

Fractional corner charges in threefold-symmetric two-dimensional materials with fragile topology

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(Received 11 March 2024; accepted 7 May 2025; published 20 June 2025)

We perform a systematic study of the signatures of fragile topology in over 50 nonmagnetic two-dimensional materials with formula AB_2 , belonging to space group $P\bar{3}m1$. Using group theory analysis in the framework of topological quantum chemistry, we find fragile bands near the Fermi level for all the materials studied. Since stable topological bands are also present in these systems, the interplay of both phases is discussed, showing that corner charges appear in over 80% of the materials and are linked to fragile topology. Using first-principles calculations, we predict fractionally charged corner charges protected by C_3 symmetry. Our work aims to broaden the scope of materials with experimentally accessible fragile bands.

DOI: [10.1103/qcr8-jxvn](https://doi.org/10.1103/qcr8-jxvn)

I. INTRODUCTION

Since the proposal and subsequent discovery of the first topological insulators [1,2], topology has enriched the electronic properties of a great number of materials. Different types of Dirac and Weyl fermions have been discovered in analogy to high-energy physics [3–5]. The development of symmetry indicators and topological quantum chemistry (TQC) [6–13] has further extended and standardized the variety of topological phases of matter. Higher-order topological insulators (HOTIs) and fragile topology are the latest additions; the former was first established in topological insulators characterized by a mirror Chern number [14,15], while the latter has been theoretically proposed in twisted bilayer graphene [16–20]. Both phases share the absence of topological gapless modes on their surfaces or edges, in contrast to standard topological insulators. Whereas d -dimensional n -th-order topological insulators are known to host topological states in $d - n$ dimensions, the same does not always apply to fragile topology. Interestingly, while nearly 90% of all classified bulk materials have at least one topological band [13,21], only about 8% show fragile states. Thus, the search for new materials that could provide more information on signals of fragile topology is highly desirable.

Fragile topology is based on the fact that a set of fragile bands can be trivialized by adding a suitable set of trivial bands [16,17]. The starting point for every analysis of symmetry-indicated topology is to characterize the form in

which the electronic bands transform at high symmetry points in reciprocal space, under the action of the space group of the system. This allows us to classify each band using the eigenvalues of the symmetry operations of the material, which corresponds to the characters (traces) of the irreducible representations (irreps). Due to real space periodicity, a set of orbitals located at specific Wyckoff positions (WP) will induce a well-defined set of irreps in the momentum space description of the bands. The key point is that in the atomic limit, that is, no interaction among the orbitals is considered, the orbitals will induce what is called an elementary band representation (EBR). These EBRs are the building blocks that allow discriminating the type of band topology in a material [9,10,12]. Thus, a band is said to be topologically trivial if it can be expressed as a linear combination of EBRs where all coefficients are positive integers [10,12]. Unlike trivial bands, fragile bands can be expressed as a combination of EBRs with integer coefficients, but at least one of them must be negative [10]. This way, when more bands are added to a fragile one, the negative EBRs can cancel out, giving rise to an all-positive linear combination of EBRs and thus trivializing the band set [8,9,12,13,16,18,21]. Hence, even if the fragile state is near the Fermi energy, the lower energy bands can trivialize it. This trivialization can explain the scarcity of topological materials with fragile topology features. For its part, a band has a stable topology (stable upon band addition) if it can be written in terms of EBRs and at least one coefficient is fractional [8–10,12,13,21].

From the above discussion, fragile topology cannot be captured by stable topological invariants such as the $\mathbb{Z}_2$ index used in spin Hall systems. Thereby, TQC stands as one of the most useful tools to diagnose this kind of topology, together with the most general study of the evolution of Wannier charge centers along appropriate directions in reciprocal space [18,22–27]. Beyond TQC, stable topological phases were al-

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ready established in relation to the tenfold classification of systems attending to their (noncrystalline) symmetries [28] and within K-theory [29]. Note that, in a similar way, fragile phases can also arise without crystalline protection and even beyond symmetry indicators [27], as is also the case for other recently-discovered topological phases [30]. However, crystalline symmetries will play an important role in this work. In addition, although a bulk-boundary correspondence can be established for fragility using twisted boundary conditions [26], this is difficult to implement in electronic systems, so a case-by-case analysis is still justified. In order to have a complete picture of fragile topological materials, a study of fragile bands for all space groups in bulk materials within the framework of TQC has been performed in Ref. [31], and high-throughput calculations have very recently classified two-dimensional materials attending to TQC and including fragile topology [32].

