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J. Appl. Phys. 119, 044903 (2016)

<https://doi.org/10.1063/1.4940723>



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Mechanical and electronic properties of antiperovskite Ti-based compounds AXTi_3 ($X = \text{C}, \text{N}$): A first-principles investigation

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(Received 1 September 2015; accepted 12 January 2016; published online 27 January 2016)

In this paper, we systematically studied the mechanical and electronic properties of a series of antiperovskite-type Ti-based ternary carbides and nitrides AXTi_3 ($A = \text{Ba}, \text{Ca}, \text{In}, \text{Sn}, \text{Sr}, \text{Zn}, \text{Cu}, \text{Al}, \text{Ga}, \text{Cd}, \text{and La}$; $X = \text{C}, \text{N}$) from first-principles calculations. By calculating the formation energies, elastic constants, and other mechanical parameters, we predicted that 7 carbides ACTi_3 and 7 nitrides ANTi_3 compounds are stable among the 22 compounds. The predicted large Young's modulus and high hardness imply a good mechanical application prospect of AXTi_3 . Particularly, SnNTi_3 was found to show ferromagnetic ground state. For the electronic structure, our results confirm that the compounds are metallic in nature, and the density of states near the Fermi energy is predominately contributed by Ti-3d states. The effect of A- and X-site atom doping on AXTi_3 can be evaluated by rigid band approximation. Our prediction will be useful for the experimental exploration of the new antiperovskite compounds. © 2016 AIP Publishing LLC.

<http://dx.doi.org/10.1063/1.4940723>

I. INTRODUCTION

The 3d transition-metal based antiperovskite compounds AXM_3 (A usually is main group element; $X = \text{B}, \text{C}, \text{and N}$; and M is 3d transition metal element) with simple cubic structure (Fig. 1) have attracted a lot of attention because of the emerging physical properties. With high amount of magnetic element Ni, MgCNi_3 shows a sizeable superconductivity.¹ Giant magnetoresistance,^{2,3} large negative magnetocaloric effect,^{4,5} giant negative thermal expansion,^{6,7} magnetostriction,⁸ and nearly zero temperature coefficient of resistivity^{9,10} emerge in Mn-based antiperovskite. Recently, Fe- and Co-based antiperovskites have also been extensively investigated.^{11–14} Theoretically, the abundant physical properties of AXM_3 originate from the high amount of 3d elements.^{15,16} One can expect that the early transition metal ($M = \text{Sc}, \text{Ti}, \text{V}, \text{Cr}$) based antiperovskites may also show novel properties. However, the early transition metal based antiperovskites are less studied. Although there are theoretical predictions of superconductivity in Sc- and Cr-based antiperovskites,^{16–22} there are few experiment reports of the synthesis and physical properties.^{18,23} For Ti-based antiperovskites, it seems that only AlCTi_3 was experimentally reported for the mechanical properties.²⁴ To the best of our knowledge, no AXV_3 is reported. The situation might be due to the difficulty of sample preparation. Therefore, it is very necessary to study the stabilities and ground states of early transition metal based antiperovskites theoretically to guide the experimental exploration.

In this work, we theoretically investigate Ti-based antiperovskite AXTi_3 ($A = \text{Ba}, \text{Ca}, \text{In}, \text{Sn}, \text{Sr}, \text{Zn}, \text{Cu}, \text{Al}, \text{Ga}, \text{Cd}, \text{and La}$; $X = \text{C}$ and N) through the first-principles

calculation based on density functional theory (DFT). The lattice parameters, formation energies, and ground states of a series of AXTi_3 are predicted. Since Ti-based alloys usually have extraordinary mechanical properties, the mechanical parameters of the predicted stable AXTi_3 are calculated. The predicted large Young's modulus and high hardness imply a good mechanical application prospect of AXTi_3 . The electronic structure is also investigated. The bands around Fermi energy (E_F) are predominately contributed by 3d electrons of Ti, while the E_F is strongly influenced by the total valence electrons. According to the Stoner's magnetism,²⁵ the spin polarization of AXTi_3 is also discussed, and we find that SnNTi_3 shows ferromagnetic (FM) ground state. Our prediction will be helpful for the experimental exploration of Ti-based antiperovskite compounds.

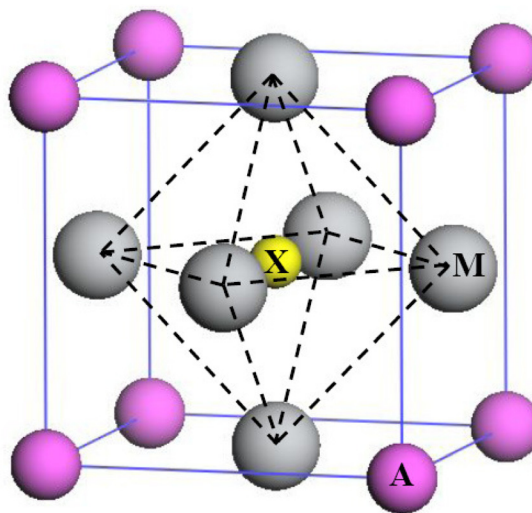


FIG. 1. Crystal structure of AXM_3 .

