Data-driven descriptor for high-throughput screening of topological insulators

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Significant advances have been made in predicting new topological materials using high-throughput empirical descriptors¹ or symmetry-based indicators²⁻⁵. This line of research has produced extensive lists of candidate topological materials that still await experimental validation. To date, these approaches have been limited to materials already known in databases, leaving a much larger portion of the materials space unexplored. Here we uncover a novel two-dimensional descriptor for fast and reliable identification of the topological characters of complex alloyed systems. Using tetradymites with widely varying stoichiometric compositions as examples, we obtain this descriptor by applying a recently developed data-analytics approach named SISSO (Sure Independence Screening and Sparsifying Operator) to training data from high-level electronic structure calculations. By leveraging this descriptor that contains only two elemental properties (the atomic number and electronegativity) of the constituent species, we can readily scan over four million alloys in the tetradymite family. Strikingly, nearly two million new topological insulators are
discovered, thus drastically expanding the territory of the topological materials world. The strong predictive power of the descriptor beyond the initial scope of the training data also testifies the increasing importance of such data-driven approaches in materials discovery.
Topological insulators (TIs) constitute a new class of quantum materials with insulating bulk but metallic boundary states. Protected by time-reversal symmetry\textsuperscript{6-9}, those boundary states possess a spin-momentum locked Dirac structure in which all the backscattering channels are suppressed, favoring dissipationless electronic conduction. Due to this salient property, TIs have immense application potential in spintronics, catalysis, and quantum computing\textsuperscript{10-14}, propelling the field to actively search for new TIs that may deliver such high technological expectations.

Theoretically, TIs are characterized by a non-vanishing topological invariant $Z_2$, which can be determined by parity considerations or by integration of the Berry curvature in momentum space through detailed electronic structure calculations\textsuperscript{15-17}. Earlier search efforts for potential TIs have been performed on a case-by-case basis, as exemplified by the successful predictions and experimental confirmations of the well-known strong TIs Bi$_2$Te$_3$, Sb$_2$Te$_3$, and Bi$_2$Se$_3$\textsuperscript{18-21}. More recently, the field has witnessed rapid advances achieved by high-throughput screening over many candidate topological materials using empirical descriptors\textsuperscript{1,22} or symmetry-based indicators\textsuperscript{2-5}. Strikingly, out of the tens of thousands of materials in the Inorganic Crystal Structure Database (ICSD), hundreds to thousands have been identified to be topologically nontrivial.

Beyond the systems listed in the ICSD and other databases, there exists a much larger materials space, e.g., compounds that can be created by alloying, i.e., by fractionally varying the stoichiometric compositions. While these immensely vast material classes were out of the scope of the above-mentioned approaches, they are the focus of the present study. Using alloyed tetradymites as a prototypical class of examples, we establish a data-driven descriptor for the prediction of TIs with fractional stoichiometry, thus covering a previously uncharted territory in materials space. To this goal, we first investigate a moderate number (hundreds) of layered tetradymites by using high-level electronic structure calculations that account for van-der-Waals (vdW) interactions\textsuperscript{23-25} and many-body effects\textsuperscript{26,27} at a perturbative level. We then employ the SISSO approach\textsuperscript{28} that is based on the compressed-sensing technique to establish a simple and physically intuitive descriptor for the
identification of the topological character. Compared with other big-data analytics approaches\textsuperscript{29-34} that rely on interpolating existing data, SISSO is advantageous since the obtained descriptor is an elementary function of key physical inputs, i.e., only the atomic number and electronegativity of the constituent atoms in the present case. Hence, the descriptor allows for its inspection and its extension well beyond the training set, as demonstrated recently for various other material properties such as the ground-state enthalpies and metal/insulator classifications of selective binary materials\textsuperscript{35-38}. Following this strategy, we rapidly identify the topological character of more than four million tetradymites with fractional stoichiometry that are not included in the original training set, from which nearly half of them are predicted to be new TIs. Selective crosschecks using first-principles calculations and available experimental data further confirm the validity and reliability of our predictions, which further testifies the predictive power of the descriptor identified.