Fragile topology has also been theoretically reported in photonic crystals and phonon spectra [33–36]. One of its potential signatures is the presence of zero-dimensional corner states with corner charges, theoretically predicted in Refs. [20,37,38]. These corner charges have been theoretically reported in recent works studying different mono- and few-layered materials with diverse rotational symmetries [30,39–49]. Moreover, higher-order Fermi arcs have also been linked to fragile and higher-order topology [50]. From an experimental point of view, fragile topology has been described in metamaterials [51–55] and quantum simulators [56], and Fermi arcs have been reported in some transition-metal dichalcogenides [57–59]. Because corner charges are a shared feature between fragile and higher-order topology, corner state measurements in real materials are often linked to the latter [60]. The potential applications of corner states as quantum dots have also been very recently highlighted, coining the concept of cornertronics [61].

It is therefore interesting to study the relation between higher-order and fragile topology. In this direction, we construct a list of two-dimensional monolayers described by space group (SG) $P\bar{3}m1$ (164). Since transition-metal dichalcogenides (TMDs) have received a great deal of attention as candidates for layered materials with higher order [30,41,45,47,48,62] and fragile topology [30,50], we have focused on various TMDs, as well as on a number of non-TMDs with the same space group. We explore a total of 52 materials belonging to this SG to find a set of experimentally suitable candidates. We demonstrate that fragile topological bands are present in all 52 materials in the region of energies near the Fermi level, and that these bands are related to the nonzero corner charges present in most of the materials and in C_3 -symmetric flakes.

This article is organized as follows: In Sec. II, the general properties of SG 164 and the materials therein are discussed. In Sec. III, we compute a set of topological invariants based on the symmetry eigenvalues of the system, particularized to the TMD case studies ZrSe_2 , ZrS_2 , and SnS_2 . In Sec. IV, we theoretically predict the corner charges linked to these materials and present the concept of partial corner charge. Our results are consistent with first-principles corner states calculations for triangular and hexagonal flakes in Sec. V.

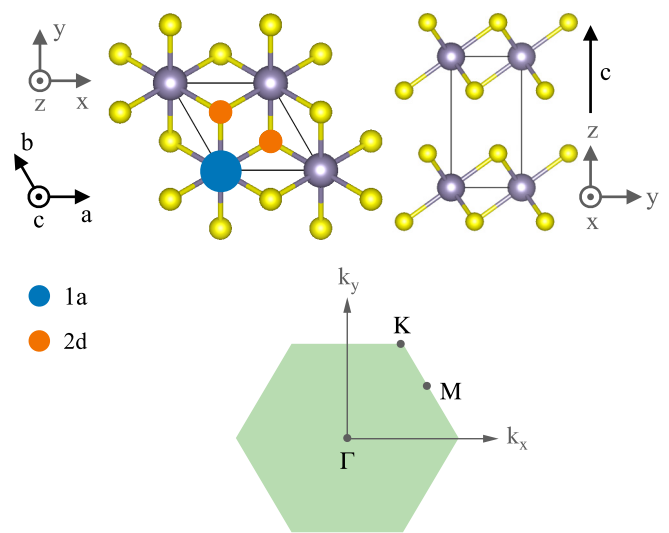


FIG. 1. Crystal structure of a unit cell belonging to SG 164: top view (upper left panel), and side view (upper right panel) displaying two layers. The structure lattice vectors, as well as the Cartesian axes, are indicated in black and gray, respectively. Blue and orange highlighted atoms indicate the 1a and 2d WPs, respectively. Bottom panel: Brillouin zone of the monolayer.

