Large family candidates for kagome topological superconductors

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A group of newly discovered non-magnetic metal kagome structures AV₃Sb₅ (A = K, Rb, Cs) have aroused widespread interest in experiment and theory due to their unusual charge density wave (CDW) and intertwined superconductivity. However, they all possess weak electron-phonon coupling (EPC) and low superconducting transition temperature. Here, we performed high-throughput first-principles calculations on novel kagome candidates with AV₃Sb₅ prototype structure, and proposed 24 dynamically stable novel kagome metals. The calculation based on Bardeen-Cooper-Schrieffer theory shows that most of these metals are superconductors with much stronger EPC than the reported AV₃Sb₅ materials, and their superconducting transition temperatures Tc are between 0.3 and 5.0K. Additionally, several compounds, such as KZr₃Pb₅ with the highest Tc, are identified as Z₂ topological metals with clear Dirac cone topological surface states near Fermi level. NaZr₃As₅ is shown to have possible CDW phases. Our results provide rich platforms for exploring various new physics with the prototype kagome structure, in which the coexistence of superconductivity and nontrivial topological nature provides promising insights on the discovery of topological superconductors.

Introduction.—In 2019, a new class of nonmagnetic metals AV₃Sb₅ (A = K, Rb, Cs) with perfect vanadium kagome net were synthesized [1]. Since then, surprises have emerged in the study of these structures. The electronic structures of AV₃Sb₅ show Dirac nodal lines, nontrivial Z₂ topological indices of bands and clear topological surface near Fermi level, showing that their normal states are Z₂ topological metals [1–4]. The superconducting transition temperatures Tc of KV₃Sb₅, RbV₃Sb₅ and CsV₃Sb₅ are 0.93 [2], 0.92 [5] and 2.5K [3] (2.3K [6, 7]), respectively, in which the corresponding transition temperatures T* of charge density wave (CDW) order are 78 [8], 102 [9] and 94K [10], respectively. The exotic CDW states without electron-phonon coupling (EPC) mechanism [9] display many unconventional characteristics. The CDWs in these three compounds exhibit chiral anisotropy [11–13] and reduce the density of electronic states near the Fermi level [11, 14–16]. Various evidence including giant anomalous Hall response even without magnetic field [17, 18], the chirality of CDW that can be tuned by a magnetic field [11–13], edge supercurrent [19] and spontaneous internal magnetic field [20] indicates that the charge order may break the time-reversal symmetry, which has also been verified theoretically [11, 21, 22]. Moreover, it has been found that CsV₃Sb₅ samples have the roton pair density wave [7], which is analogous to the one in unconventional high-Tc cuprate superconductors [23]. The coexistence of V- and U-shaped superconducting gaps in CsV₃Sb₅ [24] and the anisotropic superconducting properties [25] imply a possible multi-band superconducting pairing. Intertwined superconductivity with CDW shows many new features. For instance, Tc exhibits an unconventional double dome behavior, and T* decreases rapidly with increasing pressure [10, 26, 27]. The second dome of Tc and the disappearance of T* emerge at the same pressure. The superconducting properties and charge order of AV₃Sb₅ can also be tuned by magnetic impurities [24], strain [28], thicknesses [29–31], which dramatically enrich the phase diagram. The experimental and theoretical studies on AV₃Sb₅ show a complementary and rapid trend. However, to further explore the exotic properties of AV₃Sb₅, more candidate compounds based on AV₃Sb₅ prototype structure appear to be needed.

In this paper, we first apply the high-throughput first-principles calculations on 800 new kagome structures based on AV₃Sb₅ prototype. We found 24 dynamic stable new metal compounds. Then, we calculated their superconducting and topological properties. The results show that 14 novel compounds are superconductors with superconducting transition temperatures between 0.3 and 5.0K. Some compounds, including KZr₃Pb₅ with the highest superconducting transition temperature, have strong Z₂ indices with abundant nontrivial topological surface states near Fermi surface, showing they are Z₂ topological metals. The coexistence of superconductivity and nontrival topology in KZr₃Pb₅ and some other compounds opens a door for the possible discovery of topological superconductor based on the kagome net. Additionally, we also found two possible CDW phases in NaZr₃As₅, which exhibit soft modes in phonon spectrum, and may provide useful information for further understanding the CDW phases in AV₃Sb₅.