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TABLE I. Lattice parameter a , magnetic moments M , and the formation energies ΔE of AXTi_3 .

ACTi_3	a (Å)	ΔE_{NM} (eV/cell)	ΔE_{FM} (eV/cell)	M (μ_B /cell)	ANTi_3	a (Å)	ΔE_{NM} (eV/cell)	ΔE_{FM} (eV/cell)	M (μ_B /cell)
BaCTi ₃	4.459	1.192	1.193	0	BaNTi ₃	4.377	3.737	3.737	0
CaCTi ₃	4.406	0.348	0.337	0	CaNTi ₃	4.327	1.999	1.999	0
InCTi ₃	4.243	-2.788	-2.789	0	InNTi ₃	4.191	-0.896	-0.896	0
SnCTi ₃	4.243	-2.941	-2.941	0	SnNTi ₃	4.200	-0.947	-0.948	1.01
SrCTi ₃	4.467	1.508	1.508	0	SrNTi ₃	4.386	3.280	3.280	0
ZnCTi ₃	4.165	-2.498	-2.492	0	ZnNTi ₃	4.087	-1.033	-1.033	0
CuCTi ₃	4.146	-1.860	-1.868	0	CuNTi ₃	4.061	-0.643	-0.643	0
AlCTi ₃	4.178	-3.013	-3.029	0	AlNTi ₃	4.124	-1.314	-1.314	0
GaCTi ₃	4.158	-3.190	-3.188	0	GaNTi ₃	4.105	-1.462	-1.462	0
CdCTi ₃	4.236	-2.295	-2.285	0	CdNTi ₃	4.179	-0.643	-0.643	0
LaCTi ₃	4.412	0.067	0.067	0	LaNTi ₃	4.341	1.755	1.755	0

II. COMPUTATIONAL DETAILS

DFT calculations are performed by means of the plane-wave pseudopotential representation through the Quantum-Espresso (QE) program.²⁶ The ultrasoft pseudopotentials are used to model the electron-ion interactions. We adopt the generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) parametrization²⁷ for the exchange correlation potentials. The cutoff energy and k-point sampling are checked for energy convergence. The cutoffs for wave functions and charge density are 60 Ry and 600 Ry, respectively. The electronic integration is performed over a $12 \times 12 \times 12$ -k-point mesh in the Brillouin Zone (BZ). Since all the compounds are metallic in nature, in our calculations, we use Marzari-Vanderbilt smearing method²⁸ with degauss equals to 0.02 Ry. The non-magnetic (NM) and FM states are studied in this work.

III. RESULTS AND ANALYSIS

A. Structural parameters and formation energies

We use the reported lattice parameters of antiperovskite compound AlCTi_3 ²⁹ to initiate the structural optimization for antiperovskite Ti-based compounds AXTi_3 . The optimization of atomic positions and unit cell is finished when the total energy changes less than 10^{-6} ha and the force on each atom is less than 10^{-5} ha/Bohr. The optimized lattice parameters of AXTi_3 are listed in Table I. The results show that the lattice parameter of AXTi_3 is basically proportional to the radius of A-site elements (see Fig. 2). The obtained lattice parameters are very close to the previous results.^{29–32}

One of the common methods of preparation of antiperovskite compounds is solid-state synthesis from fully mixed raw materials. Therefore, we assume that the AXTi_3 ($X = \text{C}, \text{N}$) could be synthesized using the same way. The formation energy ΔE is defined as the difference between the total energies of initial elements and final compounds

$$\Delta E_{\text{ACTi}_3} = E_{\text{tot}}^{\text{ACTi}_3} - (E_{\text{tot}}^{\text{A}} + E_{\text{tot}}^{\text{C}} + 3E_{\text{tot}}^{\text{Ti}}), \quad (1)$$

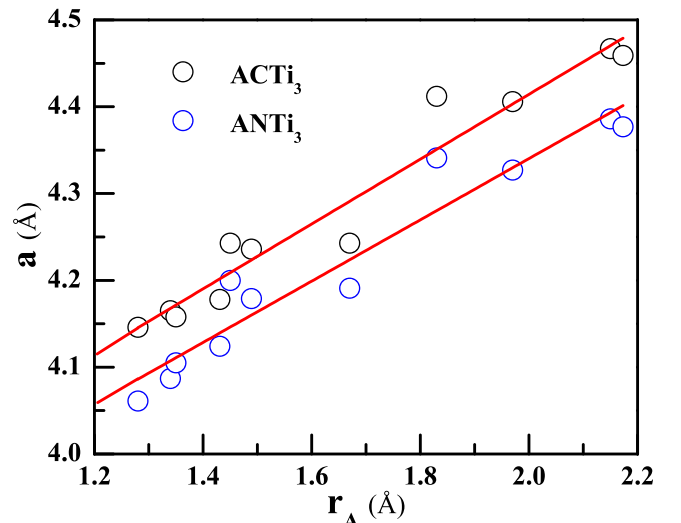
and

$$\Delta E_{\text{ANTi}_3} = E_{\text{tot}}^{\text{ANTi}_3} - (E_{\text{tot}}^{\text{A}} + E_{\text{tot}}^{\text{TiN}} + 2E_{\text{tot}}^{\text{Ti}}). \quad (2)$$