II. COMPUTATIONAL METHODS AND GENERAL BACKGROUND OF SPACE GROUP 164 MATERIALS

Electronic structure calculations for all materials were performed using the Quantum ESPRESSO first-principles code [63,64] employing the generalized gradient approximation (GGA) and Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional. Spin-orbit coupling was considered throughout the self-consistent calculations in all cases. A kinetic energy wavefunction cutoff of 100 Ry and a $8 \times 8 \times 1$ Monkhorst-Pack reciprocal space grid were used. All structures were relaxed until the forces were less than 0.001 eV/Å. The initial crystal structures were obtained from the Computational 2D Materials Database (C2DB) [65,66] and checked against the Topological Materials Database [9,13,67] for further relaxation. Subsequently, a group theory analysis was performed using the IrRep code [68]. For the flake calculations, the SIESTA code [69,70] was used, including spin-orbit coupling and considering the same GGA-PBE approximation.

SG 164 has inversion symmetry and includes rotational symmetries C_{3z} and C_{2x} , with a total of 12 symmetry operations. As shown in Fig. 1, we focus on AB_2 compounds that display a layered structure. The A atom, which is usually (but not necessarily) a transition metal, belongs to the high-symmetry real space WP 1a, whereas the B atom is described by the 2d WP. The spatial location of these positions within the unit cell is highlighted in blue and orange, respectively, in Fig. 1. For the WPs, as well as for the symmetry operations and the SG, we follow the notation of the Bilbao Crystallographic Server [71–73].

We screen the C2DB by restricting the search to dynamically stable monolayers with the SG 164 and AB_2 formulas that possess a PBE band gap greater than 0.1 eV and a nonmagnetic ground state. Additionally, we also mention examples of semimetallic systems that allow for a formal

definition of a set of valence bands separated from the upper conduction bands by a nonabsolute gap. A complete list of materials identified in this work is presented in Table III.

In the following sections, we will focus on three illustrative materials of this collection that have already been synthesized in monolayer form [74–76], namely, semiconductors ZrSe₂, ZrS₂, and SnS₂. The semimetals ZrTe₂ and NiTe₂ are also briefly commented on. In addition to the aforementioned compounds, other materials encompassed in this work such as PtSe₂, SnI₂, PbI₂, PdS₂, PtS₂, and PtTe₂ are also experimentally available as monolayers [77–81]. Note that the fragile topology database described in Ref. [31] may not apply here, since for monolayers the combination of EBRs is now restricted to the two-dimensional high-symmetry points of the Brillouin zone (BZ).

III. BAND TOPOLOGY OF $P\bar{3}m1$ MONOLAYERS

A. Topological quantum chemistry analysis

We perform a TQC analysis of all individual valence bands, as well as of the full valence band manifold. The basic ingredient to start the topological description is to consider that time-reversal symmetry and spatial inversion are both preserved for all cases. This immediately implies that all bands will be twofold degenerate along the entire BZ. In addition, since spin-orbit is not negligible, double-space group irreducible representations should be employed to characterize the bands at high symmetry points. In double SG 164, the highest degeneracy that a set of bands can have is two [82], so all doubly degenerate bands will always be isolated from each other. This allows for the topological classification not only of the valence band manifold as a whole, but also for the characterization of each twofold set of bands. This basic set of bands is described by the labels of the irreps at high symmetry points Γ , M , and K , which comprises what is known as a band representation [9].

Following the notation in the Bilbao Crystallographic Server, we list in Table I all possible 16 band representations that are allowed by the compatibility relations of the group. These sixteen band representations are classified as fragile, stable topological with $\mathbb{Z}_2 = 1$, and trivial. If a set of bands corresponds to a combination of EBRs with integer coefficients and at least one of them is negative, the set is fragile [10]; if at least one is fractional, the set has stable topology. Otherwise, if all coefficients are positive integers, the set is generally said to be in an atomic limit and trivial [12]. To identify these phases, we follow the Smith decomposition procedure [10] as detailed in the Supplemental Material (SM) [83], and define a strong topological invariant indicated by symmetry eigenvalues $\mathbb{Z}_2$ as

$$\mathbb{Z}_2 = c_6 \bmod 2, \quad (1)$$

where c_6 is the 6th element of the c -vector, obtained from the multiplicities of the irreps of each band set, and whose computation is detailed in the SM.

