Editors' Suggestion

Filling-enforced obstructed atomic insulators

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Topological band theory has achieved great success in the high-throughput search for topological band structures both in paramagnetic and magnetic crystal materials. However, a significant proportion of materials are topologically trivial insulators at the Fermi level. In this paper, we show that, remarkably, for a subset of the topologically trivial insulators, knowing only their electron number and the Wyckoff positions of the atoms we can separate them into two groups: the obstructed atomic insulator (OAI) and the atomic insulator (AI). The interesting group, the OAI, have a center of charge not localized on the atoms. Using the theory of topological quantum chemistry, in this work we first derive the necessary and sufficient conditions for a topologically trivial insulator to be a filling enforced obstructed atomic insulator (feOAI) in the 1651 Shubnikov space groups. Remarkably, the filling enforced criteria enable the identification of obstructed atomic bands without knowing the representations of the band structures. Hence, no *ab initio* calculations are needed for the filling enforced criteria, although they are needed to obtain the band gaps. With the help of the Topological Quantum Chemistry website, we have performed a high-throughput search for feOAIs and have found that 957 ICSD entries (638 unique materials) are paramagnetic feOAIs, among which 738 (475) materials have an indirect gap. The metallic obstructed surface states of feOAIs are also showcased by several material examples.

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I. INTRODUCTION

The development of topological quantum chemistry (TQC) [1–3] and equivalent methods of symmetry indicator [4,5] have led to high-throughput discoveries of topological quantum materials [6–10]. (See the Topological Quantum Chemistry website for examples.) In the theory of TQC [1], topologically trivial insulators are defined as band representations (BRs), which are equivalent to a set of symmetric exponentially decayed Wannier functions. Any BR can be spanned by the elementary BRs (EBRs), which are induced from irreducible representations (irreps) at maximal Wyckoff positions (WPs) [1,2,11–13]. For a given material, a set of isolated bands below the Fermi level can be characterized by an integer vector, the symmetry-data-vector, whose components are the multiplicities of irreps formed by the bands at the high symmetry momenta [11,12,14–18].

If the symmetry-data-vector can be expressed as a nonnegative integer linear combination of the symmetry-data-vectors of EBRs, the set of bands is eigenvalue-diagnosed as trivial by TQC, and we will refer to the material as a "TQC trivial insulator." Otherwise the material must be topological (with strong or fragile topology [1–4,19–37]) or enforced semimetal [1,4,11].

As schematically shown in Fig. 1, several high-throughput calculations [6–9] have identified thousands of compounds that belong to different topological categories. However, among the topologically trivial insulating materials, there are still interesting cases in which the valence bands are BRs (in terms of irreps) but not BRs induced from the occupied WPs. In other words, these insulators are not atomic insulators where electrons fill atomic orbitals at the atom sites. We refer to such materials as the obstructed atomic insulators (OAI) [1,14,16,19,38–40]. In the decomposition of the symmetry-data-vector of an OAI, there must be at least one BR induced from an empty Wyckoff position. We refer to this empty site as an obstructed Wannier charge center (OWCC). Given an OAI with the cleavage terminations cutting through an OWCC, which is off the occupied sites, there has to exist metallic

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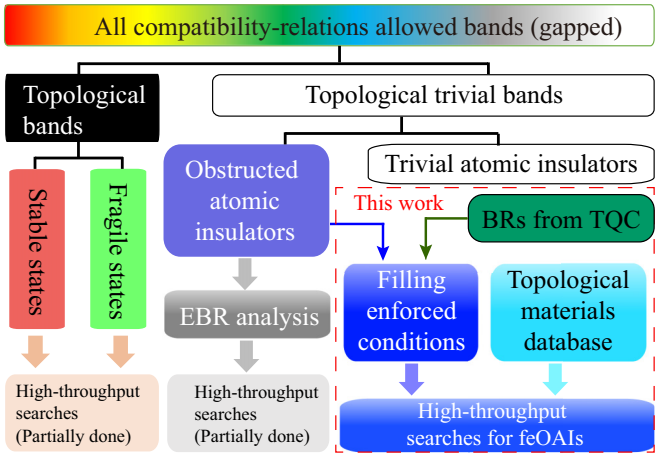

FIG. 1. Topological classification of the gapped bands satisfying compatibility relations. High-throughput searches of topological bands, including strong topological bands and fragile bands, are partially done. Topologically trivial bands can be classified into obstructed atomic limit bands and trivial atomic bands. Although a full topological classification of obstructed bands has not been achieved, we perform high-throughput search of filling enforced obstructed bands in the present work.

surface states in the gap between valence and conduction bands, which is also referred to as the filling anomaly—a mismatch between the number of electrons required to simultaneously satisfy charge neutrality and the crystal symmetry [41–43].