Here, $E_{\text{tot}}^{\text{AXTi}_3}$ is the total energy of final compounds, and $E_{\text{tot}}^{\text{A}}$, $E_{\text{tot}}^{\text{C}}$, $E_{\text{tot}}^{\text{TiN}}$, and $E_{\text{tot}}^{\text{Ti}}$ are the total energies of the initial

elements/compounds. One can expect that the compounds will be stable with respect to a mixture of the initial elements when $\Delta E < 0$. On the contrary, if $\Delta E > 0$, the compounds are unlikely to be synthesized under normal conditions. The calculated ΔE are shown in Table I. BaXTi_3 , CaXTi_3 , SrXTi_3 , and LaXTi_3 ($X = \text{C}, \text{N}$) show positive ΔE , implying that these compounds are hard to be synthesized under normal conditions. Indeed, the 3d transition metal based antiperovskites AXM_3 with $A = \text{Ba}, \text{Ca}, \text{Sr}$, and La have never been experimentally reported, which might be due to that these atoms with large radius strongly influence the MX_6 octahedra. Other AXTi_3 compounds seem to be stable according to the negative ΔE . Moreover, in the calculation of FM state, the magnetic moments of almost all the compounds considered are converged to zero except for SnNTi_3 (Table I). The spin polarization in AXTi_3 will be discussed later.

To check the dynamical stability, we calculate phonon dispersions of two typical compounds, BaCTi_3 and AlCTi_3 , which show positive and negative formation energies, respectively. The phonon results are consistent with the calculated formation energy results. As shown in Fig. 3(a), BaCTi_3 shows strong instability in the phonon dispersion, while for AlCTi_3 , the phonon dispersion suggests the dynamical stability of this compound (Fig. 3(b)).

FIG. 2. Lattice parameters of ACTi_3 and ANTi_3 .

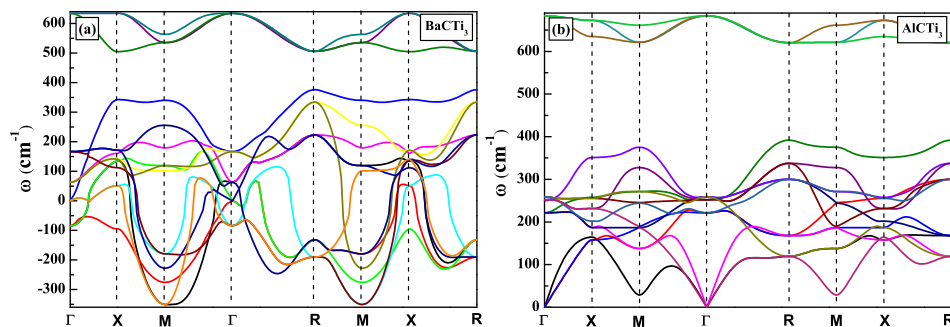


FIG. 3. The phonon dispersion curves of (a) BaCTi₃ and (b) AlCTi₃.

B. Mechanical properties

We calculate the elastic constants according to the finite-strain continuum elasticity theory.³³ The strain energy $\phi(\xi)$ per unit mass can be written as an expansion in the strain parameter ξ ³⁴

$$\phi(\xi) = \frac{1}{2}A_2\xi^2 + \frac{1}{6}A_3\xi^3 + o(\xi^4). \quad (3)$$

Here, A_2 and A_3 are the second- and third-order elastic constants, respectively. There are three independent second-order elastic constants (C_{11} , C_{12} , and C_{44}) for cubic structure. It is necessary to impose three strain tensors η_α in terms of ξ . η_α ($\alpha = 1, 2, 3$) and the corresponding coefficients A_2 are listed in Table II.

To obtain the elastic constants accurately, we change ξ with a step of 0.0025 for each η_α . As an example, the strain energy and the fitted polynomials for AlCTi₃ are shown in Fig. 4. The calculated elastic constants for the 14 stable ACTi₃ and ANT₃ are shown in Tables III and IV. It is well known that the generalized criteria for mechanically stable cubic crystals are $C_{11} > C_{12}$, $C_{44} > 0$ and $C_{11} + 2C_{12} > 0$.³⁵ Therefore, from the calculated values of elastic constants, we can conclude that almost all of compounds are mechanically stable, consistent with the result predicted by the formation energy calculation.

