

High-throughput computational design of $\text{Mo}_3\text{Al}_2\text{C}$ -like noncentrosymmetric superconductors with multifold degenerate fermions

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Nonsymmorphic chiral superconductors, like $\text{Mo}_3\text{Al}_2\text{C}$, are promising candidates to explore parity mixing and multifold degenerate fermions. However, only $\text{Mo}_3\text{Al}_2\text{C}$ and $\text{W}_3\text{Al}_2\text{C}$ in the $\text{Mo}_3\text{Al}_2\text{C}$ family have been identified up to now. We carry out a high-throughput materials screening procedure on $\text{Mo}_3\text{Al}_2\text{C}$ -like crystals based on first principles calculations. We report 21 crystals in this family based on systematic stability evaluations and perform electron-phonon coupling strength calculations for all of them. Additionally, the band structures of these compounds indicate that almost all of these compounds can hold multiple fermions near the Fermi level. This study may contribute to the discovery of more novel NCSs with multiple degenerate fermions.

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I. INTRODUCTION

Recently, there has been an increasing interest in superconductors without inversion centers, called noncentrosymmetric superconductors (NCSs) [1–14]. An intriguing phenomenon arises in NCSs is the antisymmetric spin-orbit coupling (ASOC) effect, which makes the $(s + p)$ -wave pairing below the superconducting transition temperature (T_c) possible [15]. This suggests that NCSs can hold the Majorana modes which can be manipulated to construct topological quantum computations [16,17]. Moreover, NCSs can exhibit distinctive characteristics that surpass conventional Bardeen-Cooper-Schrieffer (BCS) limits [18], including unconventional nodal gapless pairing [9], Ising superconductivity [19], and spontaneous time-reversal symmetry (TRS) breaking [9,20,21].

The research of NCSs was initiated following the discovery of unusual line nodes in the heavy fermion superconductor CePt_3Si [1–3]. Several other compounds, such as PbTaSe_2 [22–26], $\text{K}_2\text{Cr}_3\text{As}_3$ [27], LaNiC_2 [4,20], $\text{Li}_2\text{Pt}_3\text{B}$ [28–35], and $\text{Mo}_3\text{Al}_2\text{C}$ [36–39], also display attractive superconducting and electronic properties. In recent years, significant attention has been paid to $\text{Mo}_3\text{Al}_2\text{C}$, which possesses a β -Mn-type structure with space group (SG) $P4_132$, having a relatively high $T_c = 9\text{ K}$ [39]. In this system, some observations suggest strong indications of the superconducting behavior deviating from the standard BCS model [39], while other techniques diagnose $\text{Mo}_3\text{Al}_2\text{C}$ as nodeless electron pairing [40]. More recently, an isostructural compound of $\text{Mo}_3\text{Al}_2\text{C}$, that is, $\text{W}_3\text{Al}_2\text{C}$ ($T_c = 7.6\text{ K}$), has been successfully synthesized, and a zero-field and transverse-field muon

spin relaxation/rotation (μSR) measurement indicates the unconventional nature of superconductivity from the $T_c/\lambda_{\text{eff}}^{-2}$ ratio [41,42].

More intriguingly, crystals with a SG number of 213 were proposed as excellent candidates for exploring exotic multiple degeneracy, i.e., sixfold degenerate fermions in the presence of TRS [43]. Although NCSs with $\text{Mo}_3\text{Al}_2\text{C}$ structure contains a wealth of physical images, most of the exploratory work has been on $\text{Mo}_3\text{Al}_2\text{C}$ and $\text{W}_3\text{Al}_2\text{C}$. In this work, a high-throughput screening based on first principles calculations has been carried out on NCSs with $\text{Mo}_3\text{Al}_2\text{C}$ structure to obtain candidate materials with good stability for experimental synthesis. In addition, the electronic and superconducting properties have been calculated.

II. METHODOLOGY

The major calculations were carried out by using the Vienna *ab initio* simulation package (VASP) based on density function theory (DFT), and the projector augmented wave (PAW) method was utilized [44,45]. Besides, the Perdew-Burke-Ernzerhof (PBE) scheme within the framework of the generalized gradient approximation (GGA) for the exchange-correlation potential was utilized [46]. In order to reduce numerical errors, the pseudopotential types and the plane-wave basis energy cutoff (520 eV) were the same as that in the Materials Project (MP) [47] database. The force criterion was set to 0.001 eV/Å. Moreover, the Brillouin zone was sampled with a Γ -centered $5 \times 5 \times 5$ k -point mesh in relaxation and a $9 \times 9 \times 9$ k -point mesh in self-consistent calculation. In total, 2000 k points were utilized in band calculations. In phonon calculations, $2 \times 2 \times 2$ supercells were performed with the PHONOPY package and the density functional perturbation (DFPT) theory [48,49]. The maximally localized Wannier

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functions (MLWFs) were constructed with WANNIER90 [50] package and the Mo d orbital was utilized for the initial projection. In addition, the surface states were calculated with the WANNIERTOOLS [51] package. In addition, the VASPKIT [52] and PYPROCAR [53] codes were also used in data processing and figure plotting.