In general, the OAI can be detected from the identified irreps at all the high symmetry momenta through the real space invariants (RSI) introduced in 2D plane groups in Ref. [21]. It requires the extension of the RSIs to 3D. However, in some special cases, it is possible to identify the OAIs just by electron counting without *ab initio* calculations.

In some space groups (SGs) and magnetic space groups (Shubnikov space groups, in general [44]), knowing the number of valence electrons and the occupied Wyckoff positions (WPs) is sufficient for the identification of topologically trivial materials as OAIs. We denote this special type of OAI as filling enforced obstructed atomic insulator (feOAI). This special case of OAI does not depend on the specific order of the eigenstates (irreps) in the band structure, but only on the number of electrons. Therefore, independently of the specific band structure and of the order in energy of the eigenstates (irreps) at every maximal k vector, when the material is an insulator, it must be topological (stable or fragile) or it must be an OAI. In principle, in a material whose band structure corresponds to an OAI (but it is not an feOAI), it is possible to induce a phase transition through band inversion so that the resulting band structure corresponds to an atomic insulator. This is not possible when the material is a feOAI. The present work is focused in the search of this special subset of materials. Note also that the blind application of the tables of RSIs cannot differentiate feOAIs from general OAIs, unless the RSI algorithm includes also the electron counting. Figure 2(a) shows a simple example of a feOAI. It represents a Su-Schrieffer-Heeger (SSH) chain model [45] in the space group $P\bar{1}$ with $2i$ sites occupied by atoms. A necessary condition for this atomic

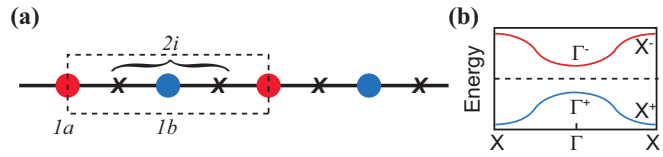

FIG. 2. FeOAI in 1-d. (a) A 1-d atomic chain with a Wyckoff position $2i$ occupied by atoms. (b) Schematic diagram of the band structure of the 1-d model in (a). The blue and red bands are valence and conduction bands, respectively.

chain to be a band insulator is that the number of electrons N_e in a unit cell is even, i.e., $N_e = 2n(n = 1, 2, 3, ...)$. As the dimension of the BR induced from single orbitals at $2i$ is four, when the number of electrons is an odd multiple of two, i.e. $N_e = 4n + 2(n = 0, 1, 2, ...)$, the decomposition of the BR into EBRs needs at least one EBR induced from an empty WP, $1a$ or $1b$, because these EBRs have dimension two. Thus, the filling enforced condition $N_e = 4n + 2(n = 0, 1, 2, ...)$ plus the x-ray diffraction (XRD) information that the atoms are placed at the $2i$ Wyckoff position alone can identify whether an insulator is feOAI or not without any information of the wavefunction at the high symmetry points. To obtain the OWCC of feOAI (in our example, to elucidate whether the needed EBR or EBRs out of WP $2i$ are those of $2a$ or $2b$), one needs to analyze the specific BR. As schematically shown in Fig. 2(b), when the irreps of the valence band are $\{\Gamma^+X^+\}$, which are induced from $A_g@1a$, the OWCC is sitting at $1a$.

In this paper we first derive in Sec. II the filling enforced conditions of topologically trivial bands to be obstructed for all the 1651 Shubnikov space groups (SSGs). In Sec. III, using the obtained filling enforced conditions, we perform the first high-throughput search for feOAIs from the Topological Quantum Chemistry website and analyze the surface states for several material examples.

II. FILLING ENFORCED CONDITIONS

In this section we will obtain the filling enforced conditions of OAIs in all 1651 SSGs, which contain as a particular case the SGs of nonmagnetic structures, both with and without spin-orbit coupling (SOC).

