Screening promising CsV$_3$Sb$_5$-like kagome materials from systematic first-principles evaluation

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Abstract

CsV$_3$Sb$_5$ kagome lattice holds the promise for manifesting electron correlation, topology and superconducting. However, by far only three CsV$_3$Sb$_5$-like kagome materials have been experimentally spotted. In this work, we enlarge this family of materials to 1386 compounds via element species substitution, and the further screening process suggests that 28 promising candidates have superior thermodynamic stability, hence they are highly likely to be synthesized. Moreover, these compounds possess several identical electronic structures, and can be categorized into five non-magnetic and three magnetic groups accordingly. It is our hope that this work can greatly expand the viable phase space of the CsV$_3$Sb$_5$-like materials for investigating or tuning the novel quantum phenomena in kagome lattice.
Introduction

In condensed matter physics, kagome lattice serves as an important quantum material system to manifest/investigate the interplay between electron correlation, topology, and lattice geometry. [1,2] For example, kagome lattice is featuring novel electronic structures, such as the flat band, Dirac cone, Van-Hove points, etc., owing to its special lattice geometry. [3] By far, several materials have been discovered to host the kagome lattices and novel kagome physics, e.g., the Fe kagome lattice within the Fe$_3$Sn$_2$ shows giant spin-orbit tunability [4,5] and the long sorted magnetic Weyl semimetals were identified in kagome Co$_3$Sn$_2$S$_2$ [6–8]. Recently, the newly discovered quasi-2-dimensional kagome materials, which are KV$_3$Sb$_5$, RbV$_3$Sb$_5$, and CsV$_3$Sb$_5$, open a new avenue for connecting the superconductivity with kagome physics [3,9–16], escalating the curiosity of physics community to uncover even more unconventional quantum phenomena from the kagome lattice.

Unfortunately, finding the desired kagome materials is a challenging task. For example, only three CsV$_3$Sb$_5$-like superconductive kagome materials (as mentioned above) have been experimentally synthesized at the time of writing, limiting the investigation of kagome superconductivity to a fairly small compound space. Hence, the development of quantum physics hinges pretty much on finding a viable material system with low dimensionality as well as various symmetry-breaking instabilities (such as superconductivity).

In order to search for promising kagome materials, this work systematically evaluates 1386 structures of kagome materials with the stoichiometry of AM$_3$X$_5$ (A for alkali elements, M for
transition metals, and X for anionic elements from III A, IV A, V A), which is derived from the CsV₃Sb₅ (space group P6/mmm). Employing the high-throughput calculations at the density functional theory level as well as the atomly.net [17] materials database, the optimized structure, thermodynamic stability (energy above hull < 5meV/atom), and electronic structures are calculated, and, in the end, 28 promising candidates are popped out from the screening process, including the CsV₃Sb₅, RbV₃Sb₅, and KV₃Sb₅ – the three known compounds that have been experimentally made according to existing literature, validating the reliability of our calculations. Among the 25 new compounds, it is found that the non-magnetic can be grouped into five non-magnetic categories based on their electronic structures. There are also a handful of magnetic kagome materials that fall out of the screening, and they are likely the feasible compounds to materialize the spin-related quantum phenomena in kagome lattice. This work charts a synthesizability “treasure hunt map”, from the theory- and data-driven approach, for quantum material community to discover the viable kagome materials.

**Methodology**

The theoretical calculations are performed at Density Functional Theory (DFT) [18] level in a high-throughput mode to evaluate the properties of AM₃X₅ kagome system. The DFT calculations are carried out using the Vienna ab initio software package (VASP) [19,20] with the projector augmented-wave (PAW) [21,22] method to describe the nucleus-electron interactions and the generalized gradient approximation (GGA) within the Perdew-Burke-Ernzerhof (PBE) [23] framework to describe the exchange-correlation in-between electrons. The plane-wave cutoff energy is 520 eV, the energy convergence criterion is 5*10⁻⁶ eV, and the K-points grid density of 100 k-points/Å⁻¹ is adopted for all the calculations. All the
calculations are conducted in a high-throughput mode by employing the standardized parameters to ensure that the calculation results (especially the formation energy) are mutually comparable to each other.