Crystal structures of AV₃Sb₅.—The AV₃Sb₅ crystalize in the hexagonal structure with the space group of P6/mmm (No.191) as shown in Fig. 1. As we can see, these three-dimensional (3D) compounds form a layered structure. The perfect kagome net of V atoms mixed with a simple triangular net of Sb atoms is located in the middle layer, which is sandwiched by two additional
honeycomb layers of Sb atoms. The upper and lower triangular layers of alkali metal A atoms have large bond distances with respect to the middle V-Sb layer and are loosely bonded to them.

Searching new structures.—The high-throughput first-principles calculations are used to search for kagome topological superconductor candidates (as indicated in Fig. S1 in Supplementary Material (SM)). Based on the prototype structure of AV\(_3\)Sb\(_5\), 800 new compounds are constructed by replacing A with alkali metal elements Li, Na, K, Rb and Cs, replacing V with all transition metal elements in the fourth and fifth periods of the periodic table, and replacing Sb with its neighboring elements (Ge, As, Sn, Sb, Te, Pb, and Bi). These new compounds will be abbreviated as AB\(_3\)C\(_5\) below. For all these new compounds, we first carry out fully geometric relaxation in different magnetic configurations (shown Fig. S2). Then, by comparing the total energies of different magnetic configurations, each AB\(_3\)C\(_5\) member can be classified according to nonmagnetic (NM), ferromagnetic (FM) and antiferromagnetic (AFM) configurations. The phonon spectrum is calculated to determine the dynamic stability of these AB\(_3\)C\(_5\) members. Compounds without imaginary frequency in phonon spectra will be further analyzed for corresponding electronic structures, superconductivity, and topological properties. On the other hand, the phonon spectra with imaginary frequency will be used to discuss possible CDW phases.

In doing so, we discovered 24 stable novel AB\(_3\)C\(_5\) members, including 22 non-magnetic structures, one FM CsTi\(_3\)Pb\(_5\) with a magnetic moment of 0.69 \(\mu\)B per Ti atom and one AFM RbCr\(_3\)Te\(_5\) with a magnetic moment of 2.33\(\mu\)B per Cr atom. Their lattice information is listed in Table S1. The electronic structures show that they are all metals similar to AV\(_3\)Sb\(_5\). Furthermore, 22 members keep the same crystal structure as AV\(_3\)Sb\(_5\) after structural optimization (as listed in Fig. 1), except for CsRu\(_3\)Ge\(_5\) and RbCr\(_3\)Te\(_5\), whose triangles in the kagome nets are twisted, which changes their space group to P6\(_2\)m.

Superconductivity.—The metallicity of these 24 AB\(_3\)C\(_5\) members enables us to perform further calculations on superconductivity. We calculated the Eliashberg electron-phonon spectral function \(\alpha^2F(\omega)\) and cumulative frequency dependent EPC \(\lambda(\omega)\) of these materials at ambient pressure, and then the superconducting transition temperature \(T_c\) can be estimated with the McMillan-Allen-Dynes approach of Bardeen-Cooper-Schrieffer (BCS) theory (See SM for detailed calculations). After careful calculation and screening, we found that 14 of these 24 members have superconducting ground states as listed in Table I, where KZr\(_3\)Pb\(_5\) possesses the highest \(T_c\) of 5.027K, which is more than twice the experimental values of AV\(_3\)Sb\(_5\) (see Table II) [2, 3, 5-7].