The electron-phonon coupling (EPC) strength calculations were carried out with the QUANTUM ESPRESSO (QE) package [54,55]. All structures were reoptimized using QE before electron-phonon calculations. The superconducting transition temperatures (T_c) were calculated from the Allen-Dynes equation [56,57].

$$T_c = \omega_{\log} \frac{f_1 f_2}{1.2} \exp\left[\frac{-1.04(1 + \lambda)}{\lambda - \mu^*(1 + 0.62\lambda)}\right], \quad (1)$$

$$f_1 f_2 = \left[1 + \left(\frac{\lambda}{2.46(1 + 3.8\mu^*)}\right)^{\frac{3}{2}}\right]^{\frac{1}{3}} \times \left[1 - \frac{(1 - \frac{\omega_2}{\omega_{\log}})\lambda^2}{3.312(1 + 6.3\mu^*)^2 + \lambda^2}\right], \quad (2)$$

where ω_{\log} stands for the logarithmic average frequency and ω_2 is the mean-square frequency. μ^* was set to 0.1 and the EPC constant (λ) can be defined as

$$\lambda = \sum_{qv} \lambda_{qv} = \int \frac{2\alpha^2 F(\omega)}{\omega} d\omega. \quad (3)$$

In QE calculations, the optimized norm-conserving Vanderbilt (ONCV) pseudopotentials were utilized [58]. The plane-wave basis energy cutoff was set to 60 Ry, the k -point mesh was set to $12 \times 12 \times 12$, and the q -point mesh was set to $4 \times 4 \times 4$.

III. RESULTS AND DISCUSSIONS

As can be found in Fig. 1(a), the $\text{Mo}_3\text{Al}_2\text{C}$ -like compounds were labeled as M_3T_2X . The screening was started from element combinations based on M_3T_2X structure. Taking the element combinations of some already synthesized 3:2:1 compounds into account [41,59,60], in this work, M -site atoms were replaced with transition metals, Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W, Mn, Tc, Re, Fe, Ru, Os, Co, Rh, Ir, Ni, Pd, and Pt. T -site atoms were substituted with Cu, Ag, Au, Zn, Cd, Al, Ga, In, and Tl. X -site atoms were replaced with B, C, N, Si, P, Ge, and As, and 1323 phases in total were constructed and then were well relaxed by DFT calculations with switching symmetry on (ISYM = 2) and considering spin polarization (ISPIN = 2).

We then utilized the convex hull formation energy map to establish connections between phases that possess the lowest formation energy position at different compositions [61]. Generally, phases on the convex hull line (the energy above hull, i.e., $E_{\text{hull}} = 0$) are considered as thermodynamically stable. In addition, phases positioned above the convex hull ($E_{\text{hull}} > 0$) can be classified as thermodynamically metastable or unstable. A commonly used criterion for material synthesis is an E_{hull} value of 100 or 200 meV/atom; an E_{hull} below 50 meV/atom indicates a high success rate of synthesis [62–64]. We took the possible numerical errors in formation energy

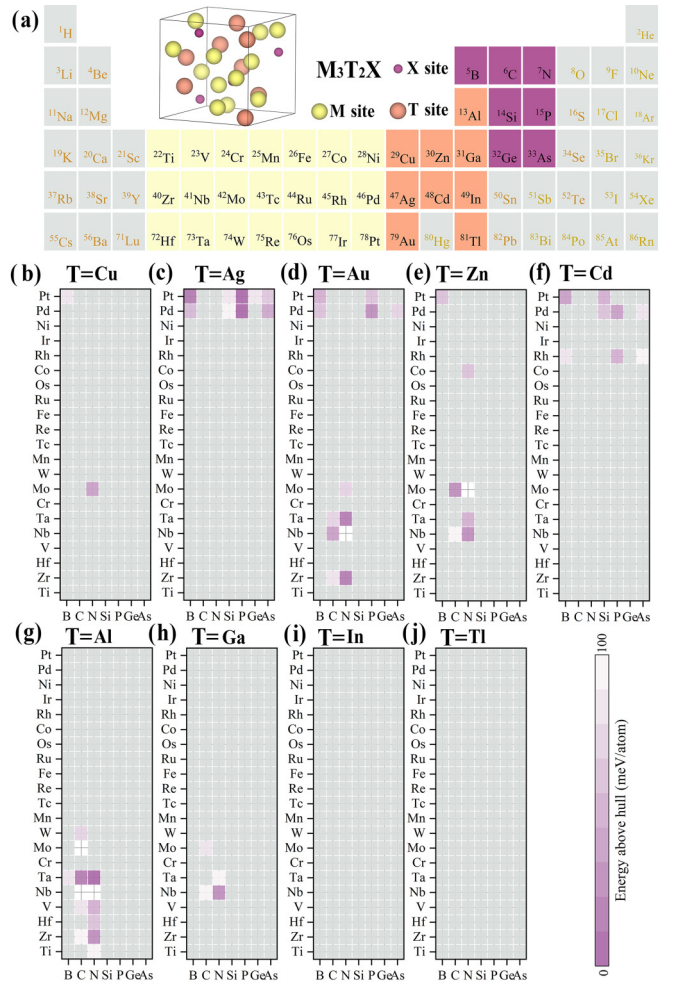


FIG. 1. (a) Crystal configuration of $\text{Mo}_3\text{Al}_2\text{C}$ -like phases and the corresponding atomic site. (b)–(j) The results on hull energy calculation for each system with different T -site atoms. The gray rectangles indicate the hull energies are over 100 meV/atom.

calculations or competing phases listed in the MP database into account. Then a medium threshold of 100 meV/atom was employed to screen out proper candidates with good thermodynamic stability that may be experimentally synthesized.