Results

In order to search for CsV₃Sb₅-like compounds that are highly synthesizable, 1386 structures are generated by employing the CsV₃Sb₅ (space group P6/mmm) as the structural template, then an element substitution process (as shown in Fig. 1a) is performed by replacing Cs site with (H, Li, Na, K, Rb, Cs), substituting V site with (Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W, Mn, Tc, Re, Fe, Ru, Os, Co, Rh, Ir, Ni, Pd, Pt), and replacing Sb site with (Si, Ge, Sn, Pb, P, As, Sb, Bi, S, Se, Te), totaling 1386 structures (including the CsV₃Sb₅). The purpose of the procedure is to create a large pool of candidate materials for future calculation and screening.

Then the high-throughput calculations are performed with an in-house workflow for structure optimization, high precision static calculation and electronic structure (density of states and energy bands) calculation. The structure optimization process relaxes the cell volume and the position of each atoms in the structure to yield the equilibrium ground state of the given structure at 0K, then the total energy obtained from the static calculation is used to justify the thermodynamic stability of the compound. In practice, the compound is put together with all available phases from the same chemical system to evaluate the phase competition. In order to get as many compounds as available from the same chemical system, we first query all the compounds from the atomly.net [17], which is an open-access materials database, to get all the relevant data. Then the data is plugged into the PhaseDiagram module [24] from the pymatgen [25] to generate the phase diagrams for each chemical system to obtain the energy above hull (Eₜₜuₜ) of each AM₃X₅ kagome material. Basically, the formation energy means the
energy released or consumed when one unit of a substance is created under standard conditions from its pure elements. [24,26] The compounds with smaller formation energy (negative value for energy release) are thermodynamically more stable. The most stable compounds open a formation energy convex hull to describe the lower boundary of the formation energies, and $E_{\text{hull}}$ simply denotes the distance between formation energy of a compound to the energy convex hull. In short, $E_{\text{hull}}$ of a compound quantitatively measures the driving force (in units of energy) to decompose the compounds to the most stable phases. The comprehensive concept of $E_{\text{hull}}$ can be found in ref. [27–29] and supplementary materials (Fig. S1). In general, smaller $E_{\text{hull}}$ represents better stability. Normally, nonmetallic compounds with $E_{\text{hull}} < 50 \text{meV/atom}$ or alloys/metals with $E_{\text{hull}} < 10 \text{meV/atom}$ are likely to exist in real world.

Fig. 1 (d-i) show the $E_{\text{hull}}$ of AM$_3$X$_5$ compounds from our calculations. It can be observed that HM$_3$X$_5$, LiM$_3$X$_5$ compounds are all thermodynamically unstable as their $E_{\text{hull}}$ are all larger than 60 meV/atom. In the rest chemical space, $E_{\text{hull}}$ of 28 compounds are under 5meV/atom (Table 1), $E_{\text{hull}}$ of 38 compounds are less than 20meV/atom (see Table S1 for complete list), and $E_{\text{hull}}$ of 90 compounds are smaller than 50meV/atom (see Table S2 for complete list).

