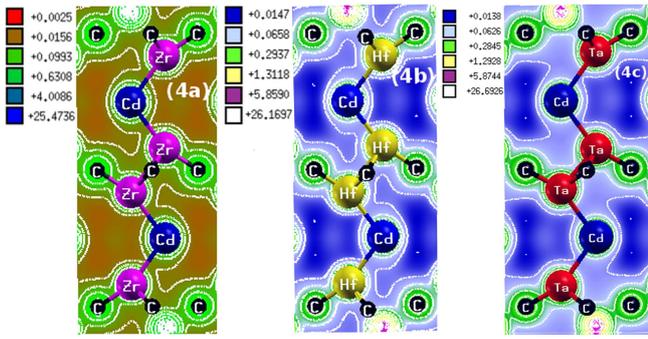


Fig. 4. Charge-density contours for: (a) Zr_2CdC , (b) Hf_2CdC , (c) Ta_2CdC . Cuts are made in the $(11\bar{2})$ plane.

has six different symmetry elements (C_{11} , C_{12} , C_{13} , C_{33} , C_{44} and C_{66}), and only five of them are independent since $C_{66} = \frac{1}{2}(C_{11} - C_{12})$. Criterion of the mechanical stability is [46, 47]:

$$\begin{cases} (C_{11} - C_{12}) > 0 \\ (C_{11} + C_{12})C_{33} - 2C_{13}^2 > 0 \\ C_{11} > 0, C_{44} > 0 \end{cases} \quad (3)$$

TABLE III

Elastic constant C_{ij} for M_2CdC with $M = Zr, Hf,$ and Ta .

	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	B/C_{44}
Ta_2CdC	408.32	106.51	107.6	218.19	151.16	150.9	1.18
Hf_2CdC	289.6	108.52	84.25	307.26	36.43	90.54	4.39
Zr_2CdC	277.55	77.38	78.12	287.28	99.80	100.09	1.45

The computations of the second-order elastic constants of M_2CdC are shown in Table III. It can be said that the M_2CdC , compounds are mechanically stable because all these elastic constants are positive and cater for the criterion of mechanical stability [47]. C_{44} module shows that the Ta_2CdC is harder than Zr_2CdC and Hf_2CdC , this result is similar to that found in the optimization part. The B/C_{44} values indicate that Hf_2CdC is more ductile than Ta_2CdC and Zr_2CdC (see Table IV). Malleable crystals are characterized by large B/C_{44} value, whereas brittle solids are characterized by small B/C_{44} value [46]. The compressibility modulus B and the shear modulus G are obtained from the Hill approximation, this approximation is based on the Reuss and the Voigt approaches with $B = (B_V + B_R) = B_H$ (the Hill bulk modulus) and $G = (G_V + G_R) = G_H$ (the Hill shear), [47]. These results are presented in Table IV. The Young modulus E and the Poisson coefficient ν for a hexagonal structure are related to the compression modulus B and shear modulus G , this module expresses the resistance of the material to a unidirectional stress are determined by the relations $E = 9BG/(3B + G)$ and $\nu = (3B - E)/6B$ [47]. In general, the Young modulus for the MAX phases is slightly less than the MAX binary. The cracks in the crystals are directly related to the anisotropy of the thermal and elastic properties to the hexagonal system and the existence

of a strong bond between the transition metal atoms and the carbon and the relatively weak bond between the metal atoms and the Cd atoms bring us back to the elastic anisotropic behavior of these compounds. [47]. The hexagonal systems can be characterized by two distinct anisotropy factors [48] For the hexagonal structure, the shear anisotropy factor is defined by two forces in the two directions [011] and [010] exerted on the (100), [49]. We define the anisotropy factor $A_G = \frac{4C_{44}}{C_{11} + C_{33} - 2C_{13}}$. The compressibility anisotropy factor is defined as the ratio of the unidirectional mass modulus along [001] and [100], [49]: by: $A_B = \frac{(C_{33} - C_{13})}{(C_{11} - C_{13}) - (C_{13} - C_{12})}$. The shear anisotropy is more important than the incompressibility of the anisotropy and any deviation greater or less than 1 corresponds to an elastic anisotropy [49] From the Criterion of Pugh [48], a material must behave ductile if $G/B < 0.5$, otherwise it should be fragile. Finally, the ratio between the linear coefficients of compressibility k_c/k_a of the hexagonal crystals can be obtained from the index $f = \frac{k_c}{k_a} = (C_{11} + C_{12} - 2C_{13})/(C_{33} - C_{13})$ [50]. The results show that for Ta_2CdC , Hf_2CdC and Zr_2CdC , $f = (2.7, 1.03, 0.95)$ respectively, it can be said [51] that if:

- 1) $f = 1$, the material is isotropic;
- 2) $f < 1$ the compressibility of crystal along c axis is less than that of a -axis;
- 3) $f \geq 0$ the material is soft in c direction.

We observe, according to the results shown in Table IV, the Young E modulus, compression B , shear value G and the Poisson coefficient ν of the three compounds studied are comparable to those of the MAX phases [52], it is indicated that Ta_2CdC is harder than Zr_2CdC and Hf_2CdC .

TABLE IV

The bulk modulus B , shear modulus G , the Young modulus E (all in [GPa]), the Poisson ratio ν , anisotropic factors A_G , A_B linear compressibility ratio $f = \frac{k_c}{k_a}$ for M_2CdC with $M = Zr, Hf,$ and Ta .

	E	B	G	A_G	A_B	ν	f	G/B
Ta_2CdC	320.02	178.84	133.15	1.47	0.33	0.2	2.7	0.74
Hf_2CdC	173.54	160.05	65.77	0.34	-0.44	0.3	1.03	0.41
Zr_2CdC	245.09	145.5	100.51	0.98	1.42	12.56	0.95	0.6

4. Conclusion

The structural, electronic and elastic properties of the three superconducting MAX phases Zr_2CdC , Hf_2CdC , and Ta_2CdC were investigated by using the first-principle calculations of DFT. The computed lattice constants are very consistent with other calculations. The band structures and total densities of states reveal that the three materials exhibit metallic conductivity. From elastic constants and the stability conditions, we have found that these compounds are mechanically stable in the hexagonal MAX phase. Besides, we have calculated their shear modulus G , Young modulus E and the Poisson ratio ν . The carbide phase is found to be brittle, while the nitride

phase is less fragile (near the Border line). We have calculated the energy of formation (E_{form}) per atom; this energy indicates that these materials are formed. The M–d and C–p bonds are stronger than the M–d and Cd–p bonds. M_2CdC has a metal-covalent-ionic character in nature.

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