Based on our DFT calculations, the PHASEDIAGRAM module [65] from PYMATGEN [66] was then used to calculate the E_{hull} for each constructed compound in this work combined with the MP database. The map of E_{hull} for each system with different T -site atoms from first-principles calculations and the MP database are shown in Figs. 1(b)–1(j). The gray rectangles indicate that the E_{hull} of related phases were more than 100 meV/atom. At first glance, we can find that a series of combinations satisfies the E_{hull} criterion where T -site atoms were substituted with Cu, Ag, Au, Zn, Cd, Al, and Ga. In addition, in the $\text{M}_3\text{In}_2\text{X}$ and $\text{M}_3\text{Tl}_2\text{X}$ systems, no phases show good thermodynamic stability. In this procedure, 55 phases were screened out.

The phonon spectrum can be utilized to check the dynamic stability of a specific solid crystal and a crystal can be verified as dynamically stable if its phonon dispersion displays without imaginary frequency modes. The calculated

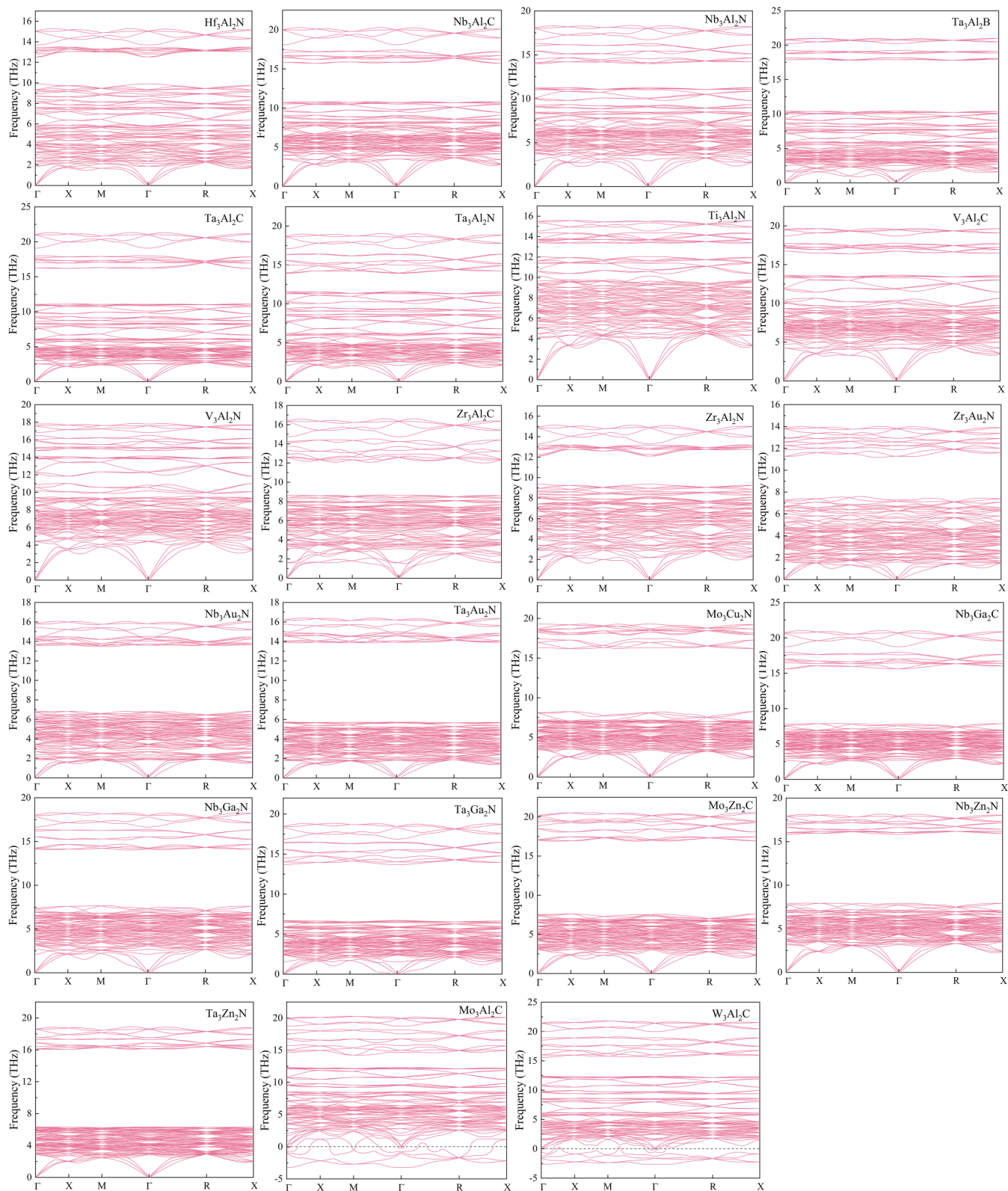


FIG. 2. Calculated phonon dispersions of $\text{Mo}_3\text{Al}_2\text{C}$, $\text{W}_3\text{Al}_2\text{C}$, and the other 21 $\text{Mo}_3\text{Al}_2\text{C}$ -like compounds. The results show that except for $\text{Mo}_3\text{Al}_2\text{C}$ and $\text{W}_3\text{Al}_2\text{C}$, the other 21 compounds are dynamically stable.

phonon spectra of these 55 compounds were displayed in Fig. 2 and Figs. S2–S5 in the Supplemental Material [67]. As we mentioned above, the parent structures $\text{Mo}_3\text{Al}_2\text{C}$ and $\text{W}_3\text{Al}_2\text{C}$ were retrieved from experimental x-ray diffraction

data [39,42]. Intriguingly, we can find from Fig. 2 that $\text{Mo}_3\text{Al}_2\text{C}$ and $\text{W}_3\text{Al}_2\text{C}$ were dynamically unstable because large imaginary frequency modes occur, which indicated that intrinsic vacancies must appear to stabilize the crystal

TABLE I. The calculated lattice parameters, independent elastic constants C_{ij} , Vickers hardness, and averaged band splitting energies at Fermi level E_{ASOC} of the 23 $\text{Mo}_3\text{Al}_2\text{C}$ -like compounds with good thermodynamic and dynamic stabilities.