Table 1 presents the full list of the 28 compounds that fall out of the $E_{\text{hull}} < 5\text{meV/atom}$ screening. It is found that three known compounds, which are CsV$_3$Sb$_5$, RbV$_3$Sb$_5$, and KV$_3$Sb$_5$, show up on the list, suggesting that the screening treatment is fairly effective and accurate. It can be observed that, the stable AM$_3$X$_5$ structures can be found in AV$_3$Sb$_5$ (A=Na, K, Rb, Cs), ANb$_3$Bi$_5$ (A=K, Rb, Cs), ATi$_3$Bi$_5$ (A=Na, K, Rb, Cs), AMn$_3$Sb$_5$ (A=K, Rb, Cs), AFe$_3$Bi$_5$ (A=K, Rb, Cs), CsTi$_3$Te$_5$, CsTi$_3$Sb$_5$, CsV$_3$Bi$_5$, CsFe$_3$Ge$_5$, CsFe$_3$Sn$_5$, CsZr$_3$Bi$_5$, CsZr$_3$Te$_5$, CsHf$_3$Te$_5$, CsTa$_3$Sb$_5$, CsRh$_3$Pb$_5$, and CsPd$_3$Pb$_5$. It is also found that the stability of
AM$_3$X$_5$ decreases sequentially when A site is occupied by H, Li, Na, K, Rb, Cs, and the later transition metal on M site is unlikely to yield stable AM$_3$X$_5$. Cs on A site can stabilize the structure as 16 out of 28 stable compounds in Table 1 are Cs-containing compounds, and it seems that the stability of AM$_3$X$_5$ is largely determined by the M-X layer as V-Sb, Nb-Bi, Ti-Bi, Mn-Sb, and Hf-Bi combinations are more stable. Overall, the viable AM$_3$X$_5$ kagome lattices are limited to a small phase space based on our screening, and Figure 1 and Table 1 chart a likelihood ‘map’ for discovering the viable CsV$_3$Sb$_5$-like compounds.

Since the electronic structures, especially the flat-band (FB), Dirac-point (DP), and Van Hove singularity (VHS), are fairly important properties of kagome lattice, the electronic structures of all the CsV$_3$Sb$_5$-like compounds (1386 of them in total) are calculated at GGA-PBE level without considering the spin orbital coupling. It is found that the AM$_3$X$_5$ can be classified into five non-magnetic groups and three magnetic groups according to their energy bands and Fermi surface. Figure 2 shows the representative compounds of the five non-magnetic types, and their electronic structures. The CsV$_3$Sb$_5$ is the most known type, and the DP is below the Fermi surface and VHS is close to or at the Fermi surface. Other than AV$_3$Sb$_5$ (A = Na, K, Rb, Cs), CsV$_3$Bi$_5$ is also in this group. For the RbNb$_3$Bi$_5$-type, the DP is below the Fermi surface, the VHS is close to or at the Fermi surface, but the bands, except the VHS band, at the M point open up a gap. KNb$_3$Bi$_5$, RbNb$_3$Bi$_5$, CsNb$_3$Bi$_5$, and CsTa$_3$Sb$_5$ belong to this type of compound. The CsTi$_3$Bi$_5$-type shots up both the DP and VHS as those compounds have less valence electrons than that of CsV$_3$Sb$_5$-type, hence it can be regarded as the hole-doped CsV$_3$Sb$_5$-type and the Fermi surface is moved downward to some extent. AT$_3$Bi$_5$ (A=Na, K, Rb, Cs), AHf$_3$Bi$_5$ (A=K, Rb, Cs), CsTi$_3$Sb$_5$, and CsZr$_3$Bi$_5$ can be classified into this electronic structure type. In CsTi$_3$Te$_5$-type compounds, the VHS band is vanished and the DP is located fairly close to the Fermi surface, forming a simple Fermi surface in reciprocal space as there
are fewer bands around. CsTi₅Te₅, CsZr₅Te₅, CsHf₅Te₅, are the similar type of compounds. CsRh₃Pb₅-type compounds are more three-dimensional losing the typical feature of two-dimensional Kagome lattice. CsRh₃Pb₅ still has the VHS band near the Fermi surface but lacks the DP bands, and CsRh₃Pb₅, CsPd₃Pb₅ are this type of compounds.

For the Mn- and Fe-containing AM₃X₅ structures, the compounds are spin-polarized and show ferromagnetism as shown in Fig. 3. There are only a few of this type of compounds, those are AM₃Sb₅ (A=K, Rb, Cs), CsFe₃X₅ (X=Ge, Sn). It is fairly special that the kagome sites in those compounds are spin-polarized, making them the viable material systems to materialize the spin-related phenomenon. [1,2,30,31] At the collinear level of treatment for the system, it is observed that the Mn or Fe kagome sites hold the prominent amount of magnetic moment, e.g. the magnetic moment of Mn sites in CsMn₃Sb₅ is around 2.5-2.7 \( \mu_B/\text{atom} \) while the total magnetic moment of the compounds is around 7.5-8.0 \( \mu_B \) per formula.