The elastic anisotropy factor A of cubic crystal can be described as

$$A = \frac{2C_{44}}{C_{11} - C_{12}}. \quad (4)$$

For a completely isotropic system, the anisotropy factor A takes the value of unity, and the deviation from unity measures the degree of elastic anisotropy.³⁶ According to our calculation, ANT₃ is more anisotropic than ACT₃, which can be understood by the following analysis. The elastic constant C_{44} represents the shear resistance in the [100] direction, which is related to the X-Ti bonding.²² It can be noted that

TABLE II. The coefficient A_2 and strain tensors η_α .

η_α	A_2
$\eta_1 = (\xi, 0, 0, 0, 0, 0)$	C_{11}
$\eta_2 = (\xi, \xi, 0, 0, 0, 0)$	$2C_{11} + 2C_{12}$
$\eta_3 = (\xi, \xi, \xi, 0, 0, 0)$	$C_{11} + 4C_{44}$

the calculated C_{44} of ACT₃ is slightly larger than that of ANT₃ with the same A-site atom, indicating that the C-Ti bonding is stronger, which is consistent with the previous calculations of AlXT₃ (X = C and N).³² On the other hand, $C_{11} - C_{12}$ turns out to be the stiffness associated with a shear in the [110] direction, which can be connected with the A-Ti bonding.²² Although A-M bonding is usually very weak in antiperovskite AXM₃, it can still influence the anisotropy of the material. For the present AXT₃, lattice parameter of ACT₃ is larger than that of ANT₃ with the same A-site atom. One can expect stronger A-Ti bonding in the nitrides, which leads to a bigger $C_{11} - C_{12}$ in ANT₃. Therefore, the ANT₃ is generally more anisotropic than ACT₃.

For cubic crystal, Voigt defined the bulk modulus B_V and shear modulus G_V as

$$B_V = \frac{C_{11} + 2C_{12}}{3}, \quad (5)$$

$$G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5}. \quad (6)$$

On the other hand, Reuss defined the bulk modulus B_R and shear modulus G_R as

$$B_R = B_V, \quad (7)$$

$$G_R = \frac{5(C_{11} - C_{12})C_{44}}{4C_{44} + 3(C_{11} - C_{12})}. \quad (8)$$

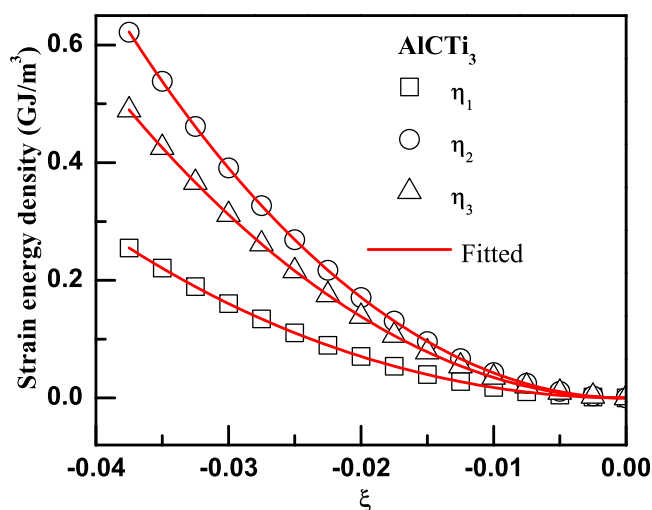


FIG. 4. The strain energy of AlCTi₃.

TABLE III. The elastic constants and related mechanical parameters of ACTi₃.

ACTi ₃	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	C_p (GPa)	B (GPa)	G (GPa)	B/G	E (GPa)	A	σ	Θ_D (K)	H_V (GPa)
CuCTi ₃	388.16	55.51	85.00	-29.49	166.39	111.60	1.49	237.62	0.51	0.26	580.09	16.84
ZnCTi ₃	381.26	56.03	89.42	-33.39	164.44	113.88	1.44	227.56	0.55	0.22	586.90	17.25
CdCTi ₃	426.41	65.95	89.36	-23.40	186.11	118.82	1.57	293.92	0.50	0.24	600.79	18.12
AlCTi ₃	362.29	68.58	86.61	-18.04	166.48	107.16	1.55	264.70	0.59	0.24	689.12	16.06
GaCTi ₃	479.95	69.84	81.29	-11.45	206.55	118.98	1.74	299.45	0.40	0.26	651.24	18.15
InCTi ₃	425.10	77.96	82.60	-4.63	193.67	111.75	1.73	281.16	0.48	0.26	581.94	16.87
SnCTi ₃	270.86	121.22	44.35	76.87	171.10	54.76	3.12	148.44	0.59	0.36	409.51	6.79

In order to obtain accurate result, we use the Voigt-Reuss-Hill approximation³⁷ to calculate the bulk modulus B and shear modulus G

$$B = \frac{B_R + B_V}{2}, \quad (9)$$

$$G = \frac{G_R + G_V}{2}. \quad (10)$$

The bulk modulus B evaluates volume changing of isotropic resistance under hydrostatic strain. And the shear modulus G responses to resistance to anisotropic shear strain. Using the bulk modulus B and shear modulus G , we can obtain the Young's modulus E , which can be expressed as

$$E = \frac{9BG}{3B + G}. \quad (11)$$

The calculated B , G , and E for ACTi₃ and ANT₃ are listed in Tables III and IV, respectively.