We have checked that fragile and $\mathbb{Z}_2 = 1$ bands are present near the Fermi level in all reported materials. For instance, fragile band F4 can be decomposed into EBRs as shown in

TABLE I. Basic band representations in the SG 164 monolayer, including trivial (labeled EBR), stable topological with $\mathbb{Z}_2 = 1$ (labeled S), and fragile (labeled F and numbered). Corner charges with and without inversion symmetry are gathered in the last two columns and described in Sec. IV.

	Γ	M	K	$Q_{c, \text{no inv}}$	$Q_{c, \text{inv}}$
EBR	$\bar{\Gamma}_4 \bar{\Gamma}_5$	$\bar{M}_3 \bar{M}_4$	$\bar{K}_4 \bar{K}_5$	0	0
F1	$\bar{\Gamma}_4 \bar{\Gamma}_5$	$\bar{M}_3 \bar{M}_4$	$\bar{K}_6$	4/3	2/3
S	$\bar{\Gamma}_4 \bar{\Gamma}_5$	$\bar{M}_5 \bar{M}_6$	$\bar{K}_4 \bar{K}_5$	0	3/2
S	$\bar{\Gamma}_4 \bar{\Gamma}_5$	$\bar{M}_5 \bar{M}_6$	$\bar{K}_6$	4/3	1/6
S	$\bar{\Gamma}_6 \bar{\Gamma}_7$	$\bar{M}_3 \bar{M}_4$	$\bar{K}_4 \bar{K}_5$	0	1/2
S	$\bar{\Gamma}_6 \bar{\Gamma}_7$	$\bar{M}_3 \bar{M}_4$	$\bar{K}_6$	4/3	7/6
EBR	$\bar{\Gamma}_6 \bar{\Gamma}_7$	$\bar{M}_5 \bar{M}_6$	$\bar{K}_4 \bar{K}_5$	0	0
F2	$\bar{\Gamma}_6 \bar{\Gamma}_7$	$\bar{M}_5 \bar{M}_6$	$\bar{K}_6$	4/3	2/3
F3	$\bar{\Gamma}_8$	$\bar{M}_3 \bar{M}_4$	$\bar{K}_4 \bar{K}_5$	2/3	4/3
EBR	$\bar{\Gamma}_8$	$\bar{M}_3 \bar{M}_4$	$\bar{K}_6$	0	0
S	$\bar{\Gamma}_8$	$\bar{M}_5 \bar{M}_6$	$\bar{K}_4 \bar{K}_5$	2/3	5/6
S	$\bar{\Gamma}_8$	$\bar{M}_5 \bar{M}_6$	$\bar{K}_6$	0	3/2
S	$\bar{\Gamma}_9$	$\bar{M}_3 \bar{M}_4$	$\bar{K}_4 \bar{K}_5$	2/3	11/6
S	$\bar{\Gamma}_9$	$\bar{M}_3 \bar{M}_4$	$\bar{K}_6$	0	1/2
F4	$\bar{\Gamma}_9$	$\bar{M}_5 \bar{M}_6$	$\bar{K}_4 \bar{K}_5$	2/3	4/3
EBR	$\bar{\Gamma}_9$	$\bar{M}_5 \bar{M}_6$	$\bar{K}_6$	0	0

Eq. (2) below:

$$F4 = -\bar{E}_{1g} @ 1a + \bar{E}_1 @ 2d. \quad (2)$$

The negative coefficients confirm the fragile nature of the band and are also present in the rest of the fragile bands in Table I. In all cases, fragile bands are described in terms of EBRs coming from WPs 1a and 2d, which are the occupied sites in the unit cell. The EBR decomposition of all fragile bands F1 – F4, as well as of an exemplary strong topological band with $\mathbb{Z}_2 = 1$, are explicitly stated in the SM. Note that these representations are not unique, as the general formulation for the symmetry data vector has several free parameters. These parameters are usually set to zero [10]; however, we have checked that other parameter choices do not change the resulting topological nature of each symmetry data vector. A potential interplay between strong, $\mathbb{Z}_2 = 1$ -indicated topological phases and fragile phases and their effect on corner states would be of great interest.