**Methodology**

To construct a reliable training set, we have computed the topological character of 243 tetradymites by combining group-VA elements (As, Sb and Bi) with group-VIA elements (S, Se and Te). These systems can be viewed as stackings of quintuple layers (QLs) along the $c$-direction, where vdW interactions bind neighboring QLs to each other. As an example, Fig. 1 shows the crystal structure of the tetradymite AsSbSeTeS, where the atoms As, Sb, Se, Te, and S occupy the sites $A$, $B$, $L$, $M$, and $N$, respectively. Unlike earlier approaches that relied on semi-local approximations for the electronic exchange and correlation\textsuperscript{18,39,40}, we employ high-level first-principles methods including appropriate vdW-functionals and quasiparticle corrections as detailed in Section 1 of the Supplementary Information, which are essential to obtaining reliable values for the topological invariant $Z_2$.

Based on this high-level electronic structure data, we utilize SISSO\textsuperscript{28} to single out a simple and physically intuitive descriptor from a huge number of potential candidates. In our case, SISSO is used to determine a low-dimensional representation of the materials space, in which the TIs and the normal insulators (NIs) belong to well-
defined, non-overlapping domains. In practice, a huge pool of more than ten billion candidate descriptors is first constructed iteratively by combining elemental physical properties of the constituent atoms. In our case, these are the atomic number, the Pauling electronegativity, and the spin-orbit coupling (SOC) constant41 (details can be found in Section 1 of the Supplementary Information). As discussed below, these few properties are already sufficient to obtain a physically meaningful descriptor. Secondly, the desired low-dimensional representation is obtained from this pool via compressed-sensing techniques. Since the transparent functional form of the identified descriptor reflects the mechanism underlying the topological character, it is physically meaningful and suitable for extrapolation, as also demonstrated below.

**Training data**

By performing accurate first-principles calculations for the set of 243 tetradymites, we identify 177 systems that are mechanically stable (namely, without pronounced negative phonons), while 66 are unstable. We also find that the topological characters of 230 systems do not depend on the special choice of the vdW functional, while the other 13 systems give different $Z_2$ values for the optB86b-vdW and optB88-vdW functionals mentioned in Section 1 of the Supplementary Information. Furthermore, among the 177 stable systems, there are 10 weak TIs (namely, topological surface states only exist on certain surface orientations), and 4 semimetals. Excluding all these somewhat ambiguous systems, we finally obtain a set of 152 stable tetradymites with clear TI/NI classifications as the training set. Among them, 67 systems are TIs (including 4 binary, 27 ternary, 30 quaternary, and 6 quinary tetradymites), while the remaining 85 systems are NIs (containing 3 binary, 24 ternary, 46 quaternary, and 12 quinary tetradymites). The stability and topological properties of all the 243 tetradymites are summarized in Section 2 of the Supplementary Information.

It should be noted that the training data set naturally includes the TIs Bi$_2$Te$_3$, Bi$_2$Se$_3$, Sb$_2$Te$_3$, Sb$_2$Te$_2$S, Sb$_2$Te$_2$Se, Bi$_2$Te$_2$Se, Bi$_2$Se$_2$Te and BiSbSeTe$_2$ that have already been previously identified18-21,42-44. Furthermore, the set also includes 59 new TIs, and some of those feature relatively large band gaps, such as SbBiSeSeSe (0.22 eV),
SbBiTeTeS (0.27 eV), and SbBiTeTeSe (0.23 eV), and are thus promising candidates for potential applications.

Descriptor for the classification of TIs and NIs

The SISSO training has been performed for the described data set of 152 tetradymites, yielding the following optimized two-dimensional (2D) descriptor among several possible candidates (see Section 3 of the Supplementary Information):

\[ D_1 = (Z_A + Z_B) \cdot (Z_L + Z_M) - |Z_A Z_M - Z_B Z_L|, \]  

(1)

\[ D_2 = \left( \frac{\chi_L + \chi_M}{\chi_A} \right) \cdot \frac{Z_N}{Z_A} - (Z_L + Z_M) - |Z_L - Z_M|. \]  

(2)