Young's modulus E represents the ratio between the linear stress and strain. Theoretical and experimental results have shown that the larger the value of E , the stiffer is the material. According to our calculation, E of most AXTi₃ are larger than those of normal titanium alloys.³⁸ Moreover, CuNTi₃ shows $E = 479.64$ GPa, which can be comparable to that of tungsten carbide.³⁹

We can also calculate the hardness of AXTi₃. According to Ref. 40, the value of Vickers hardness H_V^{Teter} is defined as

$$H_V^{Teter} = 0.1769G - 2.899. \quad (12)$$

The hardness is only connected with shear modulus.⁴¹ As seen from Tables III and IV, the hardness of AXTi₃ can change from $H_V \sim 2.23$ GPa for the softest one (SnNTi₃) to $H_V \sim 29.70$ GPa for the hardest one (CuNTi₃). The large Young's modulus and high hardness will lead to a good application potential of AXTi₃.

TABLE IV. The elastic constants and related mechanical parameters of ANT₃.

ANT ₃	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	C_p (GPa)	B (GPa)	G (GPa)	B/G	E (GPa)	A	σ	Θ_D (K)	H_V (GPa)
CuNTi ₃	1036.57	86.01	85.93	0.58	402.86	184.26	2.19	479.61	0.18	0.30	812.76	29.70
ZnNTi ₃	1002.34	93.64	83.02	10.62	396.54	177.45	2.23	463.24	0.18	0.31	796.83	28.49
CdNTi ₃	540.71	101.90	78.69	23.27	248.21	120.40	2.06	310.93	0.36	0.30	602.36	18.40
AlNTi ₃	336.24	144.29	51.63	92.67	208.28	66.35	3.14	179.94	0.54	0.36	543.19	8.84
GaNTi ₃	475.89	161.46	34.79	126.68	266.27	67.14	3.97	185.81	0.22	0.38	491.85	8.98
InNTi ₃	506.78	144.79	46.79	97.99	265.45	83.50	3.18	226.73	0.26	0.36	504.51	11.87
SnNTi ₃	313.60	187.18	16.18	170.99	229.32	29.03	7.90	83.53	0.26	0.44	298.92	2.23

Poisson's ratio σ can be expressed as

$$\sigma = \frac{3B - 2G}{2(3B + G)}. \quad (13)$$

The calculated σ is listed in Tables III and IV. Poisson's ratio σ generally describes the stability of the crystal against shear and takes the value between -1 and 0.5 , which are the lower and the upper bounds. The lower bound is where the material does not change its shape, and the upper bound is where the volume remains unchanged. In addition, the ratio B/G is also an index of ductility. According to Pugh,⁴² if $B/G > 1.75$, the material shows ductile nature, otherwise, the material is brittle. The Cauchy's pressure for cubic crystal is

$$C_p = C_{11} - C_{12}; \quad (14)$$

it can be an indication of ductility as well, i.e., $C_p < 0$ indicates that the material is brittle, or else the material is expected to be ductile.⁴³ All the three factors indicate that almost all the calculated ACTi₃ are more brittle except for SnCTi₃, while all the calculated ANT₃ are more ductile (Tables III and IV).

Moreover, using the calculated bulk modulus B and shear modulus G , we can obtain the longitudinal and transverse sound velocities ν_l and ν_t , which can be determined as

$$\nu_l = \left(\frac{3B + 4G}{3\rho} \right)^{1/2}, \quad (15)$$

$$\nu_t = \left(\frac{G}{\rho} \right)^{1/2}, \quad (16)$$

where ρ is the mass density. We subsequently obtain the mean sound velocity which is defined as

$$\nu_m = \left[\frac{1}{3} \left(\frac{2}{\nu_t^3} + \frac{1}{\nu_l^3} \right) \right]^{-1/3}. \quad (17)$$

According to these physical quantities, we can further obtain the Debye temperature Θ_D , which reflects the phonon contribution to the specific heat. Θ_D can be determined as

$$\Theta_D = \frac{h}{k_B} \left(\frac{3n\rho N_A}{4\pi M} \right)^{1/3} \nu_m. \quad (18)$$

Here, h and k_B are Planck's and Boltzmann's constants, N_A is Avogadro's number, n is the molecular weight, and M is the

number of atoms in the unit cell. The calculated Θ_D are listed in Tables III and IV.