Application to case studies

In light of our preceding general results, we now classify the electronic bands in the representative case studies ZrSe₂, ZrS₂ and SnS₂. Figure 2(a) shows the band structure of monolayer ZrSe₂ near the Fermi level, where a variety of topological bands, both stable and fragile, appear. All types of identified fragile bands, F1, F2, F3, and F4, shown in dashed lines and different colors, are present in the valence set near the neutrality point. Stable $\mathbb{Z}_2 = 1$ bands, highlighted in dark blue, also appear in the valence region and have been broadly labeled S for simplicity. If we extend the TQC analysis to the entire valence band set, we find that ZrSe₂ is topologically trivial, as the total set of irreps is expressed as a sum of different EBRs; the EBR decomposition of the full valence set

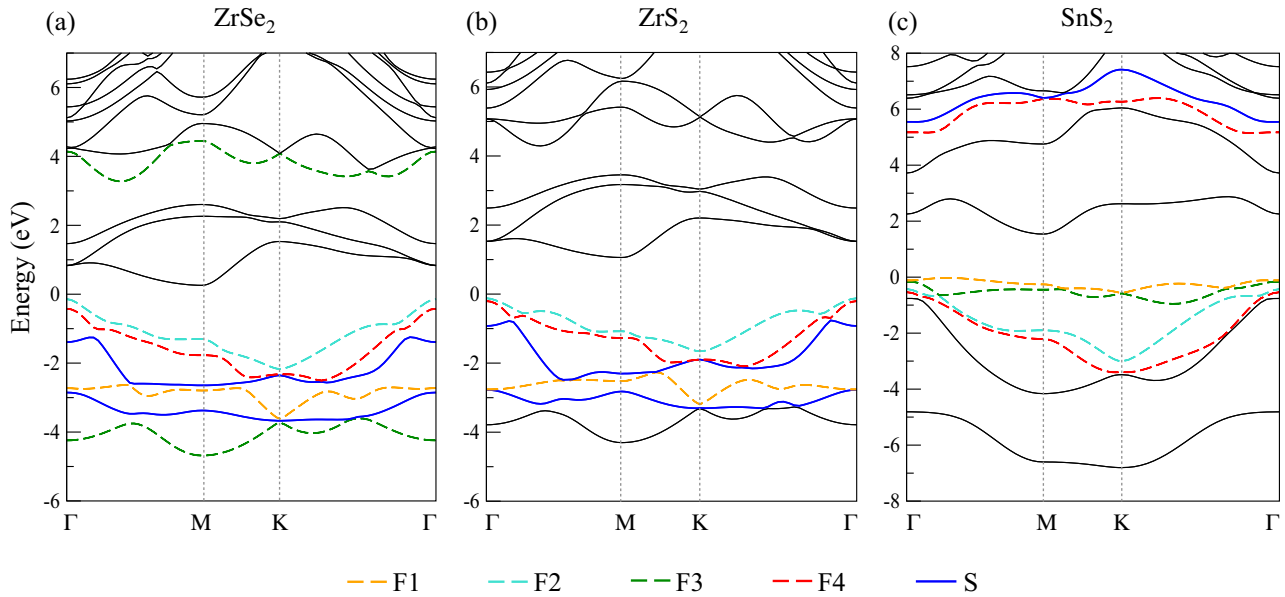


FIG. 2. Band structure of monolayer (a) ZrSe_2 , (b) ZrS_2 , and (c) SnS_2 . Fragile bands are represented in colored dashed lines, and $\mathbb{Z}_2 = 1$ bands are highlighted in dark blue.

is detailed in the SI. This is consistent with the intuitive notion of fragile bands: they are trivialized when combined with others. However, the $\mathbb{Z}_2 = 1$ bands remain topological upon addition; the only exception is the addition of an even number of $\mathbb{Z}_2 = 1$ bands, since the $\mathbb{Z}_2$ index is defined modulo 2. We emphasize that there are more topologically stable and fragile bands at lower energies, which we do not show in the figure, but have been taken into consideration in order to compute the topological properties of the valence band set.