Here, \( Z \) denotes the atomic number and \( \chi \) the electronegativity of the constituent atoms, whereby the subscripts \( A \), \( B \), \( L \), \( M \), and \( N \) refer to the sites occupied by the atoms (see Fig. 1). Using \( D_1 \) and \( D_2 \) as the \( x \) and \( y \) coordinates, we can plot a “topological phase diagram” of the 152 tetradymites as shown in Fig. 2, where the cyan and green regions are the convex envelopes of the 85 NIs and 67 TIs, respectively. The support vector machine (SVM) technique\(^{45}\) is further used to calculate the blue dividing line \( D_2 = -238.23 + 0.039D_1 \) between the TI and NI domains. We see from Fig. 2 that the obtained 2D descriptor gives a perfect classification of the training data, i.e., there is no overlap between the NI and TI domains. The robustness of the descriptor has been checked via the leave-one-out cross-validation approach, and the all-data descriptor is identified in 86% of all the 152 iterations (each descriptor is identified out of \( \sim 10^{23} \) possible candidates). Furthermore, it is remarkable that even the 66 mechanically unstable systems (open symbols) are perfectly classified by the phase diagram, despite the fact that the descriptor is obtained by using only the 152 stable ones (filled symbols) as the training set. Similarly, exactly the same 2D descriptor \( (D_1, D_2) \) is identified if the full data of 216 stable and unstable tetradymites are adopted. These striking observations further substantiate that the obtained 2D descriptor is able to capture the physical
mechanism determining the topological character in this material class.

To have a better understanding, we rewrite Eq. (1) as

\[ D_1 = \begin{cases} 
Z_A Z_L + 2Z_B Z_L + Z_B Z_M, & \text{if } Z_A Z_M - Z_B Z_L > 0 \\
Z_A Z_L + 2Z_A Z_M + Z_B Z_M, & \text{if } Z_A Z_M - Z_B Z_L < 0
\end{cases} \tag{3} \]

where we see that larger values of \( Z_A, Z_B, Z_L \) and \( Z_M \) lead to higher \( D_1 \), making the system to be in the TI region. This is consistent with the established understanding that heavier atoms usually have larger SOC, which is a key factor to induce topological band inversion\(^{18}\). For instance, the well-known TI Bi$_2$Te$_3$ exhibits the largest \( D_1 \) value of 17,264 among all the 152 tetradymites and thus represents a vertex of the convex TI envelope, since it features the largest atomic numbers of the cations (\( Z_A = Z_B = 83 \)) and anions (\( Z_L = Z_M = Z_N = 52 \)). It should also be noted that \( Z_N \) does not appear in Eq. (3), because the anions at the \( N \) sites make very minimal contributions to the highest valence band and lowest conduction band of the systems. More details can be found in Section 4 of the Supplementary Information.

Although \( D_1 \) is the decisive descriptor for a large majority of these tetradymites, it alone is not sufficient to predict the topological character in the region with \( 6806 < D_1 < 7854 \) (enclosed by two vertical lines in Fig. 2). In this case, \( D_2 \) of the 2D descriptor becomes crucial: among the 29 tetradymites located within this particular region, 14 compounds with smaller \( D_2 \) values are TIs, while the remaining 15 compounds with larger \( D_2 \) values are NIs. To better reveal the delicate physical mechanism, we rewrite Eq. (2) as

\[ D_2 = \begin{cases} 
\left( \frac{(\chi_L + \chi_M) \cdot Z_N - 2\chi_A Z_L}{\chi_A} \right), & \text{if } Z_L - Z_M > 0 \\
\left( \frac{(\chi_L + \chi_M) \cdot Z_N - 2\chi_A Z_M}{\chi_A} \right), & \text{if } Z_L - Z_M < 0
\end{cases} \tag{4} \]

In principle, \( D_2 \) is the relative electronegativity difference between the anions (at the \( L \) and \( M \) sites) and cations (at the \( A \) site). As the electronegativity difference is
approximately positively related to the band gap of an inorganic compound\textsuperscript{46,47}, a smaller $D_2$ value (smaller electronegativity difference) leads to a smaller band gap, making it easier to generate a band inversion, and the system is more likely a TI. Indeed, our first-principles calculations for the 29 tetradymites (with $6806 < D_1 < 7854$) indicate that the TIs with small $D_2$ values tend to exhibit smaller band gaps (before SOC) than the respective NIs at similar $D_1$. Details can be found in Section 4 of the Supplementary Information.