C. Electronic structure and magnetism

The band structures and density of states (DOS) of the 14 stable AXTi₃ are calculated. The effect of spin-orbit coupling (SOC) is taken into consideration. Around the Fermi energy, the electronic structure with and without SOC is

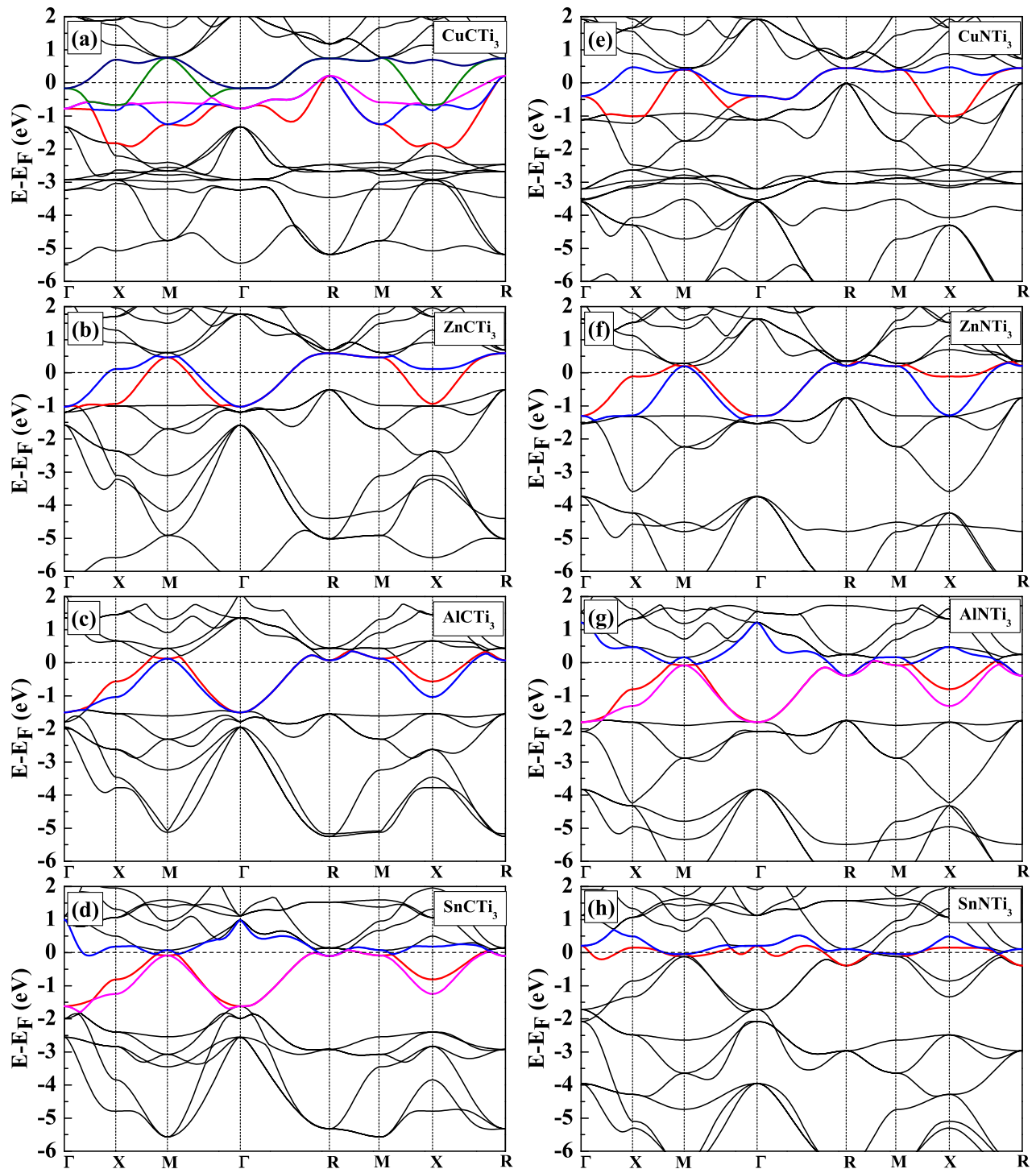


FIG. 5. The band structure of AXTi₃ compounds: (a) CuCTi₃, (b) ZnCTi₃, (c) AlCTi₃, (d) SnCTi₃, (e) CuNTi₃, (f) ZnNTi₃, (g) AlNTi₃, and (h) SnNTi₃. The horizontal dashed lines represent the Fermi level.