Phase	a (Å)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	Vickers hardness (GPa)	E_{ASOC} (meV)
$\text{Hf}_3\text{Al}_2\text{N}$	7.311	270.508	92.307	90.072	12.210	43.2
$\text{Nb}_3\text{Al}_2\text{C}$	7.129	321.232	123.522	124.802	14.693	27.1
$\text{Nb}_3\text{Al}_2\text{N}$	7.077	330.339	128.945	121.907	13.955	24.0
$\text{Ta}_3\text{Al}_2\text{B}$	7.179	308.610	125.130	123.257	13.975	91.2
$\text{Ta}_3\text{Al}_2\text{C}$	7.090	347.828	136.119	135.982	15.389	52.6
$\text{Ta}_3\text{Al}_2\text{N}$	7.039	353.990	142.363	132.100	14.406	71.4
$\text{Ti}_3\text{Al}_2\text{N}$	6.923	290.382	86.344	106.256	15.886	2.3
$\text{V}_3\text{Al}_2\text{C}$	6.674	329.323	116.726	132.019	16.681	9.0
$\text{V}_3\text{Al}_2\text{N}$	6.627	342.584	120.538	128.991	16.108	10.6
$\text{Zr}_3\text{Al}_2\text{C}$	7.477	229.582	82.920	80.629	10.977	10.1
$\text{Zr}_3\text{Al}_2\text{N}$	7.395	251.231	84.421	85.700	12.056	8.6
$\text{Zr}_3\text{Au}_2\text{N}$	7.417	222.937	132.484	86.539	6.533	53.3
$\text{Nb}_3\text{Au}_2\text{N}$	7.170	326.233	156.737	97.770	8.749	57.8
$\text{Ta}_3\text{Au}_2\text{N}$	7.137	351.895	173.563	103.072	8.707	61.2
$\text{Mo}_3\text{Cu}_2\text{N}$	6.708	385.133	178.043	139.962	12.759	32.7
$\text{Nb}_3\text{Ga}_2\text{C}$	7.107	308.072	128.648	112.266	12.236	25.4
$\text{Nb}_3\text{Ga}_2\text{N}$	7.059	312.650	135.770	105.441	10.884	25.7
$\text{Ta}_3\text{Ga}_2\text{N}$	7.028	324.263	154.135	111.559	10.282	65.7
$\text{Mo}_3\text{Zn}_2\text{C}$	6.845	344.194	154.726	129.116	12.607	49.5
$\text{Nb}_3\text{Zn}_2\text{N}$	7.035	322.448	121.071	118.288	14.141	18.0
$\text{Ta}_3\text{Zn}_2\text{N}$	6.996	357.177	133.982	128.932	14.948	72.6
$\text{Mo}_3\text{Al}_2\text{C}$	6.875	297.914	189.648	105.614	6.406	28.9
$\text{W}_3\text{Al}_2\text{C}$	6.889	312.361	219.862	135.712	6.692	90.1

lattice. We then calculated the phonon spectra of $\text{Mo}_3\text{Al}_2\text{C}$ and $\text{W}_3\text{Al}_2\text{C}$ with vacancies and the results confirmed that these vacancy structures could become dynamically stable, which was in accordance with previous reports [38,41], as shown in Fig. S1 in the Supplemental Material [67].

Additionally, the mechanical stability of those compounds was also evaluated. In the case of compounds belonging to the cubic crystal class, three independent elastic constants (C_{ij}) are necessary for the assessment. To be considered mechanically stable, a cubic crystal must meet the following conditions: $C_{11} > C_{12}$, $C_{11} + 2C_{12} > 0$ and $C_{44} > 0$ [68]. The calculated elastic constants can be found in Table I. Obviously, all of the 23 compounds were predicted to be mechanically stable. Moreover, we find that $\text{V}_3\text{Al}_2\text{N}$ and $\text{V}_3\text{Al}_2\text{C}$ have relatively larger Vickers hardness [69] (>16 GPa) than other compounds. Conversely, the Vickers hardness of $\text{Mo}_3\text{Al}_2\text{C}$ and $\text{W}_3\text{Al}_2\text{C}$ was around 6.5 GPa.

After implementing such a comprehensive stability filtering frame, a total of 23 compounds (including previously reported $\text{Mo}_3\text{Al}_2\text{C}$ and $\text{W}_3\text{Al}_2\text{C}$) emerged as promising candidate materials. Subsequently, we conducted calculations to determine the electronic properties of these compounds. The calculated energy bands with and without considering the spin-orbital coupling (SOC) effect of these compounds were displayed in Fig. 3 and Fig. S6 in the Supplemental Material [67]. The Brillouin zone and selected K path can be found in Fig. 4(a).