Overall, although the proposed 2D descriptor only depends on the atomic number $Z$ and the electronegativity $\chi$ of the constituent atoms, it correctly captures the essential physical factors of TIs, namely, the competition between the SOC strength and band gap. Compared with previous empirical models\textsuperscript{1,22}, our 2D descriptor $D_1$ and $D_2$ identified by SISSO features a much more complex functional form that enables quantitative and reliable predictions of TIs, as further demonstrated below.

**Predictions beyond the training data**

The 243 tetradymites discussed so far all feature integer stoichiometry. In fact, alloyed tetradymites with fractional stoichiometry such as $\text{Bi}_2\text{Te}_{3-x}\text{S}_x$\textsuperscript{48} and $\text{Bi}_{1.4}\text{Sb}_{0.6}\text{Te}_{1.8}\text{S}_{1.2}$\textsuperscript{49} are promising TIs for potential broader technological applications, since the variation of the stoichiometry allows to further tune their electronic and topological properties. Unfortunately, reliable first-principles data is hard if not impossible to obtain for such systems, since prohibitively large supercells are needed to represent such fractional stoichiometries $\text{As}_x\text{Sb}_y\text{Bi}_{2.4-x-y}\text{S}_a\text{Se}_{b}\text{Te}_{3-x-y}$

($0 \leq x, y \leq 2$ and $0 \leq a, b \leq 3$). Generalizing the 2D descriptor discovered above, however, allows to predict the topological characters for the complete class of tetradymites, including alloyed compounds. For this purpose, we define site-specific atomic numbers:
\[
Z_A = x_1 Z_{As} + y_1 Z_{Sb} + (1-x_1-y_1) Z_{Bi}
\]
\[
Z_B = x_2 Z_{As} + y_2 Z_{Sb} + (1-x_2-y_2) Z_{Bi}
\]
\[
Z_L = a_1 Z_S + b_1 Z_{Se} + (1-a_1-b_1) Z_{Te}
\]
\[
Z_M = a_2 Z_S + b_2 Z_{Se} + (1-a_2-b_2) Z_{Te}
\]
\[
Z_N = a_3 Z_S + b_3 Z_{Se} + (1-a_3-b_3) Z_{Te}
\]

and site-specific electronegativities:
\[
\chi_A = x_1 \chi_{As} + y_1 \chi_{Sb} + (1-x_1-y_1) \chi_{Bi}
\]
\[
\chi_B = x_2 \chi_{As} + y_2 \chi_{Sb} + (1-x_2-y_2) \chi_{Bi}
\]
\[
\chi_L = a_1 \chi_S + b_1 \chi_{Se} + (1-a_1-b_1) \chi_{Te}
\]
\[
\chi_M = a_2 \chi_S + b_2 \chi_{Se} + (1-a_2-b_2) \chi_{Te}
\]
\[
\chi_N = a_3 \chi_S + b_3 \chi_{Se} + (1-a_3-b_3) \chi_{Te}
\]

In close analogy to the virtual crystal approximation\(^{50}\) used for first-principles modelling of random alloys, these site-specific properties are weighted averages, i.e., the coefficients \(x_1, x_2, a_1, a_2, a_3, y_1, y_2, b_1, b_2, b_3\) (each may take the value between 0 and 1) denote the fractional occupancy of each site. Collectively, these coefficients define the stoichiometry of an alloyed system via \(x = x_1 + x_2\), \(y = y_1 + y_2\), \(a = a_1 + a_2 + a_3\), and \(b = b_1 + b_2 + b_3\). Utilizing these weighted elemental properties to evaluate the descriptor in Eq. (1) and (2) immediately allows to map out the topological phase diagram for the tetradymites with any fractional stoichiometry. This is illustrated in Fig. 3 using 4,084,101 compounds as yet still only a subset of the example systems, where the coefficients \(x_1, x_2, a_1, a_2, a_3, y_1, y_2, b_1, b_2, b_3\) are all multiples of 0.2. Even in this relatively small subset of alloyed tetradymites, we already obtain 1,965,047 systems located on the right side of the dividing line, i.e., they are predicted to be new TIs!