Because of the non-degenerated orbitals caused by the spin-polarization, the Fermi surface in the reciprocal space manifests much more complicated structures, and the DP and VHS are also split into two sets. Hence, our work hints that it is likely to have spin-polarized CsV₃Sb₅-like kagome materials, and a drilled-down study is worth conducting.

**Discussions**

Based on our screening, we are offering the community a ranked list for discovering new compounds that share the same crystal structure with CsV₃Sb₅. We indeed obtain a compound list of CsV₃Sb₅-like compounds, and provide a systematic evaluation of formation energy landscape for them. Considering that the formation energy of alloy is generally small compared to the ionic and covalent compounds, and the formation energy between the
compounds is still relatively close to each other, therefore, it is generally difficult to synthesize the intermetallic phases even when they are predicted to be stable.

The data that we utilized to generate the phase diagram cover a very large compound space as most ICSD [32] and materials project [33] structures are included [Here, you may need add ICSD and material project ref. or website]. More than that, we have generated and calculated ~100k new structures by replacing the element species. The large compound space can ensure the accurate gauging of the $E_{\text{hull}}$ of compounds, but there is still a small chance to overlook the most stable compounds that can stretch the hull to even lower energies. In such case, the $E_{\text{hull}}$ of most compounds can be lifted up a little, hence the value of the $E_{\text{hull}}$ may increase a little when the database grows larger.

The Table 1, S1 and S2 serve as synthesis guides for exploring the CsV$_3$Sb$_5$-like compounds, if the pure phases of those predicted compounds are hard to make, it is highly possible that the doped compounds can be experimentally realized employing the knowledge from Fig. 1. For example, hole- or electron-doping to CsV$_3$Sb$_5$ compounds could probably be experimentally realized by replacing a small amount of the V with Ti or Ni [34,35], and substituting small amount of the V with Mn or Fe can possibly introduce magnetism into these material systems. Fig. 2 and 3 provide guides on how the electronic structures can be tuned when mixing the metal elements. Although, the main text of the paper shows the 28 most stable compounds, those compounds in Table S1 also have good-to-moderate stability, and are worth looking at. For example, the CsV$_6$Sb$_6$, which has a $E_{\text{hull}}$ of $\sim$12 meV/atom based on our calculation, has been experimentally made [36].
The electronic structures of all the 28 compounds in Table 1 can be found in the supplementary material (Fig. S2). The calculated data for all the 1386 compounds is open-accessible from atomly.net [17] (for people who has a user account).

Conclusions

In summary, this work widens the knowledge of Cs$_3$Sb$_5$-family through high-throughput calculation and systematic evaluation. Via the element replacement, a large chemical space of the Cs$_3$Sb$_5$-like materials (1386 in total) are calculated at the GGA-PBE level employing the DFT, the systematic evaluation tells us that there are at least 28 compounds having excellent thermodynamic stability, and therefore it looks forward to a further experimental confirmation. The electronic structures of those materials add possibilities for rational band structure engineering of kagome quantum materials. It is our hope that useful new kagome materials can be experimentally discovered for quantum physics community based on our prediction.

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Figure 1. The structure and thermodynamic stability of the kagome compounds. (a-c) the structure and the schematic of the element substitution strategy for generating CsV₃Sb₅-like compounds, and the transition metal forms the kagome lattice in structure. (d-i) The thermodynamic stability (represented quantitatively as \( E_{\text{hull}} \)) for 1386 compounds in a heat map plotting mode. Each box shows a AM₃X₅ compound, and the darker color the more stable the compound is. Compounds with \( E_{\text{hull}} \) greater than 100 meV/atom are plotted in yellow.
Figure 2. Electronic structures of selected non-magnetic compounds with $E_{\text{hull}} < 5$ meV/atom.