In general, the strength of ASOC was found to play a significant role in determining the gap symmetry of NCSs due to the fact that many unconventional NCSs like CePt_3Si , CaPtAs , ThCoC_2 , and $\text{Li}_2\text{Pt}_3\text{B}$ have a large band splitting at the Fermi energy (E_f) [15,70,71], and the corresponding splitting

energy of a NCS at E_f from a DFT band calculation with SOC can be denoted as E_{ASOC} [15]. For example, the effect of ASOC on gap symmetry has been directly observed in the well-known system $\text{Li}_2(\text{Pd}, \text{Pt})_3\text{B}$ compound [28,30,31]. In this system, the parent phase $\text{Li}_2\text{Pd}_3\text{B}$ is demonstrated as a conventional BCS superconductor while $\text{Li}_2\text{Pd}_3\text{B}$ can transform from s -wave to ($s + p$) wave pairing with the introduction of Pt substitution to $\text{Li}_2(\text{Pd}_{1-x}\text{Pt}_x)_3\text{B}$, i.e., with the increasing ASOC strength from the presence of heavier Pt atoms than Pd. The similarity in the case of $\text{Li}_2(\text{Pd}, \text{Pt})_3\text{B}$ and $(\text{Mo}, \text{W})_3\text{Al}_2\text{C}$ both emphasize the pronounced effect of ASOC on superconducting pairing.

More intuitively, we listed some reported values of E_{ASOC} for some famous unconventional NCSs, which either possess nodal-line superconductivity or exhibit a spin-triplet dominated pairing state. Specifically, E_{ASOC} values of 150, 200, 200, 50–100, and 40 meV were reported for ThCoC_2 [71], CePt_3Si and $\text{Li}_2\text{Pt}_3\text{B}$ [15], CaPtAs [70], and LaNiC_2 [4], respectively. In contrast, BiPd [72,73] and $\text{Li}_2\text{Pd}_3\text{B}$ [15], two conventional superconductors, were found to exhibit E_{ASOC} values of 50 and 30 meV, respectively. These previous reports reveal that a large E_{ASOC} seems to be a prerequisite, though not sufficient, for the emergence of notable mixed parity pairing.

More intriguingly, Rashba-like SOC is recognized to arise as the mirror symmetry breaking [15]. In NCSs, the Rashba-like SOC typically exerts a direct influence on the spin susceptibility structure in the normal state [74], and a pronounced Rashba effect is advantageous for electrons to counteract the suppressive impact of the Zeeman field on superconductivity [74,75]. Thus it is reasonable to anticipate that a stronger ASOC or a larger E_{ASOC} in NCSs without mirror symmetry such as the $\text{Mo}_3\text{Al}_2\text{C}$ -like compounds could

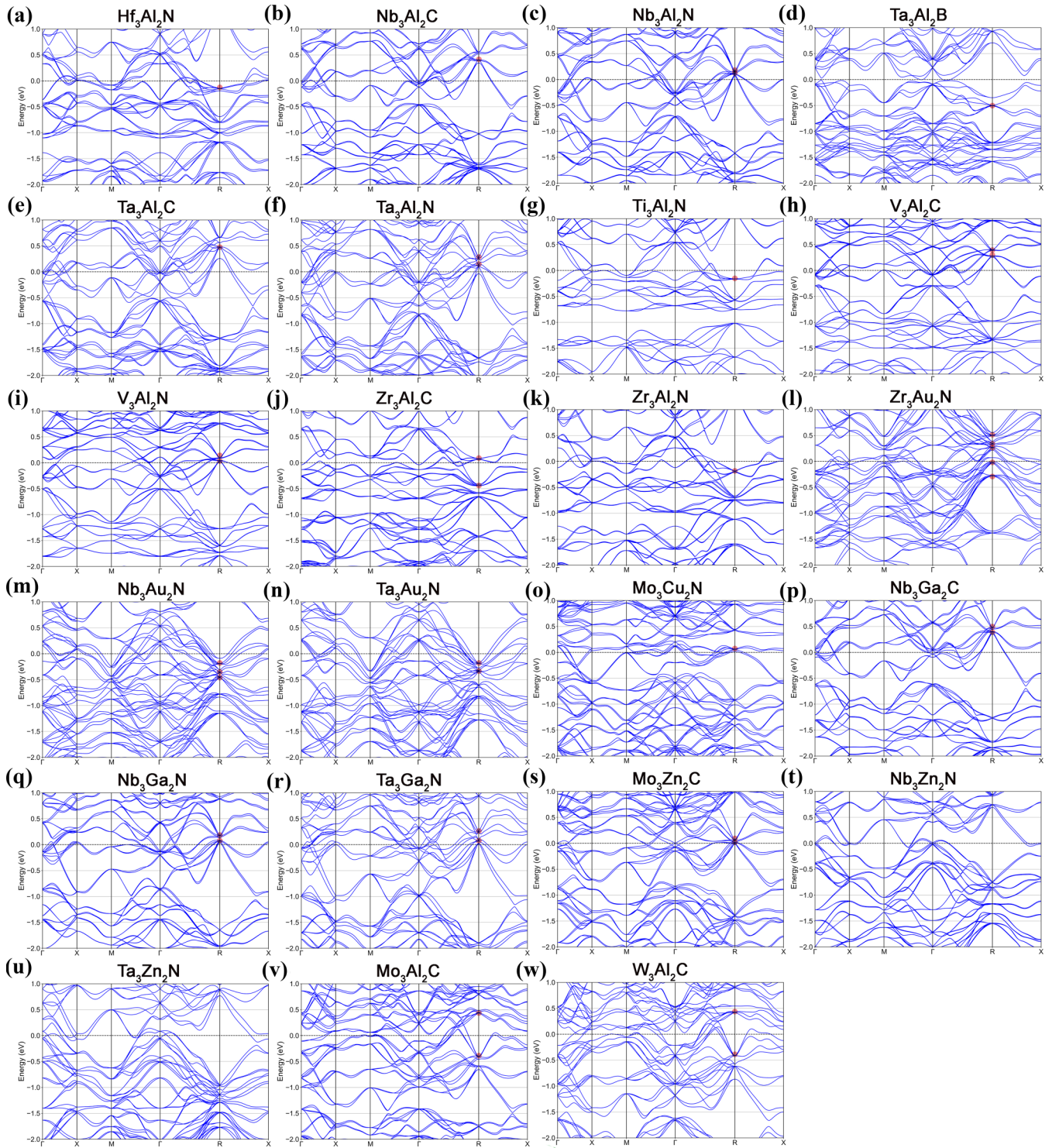


FIG. 3. (a)–(w) The energy bands of 23 $\text{Mo}_3\text{Al}_2\text{C}$ -like phases with considering SOC. The red circles denote the sixfold degeneracy around the Fermi level.