Noteworthy enough, the obtained predictions are consistent with the few available experimental data, i.e., the topologically non-trivial compounds Bi\(_2\)Te\(_{1.6}\)S\(_{1.4}\), Bi\(_{0.5}\)Sb\(_{1.5}\)Te\(_3\), Bi\(_{1.5}\)Sb\(_{0.5}\)Te\(_3\), Bi\(_{1.5}\)Sb\(_{0.5}\)Se\(_{1.3}\)Te\(_{1.7}\) and Bi\(_{1.1}\)Sb\(_{0.9}\)STe\(_2\)^{43,49,51}. This is now no longer surprising, since these Bi- and Te-rich random alloys marked by the solid asterisks in Fig. 3 feature large masses and thus large values of \(D_1\). To validate the full topological phase diagram, we have performed explicit \(ab\)-\textit{initio} calculations for
eight additional tetradymites with fractional stoichiometry that are still reasonably tractable (layered supercells with 15 atoms). Marked as the solid circles (NIs) and squares (TIs), these representative examples cover all the different areas shown in Fig. 3, including the regions close to the NI/TI boundary. Accordingly, four tetradymites sample the TI area (As\textsubscript{0.33}Sb\textsubscript{0.67}BiSe\textsubscript{2}Te, Sb\textsubscript{2}S\textsubscript{0.33}Se\textsubscript{0.67}Te\textsubscript{2}, Sb\textsubscript{1.67}Bi\textsubscript{0.33}S\textsubscript{0.67}Te\textsubscript{1.33}Se and BiSbS\textsubscript{0.67}SeTe\textsubscript{1.33}), while four systems are located within the NI area (SbBiS\textsubscript{2}Se\textsubscript{0.67}Te\textsubscript{0.33}, SbBiS\textsubscript{2.33}Se\textsubscript{0.67}, As\textsubscript{0.33}SbBi\textsubscript{0.67}S\textsubscript{1.67}Te\textsubscript{1.33} and As\textsubscript{0.33}Sb\textsubscript{0.67}BiS\textsubscript{2}Te). Notably, the TIs (Sb\textsubscript{1.67}Bi\textsubscript{0.33}S\textsubscript{0.67}Te\textsubscript{1.33}Se and BiSbS\textsubscript{0.67}SeTe\textsubscript{1.33}) as well as the NIs (As\textsubscript{0.33}SbBi\textsubscript{0.67}S\textsubscript{1.67}Te\textsubscript{1.33} and As\textsubscript{0.33}Sb\textsubscript{0.67}BiS\textsubscript{2}Te) are located in the region with $6806 < D_1 < 7854$ so that their topological character is determined by the descriptor $D_2$. For all the eight systems with fractional stoichiometry, the first-principles calculations of the $Z_2$ invariant confirm the predictions of the 2D descriptor. As an example, Fig. 4a shows the orbital-decomposed band structure of Sb\textsubscript{2}S\textsubscript{0.33}Se\textsubscript{0.67}Te\textsubscript{2}, in which a band inversion takes place at the $\Gamma$ point between the valence (mainly occupied by the $p_z$ orbitals of the Sb atoms) and conduction bands (mainly occupied by the $p_z$ orbitals of the Te atoms). Conversely, the band structure of SbBiS\textsubscript{2.33}Se\textsubscript{0.67} shown in Fig. 4b exhibits a semiconducting behavior with normal band order. The crystal structures, band structures, and the corresponding evolution of Wannier centers for these eight tetradymites are summarized in Section 5 of the Supplementary Information. Due to the moderate system sizes, these layered compounds exhibit perforce a pronounced short- and long-range order, especially if compared with the much more disordered random alloys studied experimentally. Nonetheless, the proposed descriptor achieves excellent agreement between our predictions and first-principles calculations as well as the experimental data, which further substantiates that both $D_1$ and $D_2$ are sensible, reliable, and robust descriptors for the topological character of tetradymites with either integer or fractional stoichiometry.