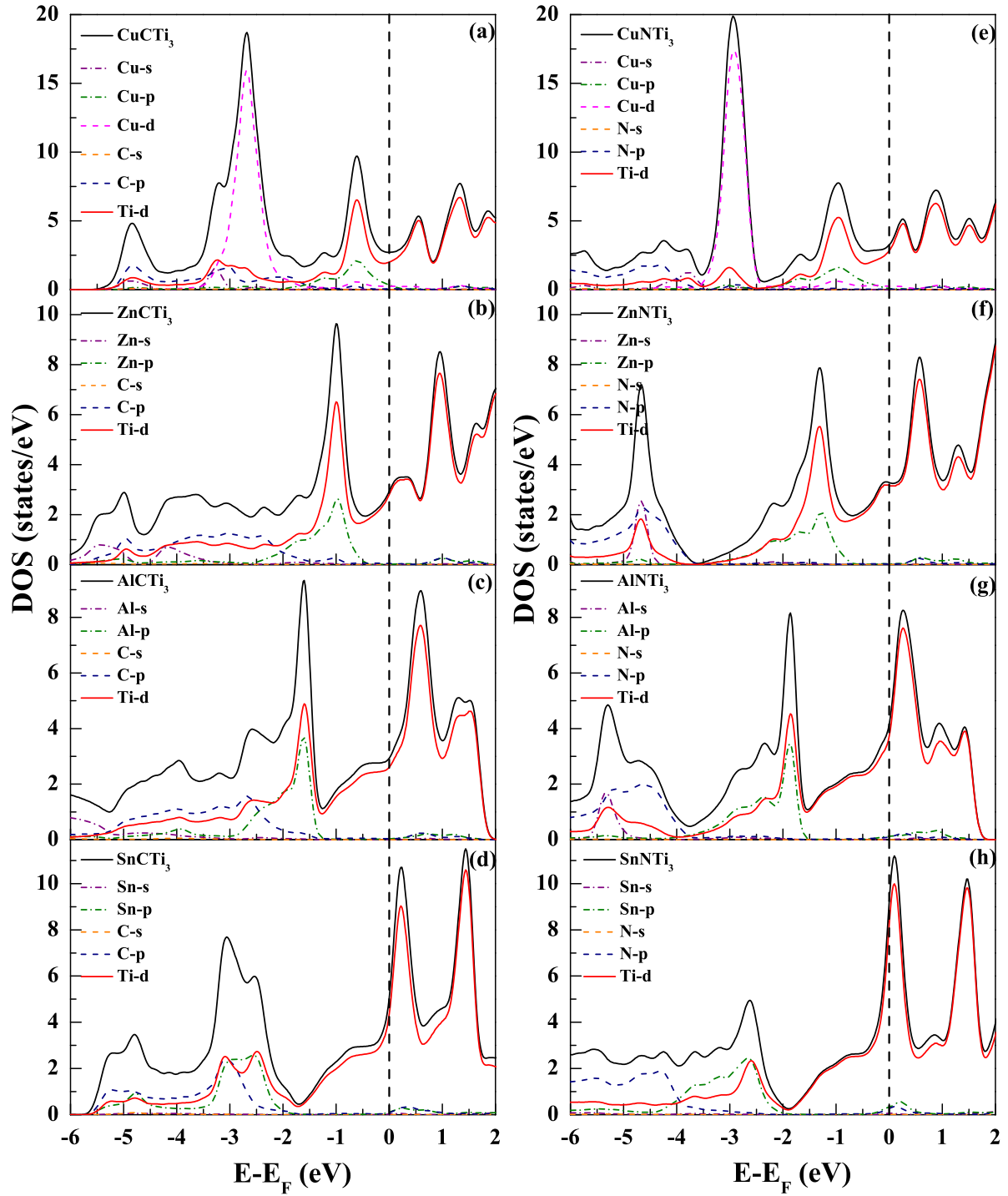


FIG. 6. The DOS of AXTi₃ compounds: (a) CuCTi₃, (b) ZnCTi₃, (c) AlCTi₃, (d) SnCTi₃, (e) CuNTi₃, (f) ZnNTi₃, (g) AlNTi₃, and (h) SnNTi₃. The vertical dashed lines represent the Fermi level.

nearly the same. Therefore, we only show the results without SOC. Previous calculation shows that the valence electrons of A-site atom strongly influence the E_F .⁴⁴ This rule still works in AXTi₃ according to our calculation. For example, we present the band structures and DOS of AXTi₃ (X = C, N; A = Cu, Zn, Al, and Sn), in which the number of valence of A varies from 1 to 4. The band structures along high symmetry lines in the first BZ and DOS are shown in Figs. 5 and 6, respectively. For the four carbides ACTi₃ (A = Cu, Zn, Al, and Sn), in Figs. 5(a)–5(d), the band structures in the vicinity

TABLE V. Calculated $N(E_F)$ for AXTi₃ compounds.