increase the likelihood of unconventional superconductivity. For example, we calculated the spin projected Fermi surfaces around the Γ point of $\text{Mo}_3\text{Zn}_2\text{C}$ with considering SOC, and the results displayed the Rashba-like spin texture, as shown in Fig. S8 in the Supplemental Material [67].

In order to determine the effective points surrounding E_f for measuring E_{ASOC} , 2000 k points in total were utilized

to calculate the energy bands; the energy eigenvalues were then computed. An additional constraint was implemented in this procedure, whereby only k points with one eigenvalue below E_f and the other above E_f were chosen for calculating the averaged SOC splitting. The predicted E_{ASOC} 's for these compounds are listed in Table I. We find that five compounds, $\text{Ti}_3\text{Al}_2\text{N}$, $\text{V}_3\text{Al}_2\text{C}$, $\text{V}_3\text{Al}_2\text{N}$, $\text{Zr}_3\text{Al}_2\text{C}$, and $\text{Zr}_3\text{Al}_2\text{N}$, had very

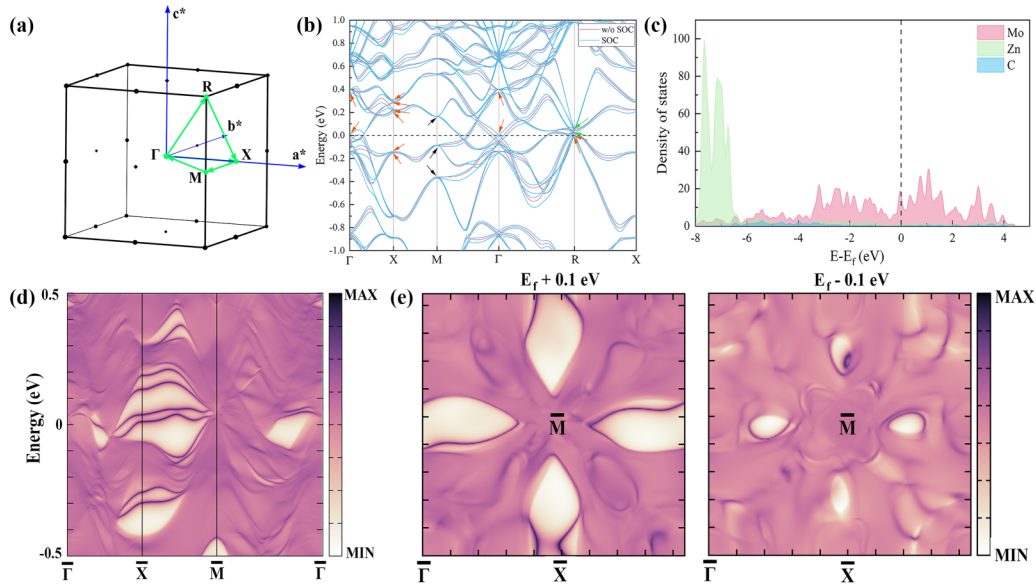


FIG. 4. (a) The Brillouin zone and selected K path of $\text{Mo}_3\text{Al}_2\text{C}$ -like compounds. (b) Energy bands of $\text{Mo}_3\text{Zn}_2\text{C}$ with and without SOC. (c) The projected density of states of $\text{Mo}_3\text{Zn}_2\text{C}$. (d) The surface band spectrum projected on the (001) surface and (e) the surface band spectra at a specific energy level of $\text{Mo}_3\text{Zn}_2\text{C}$. The orange, black, and green arrows point out the Kramers-Weyl, dKramers-Weyl, and sixfold degeneracies around the E_f , respectively.

small E_{ASOC} , only around 10 meV, while most of the other compounds had a medium E_{ASOC} value around 50 meV. This may indicate that parity mixing should be small in $\text{Mo}_3\text{Al}_2\text{C}$ -like compounds.

Recently, there has been a proposal suggesting that the presence of TRS and specific crystal symmetries in some solids can safeguard the existence of exotic fermions with degeneracies of three-, six- or eightfold [43]. This is particularly fascinating because such fermions do not have any counterparts in the realm of high-energy physics, primarily due to the constraints imposed by Poincaré symmetry [43,76,77]. The multifold fermions can originate from specific operations at particular high-symmetry points. In the case of $\text{Mo}_3\text{Al}_2\text{C}$ -like compounds, the R ($\pi/a, \pi/a, \pi/a$) point can hold sixfold fermions from the following rotation operations: $\{C_{3,111}^{-1}|000\}$, $\{C_{2x}|\frac{1}{2}\frac{1}{2}0\}$, $\{C_{2y}|\frac{1}{2}\frac{1}{2}0\}$, and $\{C_{2,1\bar{1}0}|\frac{3}{4}\frac{3}{4}\frac{3}{4}\}$ [43]. As can be found in Fig. 3, the sixfold fermions of these compounds around the E_f (± 0.5 eV) are marked with red circles. The fact that almost all $\text{Mo}_3\text{Al}_2\text{C}$ -like compounds have sixfold degeneracies around the E_f suggests that members of this family are promising candidates to detect sixfold fermions.