**Summary and Outlook**

We have performed extensive, high-level first-principles calculations to obtain
reliable information on the topological character of 243 tetradymites, of which many are discovered as new TIs. From this data set, we obtain a simple and predictive 2D descriptor for the TI/NI classification using the data-driven SISSO approach. The descriptor only depends on the atomic number and Pauling electronegativity of the constituent elements, and captures the essential physics governing the TIs. Accordingly, it exhibits perfect classification accuracy and strong predictive power, even drastically beyond the original training data. This is explicitly demonstrated for tetradymites with fractional stoichiometry, a material class that would be prohibitively expensive to investigate even using the lowest-level first-principles approaches. With the presented descriptor, we are able to identify millions of novel TIs in this complex material class in a fast and reliable fashion. We expect that the approach established here should also be applicable to the classification of the topological characters of many other classes of materials beyond the tetradymite family. Our study therefore offers a major step forward in the exploration of topological materials space, allowing us to cover complex materials with fractional occupations that go far beyond the compounds in the existing databases. The present study also testifies the increasingly important role of such data-driven approaches in materials discovery.
Figures and Captions

Fig. 1 | Tetradymite Crystal Structure. Crystal structure of the quinary tetradymite AsSbSeTeS, where (a) is the unit cell, (b) is the primitive cell, and the atoms As, Sb, Se, Te, S occupy the sites $A$, $B$, $L$, $M$, $N$, respectively.
Fig. 2 | Topological Phase Diagram. Phase diagram for the 152 tetradymites used as the training data, plotted as function of the 2D descriptor. The NI and TI phases are marked as the cyan and green areas, which are determined by connecting the outermost black points (85 NIs) and red points (67 TIs). The two vertical dashed-lines correspond to $D_1 = 6806$ and $D_1 = 7854$. For comparison, 91 additional tetradymites not included in the training set (see text) are also included.
Fig. 3 | Topological Phase Diagram for Tetradymines with Fractional Stoichiometry. A total of 4,084,101 possible tetradymines with fractional stoichiometries (As$_x$Sb$_y$Bi$_{2-x-y}$S$_a$Se$_b$Te$_{3-a-b}$) are mapped into the phase diagram using the calculated ($D_1, D_2$) values. The solid asterisks indicate 5 experimentally reported TIs with fractional stoichiometry. The topological character of the 8 tetradymines marked by solid circles (4 NIs) and solid squares (4 TIs) are confirmed by first-principles calculations.
Fig. 4 | Band Structures of two Tetradyminites with Fractional Stoichiometry.

Electronic band structures of (a) Sb$_2$S$_{0.33}$Se$_{0.67}$Te$_2$ and (b) SbBiS$_{2.33}$Se$_{0.67}$. The Fermi level is at 0 eV. The colored circles denote the contributions from different orbitals and the sizes of the markers are proportional to the magnitude of their contribution.
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Acknowledgments The authors acknowledge fruitful discussions with Carlos Mera Acosta and Zizhen Zhou. We thank financial support from the National Natural Science Foundation of China (Grant Nos. 11574236, 11634011, 51772220, and 61434002), the National Key R&D Program of China (Grant No. 2017YFA0303500), and Anhui Initiative in Quantum Information Technologies (Grant No. AHY170000). The numerical calculations in this work have been done on the platform in the Supercomputing Center of Wuhan University.

Author contributions MS and ZYZ initiated and supervised the project. GHC performed the first-principles and SISSO calculations under the co-supervision of HJL, CC, RO, and LMG. The manuscript was written by GHC, HJL, LMG, CC, and ZYZ. All authors contributed to the interpretation of the results and finalization of the paper.

Competing interests The authors declare no competing interests.

Additional information

Supplementary information is available for this paper.

Data availability: All data required to reproduce the findings is summarized in tabular form in the Supplementary Information. Additionally, the input and output files of the first-principles calculations are available on the NOMAD Repository, see http://dx.doi.org/10.17172/NOMAD/2019.05.22-1.

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