Let's consider a nonmagnetic insulator that has been identified as trivial using the TQC method [1] or a magnetic trivial insulator identified by the extension of TQC to magnetic groups [2] (it has been labeled as LCEBR in [6] or [9], respectively) in a single (double) SG with a set of WPs $\{\alpha\}$ with multiplicities $\{n_\alpha\}$. We consider here the multiplicities in a primitive unit cell (not the conventional cell used in the International Tables of Crystallography [46]). We denote the allowed corepresentations of the site-symmetry group of the WP $\{\alpha\}$ as $\{\rho_\alpha^i\}$, whose dimensions are $\{d(\rho_\alpha^i)\}$, with $i = 1 \ldots N_{\text{rep},\alpha}$, where $N_{\text{rep},\alpha}$ is the total number of corepresentations of the site-symmetry group G_α. In paramagnetic compounds, for which time-reversal symmetry is always a symmetry operation of the SG, if SOC is considered (spinful cases), the Kramers theorem implies that the dimension $\{d(\rho_\alpha^i)\}$ is always an even number. In paramagnetic spinless

(without SOC) systems the dimensions of the irreps can be odd, but two times of the dimension electrons are needed to fill each irrep due to the twofold spin degeneracy. Finally, in magnetic groups, where the time-reversal and spin $SU(2)$ symmetries are absent, there is no restriction on electron number parity as in the paramagnetic groups. All the band corepresentations $\{\rho_\alpha^i\}$ (and the corresponding dimensions $\{d(\rho_\alpha^i)\}$) induced from any WP in the 1651 double SSGs are accessible on the Bilbao Crystallographic Server through the MBANDREP program [2]. The complete set of elementary band corepresentations are also listed in this program. The subset of corepresentations of magnetic type I and type II (the last ones are the relevant groups for paramagnetic phases) and the elementary band corepresentations are also implemented in the BANDREP program [11].

Now we assume that there are M occupied WPs $\alpha_1 \ldots \alpha_M$. Some of these WPs can share the same label because they can belong to (sometimes maximal) WPs whose coordinates depend on continuous parameters, and the values of these parameters are different. If an atom sits at a given WP α_j and contributes N_j electrons (typically these are the electrons in the outer shell of the atom), the whole WP α_j contributes $n_{\alpha_j} N_j$ electrons to the total number of electrons in a primitive unit cell, with n_{α_j} being the multiplicity (in each primitive unit cell) of the Wyckoff position α_j. Then, the total number of spinless (spinful) electrons per primitive cell in the system can be expressed as

$$N_e = \sum_{j=1}^{M} n_{\alpha_j} N_j. \tag{1}$$

A necessary (but not sufficient) condition for a material to be an eigenvalue indicated topologically trivial insulator is that there exists a solution to the equation:

$$N_e = \sum_{j=1}^{\text{All WPs}} \sum_{i=1}^{N_{\text{rep},\alpha_j}} n_{\alpha_j} d\left(\rho_{\alpha_j}^i\right) N_{i,j}, \tag{2}$$

where j sums over all the WPs of the corresponding SSG, and $N_{i,j}$ are nonnegative integers that represent how many "orbitals" (representations $\rho_{\alpha_j}^i$) at WP α_j are occupied. Due to the spin degeneracy when SOC is neglected, each orbital $\rho_{\alpha_j}^i$ can be occupied by two electrons. In this case, we should multiply the right side of Eq. (2) by two. However, in order to use a single expression for the spinful and spinless cases, in Eq. (2) and in the rest of this paper, N_e will be equal to the number of electrons when the SOC is considered, and to one half the number of electrons in the absence of SOC. With this convention Eq. (2) is valid in both cases.

For each (double) SSG, the dimensions of the BRs induced from the coirreps ρ_α^i of the site symmetry group of each WP α can be expressed as

$$d\left(\rho_\alpha^i \uparrow \mathcal{G}\right) = n_\alpha d\left(\rho_\alpha^i\right). \tag{3}$$

Then Eq. (2) can be rewritten as

$$N_e = \sum_{j=1}^{\text{All WPs}} \sum_{i=1}^{N_{\text{rep},\alpha_j}} d\left(\rho_{\alpha_j}^i \uparrow \mathcal{G}\right) N_{i,j}, N_{i,j} \geqslant 0, \in \mathbf{Z}. \tag{4}$$

For symmetry eigenvalue indicated trivial insulators, the solution for Eq. (4) is in general not unique. The set of EBRs in a SSG form an overcomplete basis of the BRs in a group and, moreover, in our analysis we must consider all the WPs of the SSG, maximal and nonmaximal. It is well known [47,48] that the band corepresentations induced from nonmaximal WPs are linear combinations of EBRs (induced from maximal WPs); therefore different sets of $N_{i,j}$ coefficients can in principle satisfy Eq. (4).