We choose AZr\(_3\)Pb\(_5\) group with relative higher superconducting transition temperatures for further discussions. The phonon spectra, phonon density of states

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**TABLE I.** Electronic density of states at Fermi energy \(N(E_F)\) for per fomular unit \((eV^{-1}\text{f.u.}^{-1})\), logarithmic average frequency \(\omega_{log}(K)\), EPC \(\lambda(\omega = \infty)\) and \(T_c\) of 14 stable compounds.

| Compound       | \(N(E_F)\) \((eV^{-1}\text{f.u.}^{-1})\) | \(\omega_{log}(K)\) | \(\lambda\) | \(T_c\) \((K)\) |
|----------------|---------------------------------|-----------------|----|-------------|
| RbMo\(_3\)Sn\(_5\) | 3.60                           | 136.5           | 0.36 | 0.371       |
| KNb\(_3\)Sn\(_5\) | 4.22                           | 149.1           | 0.52 | 2.102       |
| CsRu\(_3\)Ge\(_5\) | 3.19                           | 170.8           | 0.36 | 0.353       |
| CsTi\(_3\)Bi\(_5\) | 5.96                           | 163.4           | 0.35 | 0.316       |
| KTi\(_3\)Pb\(_5\) | 7.29                           | 157.9           | 0.51 | 2.039       |
| RbTi\(_3\)Pb\(_5\) | 7.50                           | 156.5           | 0.50 | 1.857       |
| KTiSn\(_3\)Sn\(_5\) | 6.57                           | 180.3           | 0.42 | 0.974       |
| RbTiSn\(_3\)Sn\(_5\) | 6.50                           | 182.5           | 0.42 | 0.961       |
| CsTiSn\(_3\)Sn\(_5\) | 6.87                           | 174.6           | 0.45 | 1.375       |
| CsZr\(_3\)As\(_5\) | 3.40                           | 125.8           | 0.56 | 2.289       |
| KZr\(_3\)Pb\(_5\) | 6.47                           | 94.1            | 0.91 | 5.027       |
| RbZr\(_3\)Pb\(_5\) | 6.56                           | 111.9           | 0.72 | 4.154       |
| CsZr\(_3\)Pb\(_5\) | 6.53                           | 119.2           | 0.58 | 2.438       |
| CsZr\(_3\)Te\(_5\) | 2.88                           | 123.5           | 0.48 | 1.266       |

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**TABLE II.** Electronic density of states at Fermi energy \(N(E_F)\) for per fomular unit \((eV^{-1}\text{f.u.}^{-1})\), logarithmic average frequency \(\omega_{log}(K)\), EPC \(\lambda(\omega = \infty)\) and \(T_c\) of 14 stable compounds.

| Compound       | \(N(E_F)\) \((eV^{-1}\text{f.u.}^{-1})\) | \(\omega_{log}(K)\) | \(\lambda\) | \(T_c\) \((K)\) |
|----------------|---------------------------------|-----------------|----|-------------|
| KV\(_3\)Sb\(_5\) | 2.9                            | 0.38            | 0.22 | 0.93        |
| RbV\(_3\)Sb\(_5\) | 2.33                           | 0.32            | 0.05 | 0.92        |
| CsV\(_3\)Sb\(_5\) | 1.30                           | 0.25            | 0.0008 | 2.5 (2.3)  |
| KZr\(_3\)Pb\(_5\) | 6.47                           | 0.91            | 5.027 | ?           |
| RbZr\(_3\)Pb\(_5\) | 6.56                           | 0.72            | 4.154 | ?           |
| CsZr\(_3\)Pb\(_5\) | 6.53                           | 0.58            | 2.438 | ?           |
FIG. 2. The phonon spectra, projected PhDOS, Eliashberg spectral function $\alpha^2 F(\omega)$, and cumulative frequency dependent EPC $\lambda(\omega)$ of (a) KZr$_3$Pb$_5$, (b) RbZr$_3$Pb$_5$, (c) CsZr$_3$Pb$_5$.

(PhDOS), $\alpha^2 F(\omega)$ and $\lambda(\omega)$ of the three structures are plotted in Fig. 2. We can see that the phonon spectra of three compounds are very similar. Careful comparison of their phonon spectra shows that the faint phonon softening at L point gradually becomes obvious from K to Rb to Cs. It can be seen from PhDOS that the contributions of Pb and Zr atoms to PhDOS is mainly distributed in the relatively low and high frequency regions with much high peaks, respectively, while the PhDOS of alkali metal atoms distributed in the medium frequency region are very small. The relatively low frequency (<3THz) phonons corresponding to the vibration modes of Pb account for more than half of the total EPC. The $T_c$ of the three compounds decreases with the gradual increase of the atomic number of alkali metals as shown in Table I. The gradual decrease of $T_c$ from K to Rb to Cs is due to the negligible contribution of alkali metal elements to the EPC, and the increase of atomic radius from K to Cs, resulting in the gradual increase of the lattice parameters, is equivalent to applying a negative pressure (tensile strain) to the lattice, which significantly reduce the parameters related to the lattice and weakens the EPC.