More intriguingly, as one of the 41 nonsymmorphic chiral SGs, $\text{Mo}_3\text{Al}_2\text{C}$ -like compounds with SG 213 were proposed as promising candidates to explore Kramers-Weyl fermions at high-symmetry points. Generally, Kramers-Weyl fermions are distinct from other types of fermions as they do not arise from a band inversion nor rely on specific crystal symmetries [78,79]. Their existence as chiral fermions is ensured solely by the influence of TRS on the irreducible representations of the chiral point groups. Kramers-Weyl fermions, in contrast to other chiral fermions, can only be annihilated through pairwise interactions, for example, which may be achievable by subjecting them to a very strong magnetic field. Consequently, Kramers-Weyl fermions exhibit heightened resilience against

external disturbances and thus become more robust compared to other chiral fermions [78].

We take $\text{Mo}_3\text{Zn}_2\text{C}$ as an example; the corresponding Kramers-Weyl, double Kramers-Weyl (doubled by nonsymmorphic symmetries), and sixfold degeneracies around the E_f are marked with different arrows, as shown in Fig. 4(b). We can see from Fig. 4(b) that obvious band splitting occurs when considering SOC, and the Kramers-Weyl band crossing point (marked in orange arrows) appears in pairs. To further investigate the surface states of $\text{Mo}_3\text{Zn}_2\text{C}$, we then constructed the MLWFs. As can be found in Fig. 4(c), the projected density of states (PDOS) indicates that the contribution of Mo atoms dominates around the E_f . Consequently, we choose Mo d orbitals as initial projectors. The calculated energy bands from GGA+PBE and MLWFs of $\text{Mo}_3\text{Zn}_2\text{C}$ with considering SOC can be found in Fig. S7 [67]. We then calculated the surface band structures projected on the (001) surface of $\text{Mo}_3\text{Zn}_2\text{C}$ based on the constructed MLWFs. As can be found in Fig. 4(d), clear surface states can be detected at E_f . Moreover, we then calculated the surface states of $\text{Mo}_3\text{Zn}_2\text{C}$ for a different energy scheme. As shown in Fig. 4(e), non-trivial surface states were found to be almost buried in bulk states. This may indicate that the surface states of $\text{Mo}_3\text{Zn}_2\text{C}$ were only detectable around a narrow energy range. All the same, $\text{Mo}_3\text{Zn}_2\text{C}$ still becomes a promising candidate material for having Kramers-Weyl, double Kramers-Weyl, and sixfold band degeneracies around E_f simultaneously, which may be rare among numerous topological material families.

We then focus on the superconducting properties of these compounds. As we mentioned above, the pure lattice of $\text{Mo}_3\text{Al}_2\text{C}$ and $\text{W}_3\text{Al}_2\text{C}$ were dynamically unstable, which indicated that the intrinsic vacancies must appear. However, the EPC calculations on defective structures with massive vibrational modes were extremely expensive. Thus we performed electron-phonon coupling strength calculations on