The compounds are categorized into five dedicated kinds, as (a)-(c), (d)-(f), (g)-(i), (j)-(l), (m)-(o), according to their band structures, density of states and Fermi surfaces. Compounds in the same group have very similar electronic structures.
Figure 3. Electronic structures of magnetic compounds with $E_{\text{hull}} \leq 5 \text{meV/atom}$. (a)-(c), (d) and (e), (f) and (g) are band structures, density of states and Fermi surfaces of representative compounds.
Table 1. List of 28 compounds with good thermodynamic stability (E\text{hull}<5 meV/atom). The compound formula, ID in the database, Ehull value and the lattice parameters are provided.

| Formula        | ID (atomly.net) | E\text{hull} (meV/atom) | a(Å) | c(Å) | Magnetization (\mu\text{B/formula}) |
|----------------|-----------------|--------------------------|------|------|--------------------------------------|
| NaTi\text{Bis} | 1000299281      | 0                        | 5.78 | 9.18 |                                       |
| NaV\text{Sb}_5 | 1000299291      | 2                        | 5.46 | 8.91 |                                       |
| KTi\text{Bis}  | 1000299512      | 0                        | 5.79 | 9.72 |                                       |
| KV\text{Sb}_5  | 1000299522      | 0                        | 5.48 | 9.37 |                                       |
| KMn\text{Sb}_5 | 1000299544      | 0                        | 5.43 | 9.26 | FM(\mu=7.75)                         |
| KNb\text{Bis}  | 1000299600      | 0                        | 5.89 | 9.59 |                                       |
| KHf\text{Bis}  | 1000299666      | 3                        | 6.08 | 9.45 |                                       |
| RbTi\text{Bis} | 1000299743      | 0                        | 5.79 | 9.89 |                                       |
| Rh\text{V}Sb\text{S} | 1000299753 | 0                        | 5.50 | 9.38 |                                       |
| RbMn\text{Sb}_5 | 1000299775      | 0                        | 5.44 | 9.44 | FM(\mu=7.73)                         |
| RbNb\text{Bis} | 1000299831      | 0                        | 5.89 | 9.71 |                                       |
| RbHf\text{Bis} | 1000299897      | 0                        | 6.08 | 9.59 |                                       |
| CsTi\text{Sb}_5 | 1000299973      | 0                        | 5.68 | 9.81 |                                       |
| CsNb\text{Bis} | 1000299974      | 0                        | 5.83 | 9.92 |                                       |
| CsTi\text{Tes} | 1000299881      | 0                        | 6.10 | 8.91 |                                       |
| CsV\text{Sb}_5 | 1000299894      | 0                        | 5.49 | 9.89 |                                       |
| CsV\text{Bis}  | 1000299985      | 0                        | 5.64 | 10.15|                                       |
| CsMn\text{Sb}_5 | 1000300006      | 0                        | 5.44 | 9.69 | FM(\mu=7.70)                         |
| CsFe\text{Ges} | 1000300020      | 0                        | 4.89 | 9.73 | FM(\mu=4.99)                         |
| CsFe\text{Sb}_5 | 1000300021      | 0                        | 5.26 | 10.53| FM(\mu=6.50)                         |
| CsZr\text{Bis} | 1000300051      | 0                        | 6.11 | 10.09|                                       |
| CsZr\text{Tes} | 1000300058      | 0                        | 6.41 | 9.07 |                                       |
| CsNb\text{Bis} | 1000300062      | 0                        | 5.91 | 9.87 |                                       |
| CsRh\text{Pbs} | 1000300110      | 0                        | 5.71 | 9.74 |                                       |
| CsPd\text{Pbs} | 1000300121      | 0                        | 5.81 | 9.61 |                                       |
| CsHf\text{Bis} | 1000300128      | 0                        | 6.09 | 10.05|                                       |
| CsHf\text{Tes} | 1000300135      | 0                        | 6.35 | 8.76 |                                       |
| CsTa\text{Sb}_5 | 1000300138      | 2                        | 5.81 | 9.60 |                                       |

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