ZrSe_2 and ZrS_2 are semiconductors and share almost the same topological band distribution for the uppermost valence bands, as seen in Figs. 2(a) and 2(b). In both cases, the first, second, and fourth valence bands are fragile, and the third and fifth valence bands are stable topologically with $\mathbb{Z}_2 = 1$. In fact, the band structure has an overall similar appearance for both materials, as expected since they belong to a similar chemical environment. However, in ZrS_2 there are no topological bands in the conduction set near the Fermi level. As in ZrSe_2 , all valence bands add up to a trivial topological invariant.

Figure 2(c) displays an analogous band structure for the semiconductor SnS_2 . As in ZrSe_2 , all fragile bands F1, F2, F3, and F4 found in Table I are present in the figure. Interestingly, this figure does not include any $\mathbb{Z}_2 = 1$ bands; however, we have found such bands at lower energies. As in the previous cases, the whole valence manifold is topologically trivial, as explicitly detailed in the SM.

For the rest of the monolayers studied, the results are similar. Additional figures highlighting fragile and stable bands for ZrTe_2 and NiTe_2 are found in the SM. They both have a higher density of stable bands but show fragile states near the Fermi level. Since ZrTe_2 and NiTe_2 are semimetals, we have set the uppermost valence band to match previous works [9,13,67]. ZrTe_2 is the only material studied with a topologically nontrivial valence band set, with $\mathbb{Z}_2 = 1$, in agreement with experimental reports of Dirac-like edge states

[84]. In fact, all of the materials mentioned above (ZrSe_2 , ZrS_2 , SnS_2 , ZrTe_2 , and NiTe_2) are experimentally feasible in monolayer form.

B. Symmetry-indicator invariants beyond topological quantum chemistry

The former TQC analysis yields a broad range of materials with fragile and stable topological bands; however, we find that fragile bands become trivialized at the Fermi level. Moreover, even though a $\mathbb{Z}_2$ invariant is computed for stable topological bands, an invariant for fragile bands would also be useful to fully characterize the topological features of our system. A set of symmetry-indicator topological invariants, applicable to systems protected by crystalline (mainly rotational) symmetries, has been introduced in Refs. [38,39]. These invariants are computed in terms of certain symmetry eigenvalues of the system at selected high-symmetry points, and therefore characterize diverse topological phases, such as second-order HOTIs, fragile topology, or obstructed atomic limits [39].

In order to compute the corresponding symmetry-indicator invariants for our materials, we notice that all the studied monolayers belong to layer group $p\bar{3}m1$. Following Ref. [39], we focus on C_3 and inversion symmetries, present in layer group $p\bar{3}m1$, in order to define a topological invariant for such a system in the presence of spin-orbit coupling:

$$\nu_{\text{inv}} = (M_{-1}^I, K_{-1}^3), \quad (3)$$

where M_{-1}^I is the difference between the number of states at M and Γ points with the inversion eigenvalue -1 . Analogously, K_{-1}^3 is the difference between the number of states at K and Γ points with C_3 eigenvalue -1 . We will use ν_{inv} to characterize finite geometries that retain the monolayer point group ($\bar{3}m$), and also explore the case of a system in which inversion symmetry is absent, leaving $3m$ as the point group of the structure.

TABLE II. Symmetry indicator invariants related to fractional corner charges in the SG 164 monolayer unit cell with (top part) and without (bottom part) inversion symmetry.

AB ₂	#M ₋₁ ^I	#Γ ₋₁ ^I	#K ₋₁ ³	#Γ ₋₁ ³	ν _{inv}
ZrSe ₂	24	24	14	14	(0, 0)
ZrS ₂	14	14	8	6	(0, 2)
SnS ₂	8	8	10	8	(0, 2)
AB ₂	#K _{e^{iπ/3}} ³	#Γ _{e^{iπ/3}} ³	#K ₋₁ ³	#Γ ₋₁ ³	ν _{no inv}
ZrSe ₂	15	15	14	14	(0, 0)
ZrS ₂	8	9	8	6	(-1, 2)
SnS ₂	8	9	10	8	(-1, 2)

For this configuration, ν_{no inv} is the appropriate invariant to describe the topological properties:

$$\nu_{\text{no inv}} = (K_{e^{i\pi/3}}^3, K_{-1}^3), \quad (4)$$

where $K_{e^{i\pi/3}}^3$ is the difference between a number of states at K and Γ with C_3 eigenvalue $e^{i\pi/3}$.