Electronic band structure and topological property. — We plot the calculated electronic energy bands and density of states (DOS) with spin-orbit coupling (SOC) for KZr$_3$Pb$_5$ in Fig. 3(a). The electronic band structures of RbZr$_3$Pb$_5$ and CsZr$_3$Pb$_5$ are given in Figs. S21-22. The 3D Fermi surface (FS) of KZr$_3$Pb$_5$ and its 2D map at $k_z=0$ and $k_z=\pi$ slices are drawn in Figs. 3(b)-(d), which is obviously different from the FS of AV$_5$Sb$_5$ that exhibits a strong 2D feature. Furthermore, we can see the obvious Fermi surface nesting with the nesting vector parallel to A-L and A-H in the $k_z=\pi$ slice.

Unlike most magnetic kagome metal materials, AZr$_3$Pb$_5$ is nonmagnetic similar to AV$_5$Sb$_5$. So combining both time-reversal symmetry and inversion symmetries of AZr$_3$Pb$_5$, we can get their $Z_2$ topological invariants by calculating the parity of the wave functions at all time-reversal invariant momenta (TRIM) points [33]. It can be seen from Fig. 3(e) that several energy bands passing through the Fermi surface all have strong topological $Z_2$ indices, resulting in abundant Dirac cone surface states at TRIM M-point near the Fermi level as shown in Figs. 3 (g) and (h). The continuous bandgap between two energy bands in the whole Brillouin zone, the nontrivial topological surface states and the strong $Z_2$ indices of bands near the Fermi level make KZr$_3$Pb$_5$ a $Z_2$ topological metal. Similar analysis shows that many other AB$_3$C$_5$ members, such as CsZr$_3$Pb$_5$, are also $Z_2$
topological metals.

**Possible CDW phases.**—We take NaZr₃As₅ for an example to explore possible CDW phases. One may find that the phonon spectrum in Fig. 4(d) shows clear soften-ing acoustic phonon modes near M and L points at the Brillouin zone boundary, and the imaginary frequency at L point is slightly larger than that at M point, which is very similar to AV₃Sb₅ [15, 32]. The symmetry analysis on AV₃Sb₅ indicates that the irreducible representations of the imaginary modes at M and L points are M₁⁺ and L₂⁻, respectively, which is also consistent with the previous studies [15, 34]. However, similar analysis shows the irreducible representations of imaginary modes in NaZr₃As₅ are M₃⁺ and L₁⁻, which makes NaZr₃As₅ exhibit completely different distortions from AV₃Sb₅. In consideration of one M and one L points, it gives the phase as seen in Fig. 4(b). The soft mode at M point makes corner-sharing triangles in layers rotate around the corner, while the soft mode at L point makes the distortion of adjacent layers have a π-shift. Clockwise and counterclockwise distortions generate the same structure. The combination of all three unequal M and L points gives a similar phase as shown in Fig. 4(c), which differs from Fig. 4(b) in that Zr atoms in the kagome layers rotate around the center of triangles. These two structures have Ibam (No.72) and P6/mmc (No.192) space groups, respectively. Both of them reduce the C₆ rotation symmetry to C₂, but still retain the space inversion symmetry.

Their phonon spectra in Figs. 4(e) and (f) are dynamically stable with completely disappeared imaginary frequency, so both of them have possible CDW phases of NaZr₃As₅. We label them CDW I and CDW II, respectively. Compared with the pristine phase, the displacement values of Zr atoms in kagome layers in CDW I and CDW II are 0.12 and 0.15Å, respectively. The total energy as a function of displacement of Zr atoms is shown in Figs. 4(h) and (i). The total energies of the two stable CDW phases are 11.3 and 25.1meV lower than the pristine structure, respectively.