ACTi ₃	$N(E_F)$ (states/eV)	ANTi ₃	$N(E_F)$ (states/eV)
CuCTi ₃	2.799	CuNTi ₃	3.214
ZnCTi ₃	3.019	ZnNTi ₃	3.351
CdCTi ₃	3.454	CdNTi ₃	4.668
AlCTi ₃	2.817	AlNTi ₃	3.497
GaCTi ₃	3.012	GaNTi ₃	3.435
InCTi ₃	3.495	InNTi ₃	4.127
SnCTi ₃	4.847	SnNTi ₃	10.88

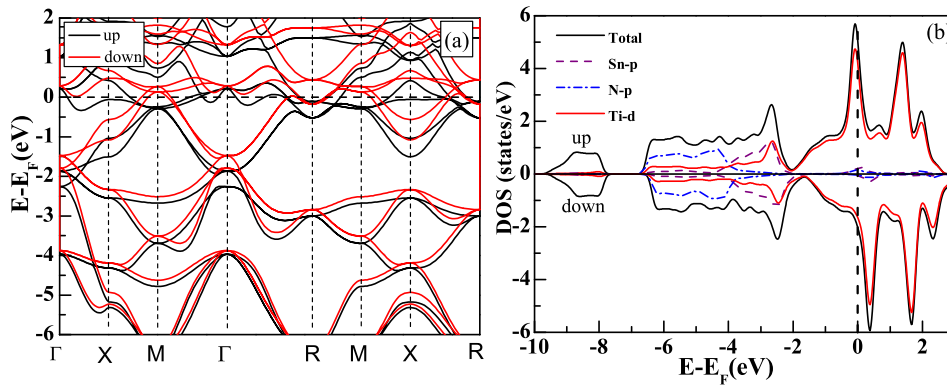


FIG. 7. The band structure (a) and DOS (b) of SnNTi₃ in FM state.

of the Fermi level are similar. The difference is that E_F moves upwards, which can be understood by the fact that the number of effective valence electrons increases from Cu to Sn. Similar behavior can be found for the band structures of four nitrides ANTi₃ ($A = \text{Cu, Zn, Al, and Sn}$) in Figs. 5(e)–5(h). Therefore, the A-site doping effect on electronic structure can be evaluated by rigid band approximation. In addition, it is seen that band structure of ACTi₃ is similar to ANTi₃ with the same A-site atom. The only difference is that the E_F of ANTi₃ moves upwards in comparison with ACTi₃. Therefore, the effect of A and X-site doping on AXTi₃ can be evaluated by rigid band approximation as well.

It can be seen from Fig. 6 that the shapes of DOS of those compounds are similar to each other. The contributions of A-s and X-s (C-2s or N-2s) to DOS are small, which is a common feature of all the compounds. Generally, A-p and X-p (C-2p or N-2p) make great contribution to DOS below the E_F . Near and above the E_F , Ti-3d electrons contribute predominately to the total DOS and are responsible for the metallic conductivity of the AXTi₃ compounds. The calculated DOS at E_F ($N(E_F)$) for AXTi₃ compounds are listed in Table V.

According to the Stoner's criterion,²⁵ a NM system will become polarized when $N(E_F)I > 1$, where I is the Stoner parameter with a value of ~ 0.3 in the 3d transition metal based antiperovskites,¹⁶ and $N(E_F)$ is in the unit of states/eV/spin. For most calculated AXTi₃, the E_F is far away from a sharp DOS peak, which leads to a moderate $N(E_F)$ (Table V). Therefore, if $N(E_F)I < 1$, the calculated magnetic moments in FM state are converged to zero. However, for SnNTi₃, the E_F just locates at a sharp DOS peak. The resulted large $N(E_F)$ of 10.88 states/eV leads to $N(E_F)I > 1$. That is why the FM state of SnNTi₃ shows lower formation energy (Table I). We present the band structure and DOS of SnNTi₃ in the FM state in Fig. 7, in which the spin-polarized behavior can be clearly seen. By comparing the band structure of SnNTi₃ in NM state in Fig. 5(h) and that in FM state in Fig. 7(a), it is seen that the bands in the FM state split into spin up and spin down branches, with the spin down branches showing higher energy than spin up ones. The potential magnetism will broaden the application of AXTi₃.

IV. CONCLUSIONS

In conclusion, we have systematically studied the mechanical and electronic properties of a series of Ti-based

antiperovskite compounds AXTi₃ ($A = \text{Ba, Ca, In, Sn, Sr, Zn, Cu, Al, Ga, Cd, and La; X = C, N}$) from first-principles calculations. The formation energies, mechanical parameters, and electronic structures of a series of AXTi₃ are studied. The predicted stable AXTi₃ shows large Young's modulus and high hardness, implying a good mechanical application value. The bands around E_F of AXTi₃ are predominately contributed by 3d electrons of Ti, while the E_F is strongly influenced by the total valence electrons. According to the Stoner's criterion, the spin polarization of AXTi₃ is discussed. Our prediction will be helpful for the experimental exploration of Ti-based antiperovskite compounds.

ACKNOWLEDGMENTS

This work was supported by the National Natural Science Foundation of China (Grant Nos. 11574108, 11104099, and 11304320), the Foundation of President of the Institute of Solid State Physics, Chinese Academy of Sciences, the Natural Science Foundation of Anhui Province (Grant No. 1408085QA12), and the Natural Science Research Project of Higher Education Institutions of Anhui Province (Grant No. KJ2015A120).

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