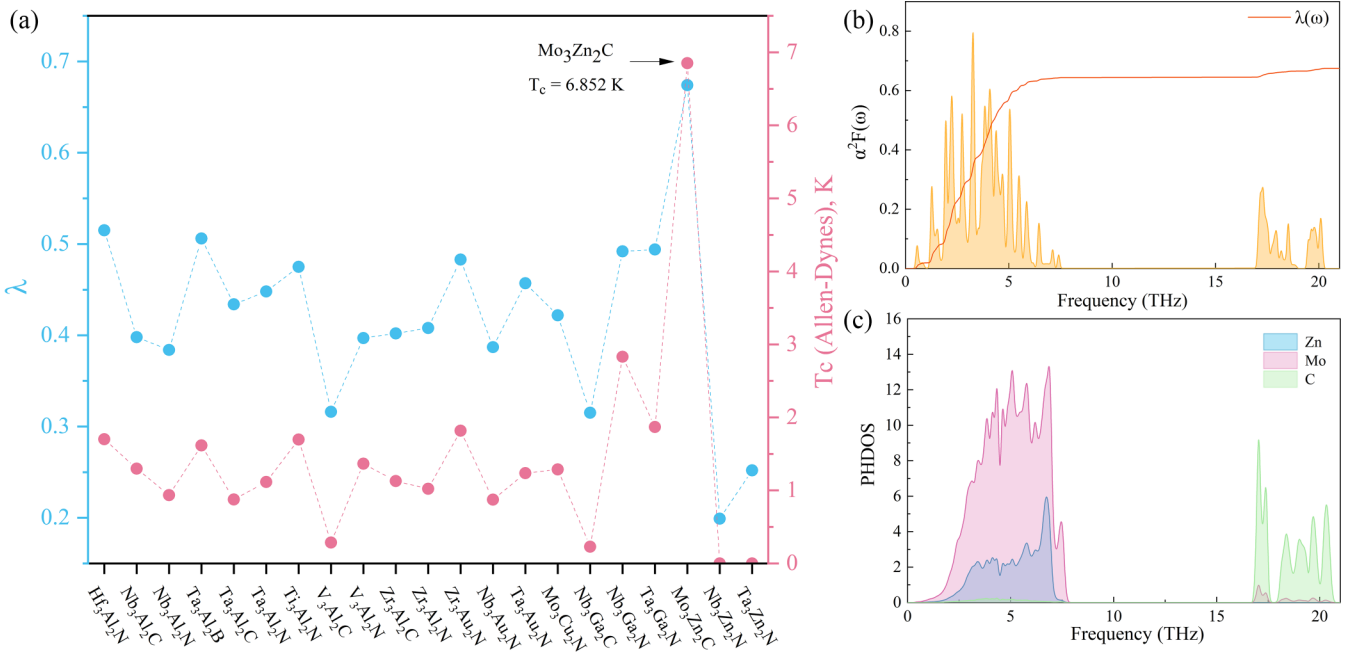


FIG. 5. (a) Superconducting properties of the 21 $\text{Mo}_3\text{Al}_2\text{C}$ -like compounds that were predicted in this work. (b) Eliashberg spectrum functions $\alpha^2F(\omega)$ and the integral EPC parameters $\lambda(\omega)$ of $\text{Mo}_3\text{Zn}_2\text{C}$. (c) The projected phonon density of states of $\text{Mo}_3\text{Zn}_2\text{C}$.

21 $\text{Mo}_3\text{Al}_2\text{C}$ -like compounds that were dynamically stable and predicted in this work. As can be found in Fig. 5(a), $\text{Nb}_3\text{Zn}_2\text{N}$ and $\text{Ta}_3\text{Zn}_2\text{N}$ were calculated to be nonsuperconducting phases and the T_c 's of $\text{V}_3\text{Al}_2\text{C}$ and $\text{Nb}_3\text{Ga}_2\text{C}$ were lower than 0.5 K. Moreover, we can find that $\text{Mo}_3\text{Zn}_2\text{C}$ was predicted to have the highest λ of 0.674 and T_c of 6.852 K among these compounds, and the T_c 's of the rest of the compounds were predicted around 2 K, displaying weak to medium coupling. The Eliashberg spectrum functions $\alpha^2F(\omega)$, integral EPC parameters $\lambda(\omega)$, and the projected phonon density of states (PHDOS) of $\text{Mo}_3\text{Zn}_2\text{C}$ were shown in Figs. 5(b) and 5(c). From PHDOS, we find that the phonon dispersions of $\text{Mo}_3\text{Zn}_2\text{C}$ consisted of two parts: the low-frequency region was mainly contributed to the vibrations of Mo and Zn atoms and the high-frequency region mainly had origins in the vibrations of carbon atoms. The results on EPC strength in $\text{Mo}_3\text{Zn}_2\text{C}$ indicated that superconductivity of $\text{Mo}_3\text{Zn}_2\text{C}$ was mainly contributed to the metal atom region at low frequency. The detailed superconducting parameters calculated in this work are listed in Table S1 [67].

Note that the T_c calculated from the Allen-Dynes equation can only represent the conventional superconducting transition. Consequently, we also calculated the T_c of these compounds based on machine learning models, the training set of which contained a series of unconventional superconductors like iron-based superconductors and cuprate superconductors like $\text{YBa}_2\text{Cu}_3\text{O}_7$ [80]. The predicted T_c from machine learning (ML) models are listed in Table S2 [67]. Both models indicated $\text{Mo}_3\text{Al}_2\text{C}$ and $\text{W}_3\text{Al}_2\text{C}$ were superconductors and the predicted T_c 's of $\text{Mo}_3\text{Al}_2\text{C}$ (3.42 K) and $\text{W}_3\text{Al}_2\text{C}$ (4.62 K) were underestimated and lower than experimental data. In addition, we can find from Table S2 [67] that 15 compounds in total predicted in this work were found to be superconducting from both ML models. Compared

with the T_c results calculated from the Allen-Dynes equation, we can infer that these compounds, $\text{Nb}_3\text{Al}_2\text{C}$, $\text{Ta}_3\text{Al}_2\text{B}$, $\text{Ta}_3\text{Al}_2\text{C}$, $\text{V}_3\text{Al}_2\text{N}$, $\text{Zr}_3\text{Al}_2\text{N}$, $\text{Zr}_3\text{Au}_2\text{N}$, $\text{Nb}_3\text{Au}_2\text{N}$, $\text{Ta}_3\text{Au}_2\text{N}$, $\text{Mo}_3\text{Cu}_2\text{N}$, $\text{Nb}_3\text{Ga}_2\text{N}$, $\text{Ta}_3\text{Ga}_2\text{N}$, and particularly $\text{Mo}_3\text{Zn}_2\text{C}$ which has the highest λ , were promising candidates to investigate superconducting transitions in the $\text{Mo}_3\text{Al}_2\text{C}$ family.

IV. CONCLUSIONS

In summary, we employed high-throughput calculations through density functional theory on $\text{Mo}_3\text{Al}_2\text{C}$ -like noncentrosymmetric superconductors. Twenty-three compounds with good thermodynamic, dynamic, and mechanical stabilities were identified as promising candidates for experimental analysis among the 1323 crystals calculated in this work. Additionally, we calculated the band structures with SOC of these compounds and the results indicated that these compounds can hold multiple fermions including Kramers-Weyl, double Kramers-Weyl, and sixfold fermions. Moreover, we have performed electron-phonon interaction calculations on compounds predicted in this work, and $\text{Mo}_3\text{Zn}_2\text{C}$ was predicted to have a relatively high T_c of 6.852 K. Besides the T_c results calculated from the Allen-Dynes equation, we also calculated the T_c of these compounds based on machine learning models. The results show the $\text{Mo}_3\text{Al}_2\text{C}$ -like family is a promising platform to explore superconductivity and topological excitation. We hope that our results may contribute to the discovery of more novel superconductors without inversion centers and topological quantum materials with multiple degeneracies.

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

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There are no conflicts of interest to declare.

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