The real CDW phase and the possible competition or cooperation between charge order and superconductivity in NaZr₃As₅ deserve the experimental exploration. Besides NaZr₃As₅, we also list those structures with obvious soft modes at high symmetry paths that may have CDW phases as well in Fig. S27.

**Discussion.**—In addition to AZr₃Pb₅, the band structures with or without SOC, DOS, FS, phonon spectra of all other dynamically stable AB₃C₅ members are presented in Figs. S3-23 in SM. The new AV₃C₅ members are not only structurally similar to AV₃Sb₅, but also inherit many attractive features, such as the existence of Van Hove singularities at high symmetry points near the Fermi level, Dirac points at the Fermi level, Dirac nodal lines, and strong 2D properties of the phonon spectrum and FS, which deserve further studies.

An important feature of those predicted structures beyond AV₃Sb₅ is their much stronger EPC strengths. The calculated Tₐ of KV₃Sb₅, RbV₃Sb₅, and CsV₃Sb₅ based on BCS theory are 0.0008, 0.05 and 0.22K, respectively [32], which are much lower than their experimental values (see Table II), because the CDW in AV₃Sb₅ reduces the DOS near Fermi level and suppresses BCS superconductivity. This indicates there may be an unconventional superconducting mechanism. This mechanism is also expected to appear in materials listed in Table I. From Table II, it can be observed that the calculated Tₑ of AZr₃Pb₅ are much higher than those of AV₃Sb₅, and thereby experimental Tₑ of AZr₃Pb₅ may be further considerably high.

The coexistence of superconductivity and topological nontrivial surface states is essentially rare [35–38]. It was reported that the robust zero-bias conductance peak in CsV₃Sb₅ exhibits similar characteristics to the Bi₂Te₃/NbSe₂ heterostructures with Majorana bound state [6]. Our new compounds with both the superconducting ground state and the nontrivial topological surface states near the Fermi surface would provide a rich platform for exploring topological superconductivity and Majorana zero-energy modes.

Mature experimental methods like flux method have been used to synthesize high-quality and stable AV₃Sb₅ compounds, which is a prerequisite for the rapid development of experimental analysis. In the initial work of Brenden et al. for the AV₃Sb₅ family, they explored the combination of (K, Rb, Cs)(V, Nb, Ta)(Sb, Bi) under different synthetic conditions [1]. However, only KV₃Sb₅,
RbV₃Sb₅, and CsV₃Sb₅ were crystallized. In this work, 800 AB₃C₅ members in the high-throughput screening process contain most of the combinations they explored. Our calculation results show that those compounds not synthesized in their experiment are dynamically unstable except KNb₃Sb₅. The agreement with the experimental results indicates that our present calculations are reasonable, and the stable structures presented here are likely to be synthesized in future experiments. Very recently, a newly discovered family of kagome metals RV₆S₄₉ (R = Gd, Ho, Y) with two V-derived kagome layers in the primitive cell was also synthesized by flux method [39, 40]. Therefore, the versatile and matured flux method could be employed to synthesize the stable structures in Table S1.

Summary.—In conclusion, we calculated 800 new kagome candidates based on the prototype structure of AV₃Sb₅ using a high-throughput DFT screening process, and discovered 24 dynamically stable novel metal compounds, including one ferromagnetic, one antiferromagnetic and 22 nonmagnetic structures. These compounds display many appealing properties similar to AV₃Sb₅. Furthermore, based on the McMillan-Allen Dynes approach, 14 compounds among them were predicted to be phonon-mediated BCS superconductors with the superconducting transition temperature $T_c$ between 0.3-5K. KZr₃Pb₅ with the highest $T_c$ exhibits strong $Z_2$ invariants of the energy bands and abundant nontrivial topological surface states near the Fermi level, revealing that it is a $Z_2$ topological metal. In addition, we also found two possible CDW phases in NaZr₃As₅. This present work would give more insights on the exploration of possible topological superconductors.

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