However, if the first summation in Eq. (4) is restricted only to the M atomic-occupied WPs and not to the whole set of WPs of the SSG, the resulting equation,

$$N_e = \sum_{j=1}^{M} \sum_{i=1}^{N_{\text{rep},\alpha_j}} d\left(\rho_{\alpha_j}^i \uparrow \mathcal{G}\right) N_{i,j}, \quad N_{i,j} \geqslant 0, \in \mathbf{Z}, \tag{5}$$

may have fewer solutions or no solution. An absence of a solution to Eq. (5) is a sufficient condition for OAI.

To summarize, a material identified as a trivial insulator by TQC always satisfies Eq. (4), but if Eq. (5) is not satisfied, mathematically

$$\nexists N_{i,j} \geqslant 0, \in \mathbf{N}, s.t. N_e = \sum_{j=1}^{M} \sum_{i=1}^{N_{\text{rep},\alpha_j}} d\left(\rho_{\alpha_j}^i \uparrow \mathcal{G}\right) N_{i,j}, \tag{6}$$

then the material is a feOAI. Although it may be possible to define a set of localized Wannier functions, at least one of them must be centered at an unoccupied WP. For example, in the case of the 1-d SSH chain in Fig. 2, when $N_e = 4n + 2$ and the atoms sit at the WP $2i$, the equation $N_e = d(\rho_{2i} \uparrow \mathcal{G}) \times N$ has no integer solution, where $d(\rho_{2i} \uparrow \mathcal{G}) = 4$ is the dimension of the BR induced from $2i$.

We stress that the simple prescription given by Eq. (6) does not rely on TQC or its derivative procedures: the only information required is the space group, the multiplicity of the occupied Wyckoff positions, the dimensions of the irreps of the site-symmetry groups of these Wyckoff positions, and the total number of electrons in a primitive unit cell.

In the Supplemental Material [59] we have tabulated the dimensions of all the BRs for all 230 space groups (SGs) and double space groups (DSGs), respectively. In the Appendices H1-H1, we have tabulated the dimensions of all the BRs for all the single and double magnetic groups (Shubnikov groups of types I, II, and IV). Once the occupied WPs in a material and the number of electrons in the primitive unit cell are known, these tables together with Eqs. (4) and (6) can be used to check whether a material that has been identified by TQC as a topologically trivial insulator is a feOAI. In Sec. H7-H14 of the Supplemental Material [59], we have tabulated the feOAI conditions for all the 230 space groups. The conditions are exactly the same for single (without SOC) and double (with SOC) space groups. In Secs. H7-H14 of the Supplemental Material [59] we have also tabulated the feOAI conditions for all 1651 SSGs. Unlike for nonmagnetic systems, the conditions are different for single and double SSGs (more discussion about this is detailed in Supplemental Material [59]).

We will apply the above analysis to a simple example. In the DSG *Pbca* (No. 61) the multiplicities of the Wyckoff positions a, b, and c are 4, 4, and 8, respectively,

and the allowed dimensions of the BRs induced from the irreps (with SOC) at a, b, and c are 8, 8, and 16, respectively (see Supplemental Material [59]). If the material has been identified as trivial insulator using TQC and the a and/or b WPs are occupied, the number of valence electrons has to be a multiple of eight, and the Wannier centers can be located at the occupied Wyckoff position(s). However, if only WP c is occupied by atoms and the number of electrons is $N_e = 8 + 16\mathbb{N}$ (with $\mathbb{N}$ being integers), the Wannier functions cannot be all located at the occupied WPs because otherwise the total electron number would be a multiple of 16. We emphasize that the filling $N_e = 8 + 16\mathbb{N}$ can be realized if, for example, a single c position is occupied by atoms and each atom at c contributes an odd number of electrons. At least one of the orbitals must be centered at a or b. The condition given by Eq. (5) cannot be fulfilled by any set of nonnegative integers $N_{i,j}$ and the material is thus a feOAI.

Equations (4) and (6) give the necessary and sufficient conditions for a material to be a feOAI once the TQC method has identified it as a topologically trivial insulator. Alternatively, there exists a simpler (but not general) equation to have a feOAI material that is easier to use than Eq. (6) (see Supplemental Material [59] for more details).

In general, Eq. (6) is analytically unsolvable and is related to the Frobenius coin problem [49]. However, for our particular case, since the number of distinct dimensions of BRs in all the SSG is small, the Frobenius coin problem is solvable by exhaustion. We have determined all the solutions to Eqs. (4) and (6) in the 1651 SSGs with and without SOC. In Supplemental Material [59] we list the feOAI conditions for the 230 SGs (type-II SSGs) relevant in the analysis of nonmagnetic structures. The table gives the conditions for spinful and spinless irreps, which are exactly the same once we consider that in the spinless case N_e represents half the number of electrons. In Supplemental Material [59] we have included the feOAI conditions for the magnetic space groups (Shubnikov groups of type I, III, and IV) with and without SOC. For magnetic groups, the solutions to Eqs. (4) and (6) with and without SOC are different, in general, and they are given in separate tables. Note that in the absence of SOC, the spinless feOAI conditions are only applied to the antiferromagnetic systems which are independent of the spin but not the ferromagnetic ones.

III. HIGH-THROUGHPUT SCREENING AND SURFACE STATES OF FEOAIS

By application of the filling enforced conditions obtained in Sec. III to all the paramagnetic trivial insulators in the Topological Quantum Chemistry website , we have performed the first high-throughput search of paramagnetic feOAIs. Among the 34 013 ICSD entries (18 133 unique materials, i.e., ICSDs sharing the same stoichiometric formula, space group, and topological property at the Fermi energy) that are identified as trivial insulators in the database, we have found 957 ICSD entries (638 unique materials) that satisfy the filling enforced conditions and hence they are feOAIs. This represents about 3% of the total number of topologically trivial insulators. Among the 957 ICSD entries (638 unique materials) identified as feOAIs, 738 (475) materials have a finite indirect band gap in the whole BZ. The full list of materials, with detailed electronic properties, and the numbers of feOAIs for each DSG are tabulated in Supplemental Material [59].

Using the filling enforced conditions of MSGs, we have also found one magnetic feOAIs candidate from the 403 magnetic materials on the Topological Magnetic Materials website. We find that the topologically trivial phase of Er_2Ni_2In with BCSID 1.195 satisfies the filling enforced condition of the type IV MSG C_amcm (No. 63.467). Hence, it is a magnetic feOAI. See Supplemental Material [59] for more details of Er_2Ni_2In.

The occupied states of symmetry-protected topological insulators are delocalized, and these systems present gapless states on lower dimensional edges or surfaces. In contrast, the occupied states of OAIs are localized. However, as all the OWCCs are localized away from the atom sites, there will be a gapless surface/edge when the cleavage cuts through the OWCCs. In Supplemental Material [59], we have also calculated the obstructed surface states of four additional feOAIs, including GaSe, GaS, IrP_2, CuP_2, and CdSb. We also provide in Supplemental Material [59] an illustrated discussion about the stability of feOAI surface states.

IV. CONCLUSIONS

In this work we have derived, for all 1651 SSGs, the filling enforced conditions that guarantee that a material identified as a topologically trivial band insulator is in the obstructed atomic insulating phase. These conditions provide an efficient *ab initio* free way to search for paramagnetic and magnetic materials in the obstructed atomic phase. Through the application of the filling enforced conditions to the nonmagnetic structures labeled as trivial insulators in the Topological Quantum Chemistry website, we remarkably find 957 ICSD entries (638 unique materials) as feOAIs, among which 750 (475) compounds have an indirect band gap. Combined with the BR analysis and first principles calculations, we have also showcased the filling anomaly metallic surface states for specific surfaces of several feOAIs. The special metallic surface states in feOAIs provide an ideal platform for the study of two-dimensional electron gases that could be detected in ARPES or STM experiments.

Note added. While this paper was under review, we completed the catalog of OAIs using real-space invariants [55] and proposed the application of OAIs on catalysis [56]. Our results in Ref. [55] are consistent with this paper. We were also aware of works about the applications of feOAIs (e.g., the feOAI material Nb_3Br_8 as predicted in this paper) on Josephson junction devices [57] and on the design of topological superconductors [58].

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[59] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevB.109.165139 for dimensions of band representations, filling-enforced conditions, the list of filling-enforced obstructed atomic insulator materials, and surface state calculations for five material examples, which includes Refs. [50–54].