The inversion-breaking scenario requires further elaboration because we are reducing the number of crystalline symmetries. To relate the topological classification developed for SG 164 to this reduced case, we must study how the irreps of this SG map to the SG without inversion, which is SG 156 ($P3m1$). As this is a subgroup of index 2 of SG 164, we can employ the subduction procedure, as explained in Ref. [10]. The result of this map can be extracted from the Bilbao Crystallographic Server, and for completeness, it is also presented in the SM. Most importantly, this map preserves the fragility of the SG 164 bands. Moreover, bands with stable topology in SG 164 are mapped to either EBRs (if the K_{-1}^3 invariant is zero) or fragile bands (if the K_{-1}^3 invariant is nonzero) in SG 156. The prevalence of fragility in SG 156 is also confirmed by the Smith decomposition procedure for this group, as it does not host stable $\mathbb{Z}_2$ phases that can be diagnosed by symmetry indicators alone (there can, however, exist other stable topological phases, as the system belongs to the class AII of the Altland-Zirnbauer classification [28]).

Application to case studies

Table II collects both symmetry indicators ν_{inv} and $\nu_{\text{no inv}}$ for the valence band set of the selected compounds ZrSe₂, ZrS₂, and SnS₂. Although the TQC analysis presented in the previous section yielded a trivial valence band set for all three compounds, nontrivial symmetry-indicator invariants are obtained for all cases except ZrSe₂. This is expected, since symmetry-indicator invariants successfully characterize topological phases whose bands at the Fermi level are an apparently trivial sum of EBRs, such as fragile topology and obstructed atomic limits. It follows that symmetry indicators are especially useful in our systems. Crucially, a nonzero ν_{inv} anticipates the presence of fractional corner charges in $C_3 + I$ -symmetric materials under open boundary conditions, whereas a nonzero $\nu_{\text{no, inv}}$ indicates a similar behavior for C_3 -symmetric systems [38,39].

On a different note, symmetry-indicator invariants are also related to the Wilson loop spectra of the bands [39], which,

due to the presence of crystalline symmetries, can be computed using the corresponding eigenvalues. As a general result for all the structures studied, we find that all fragile bands present a zero M_{-1}^I invariant, which indicates a nonwinding Wilson loop along the $\Gamma - M$ direction. This is the usual path for the characterization of the $\mathbb{Z}_2$ topology and indicates that fragile bands will show a trivial character along that direction, even when their WL spectra are calculated in isolation from other bands. Nevertheless, as has been made patent in previous works [24,25,40,44,85], fragility can be captured by other different paths, a fact that the nonzero values of $K_{e^{i\pi/3}}^3$ and K_{-1}^3 corroborate. These invariants are related to the $\Gamma - K$ path, which implies that fragile bands have nontrivial features that will show in responses related to these indicators.

IV. CORNER CHARGE ANALYSIS

In an open system, fractional corner charges are a signature of topology stemming from a filling anomaly, which arises at charge neutrality when enforcing certain crystalline symmetries in topological systems [38,39,86–88]. These systems can be trivial under periodic boundary conditions, but not under open conditions, where robust, fractionally filled corner states appear [39,50]. In particular, in the presence of C_3 and inversion symmetry, the corner charge $Q_{\text{c,inv}}$ hosted at each C_3 -symmetric sector of a flake is defined in terms of the symmetry-indicator invariants defined in Sec. III as [39]

$$Q_{\text{c,inv}} = -\frac{1}{4}M_{-1}^I - \frac{1}{3}K_{-1}^3 \bmod 2. \quad (5)$$

The allowed charge values for the three equal threefold symmetric corners, besides zero, are $1/3$, $2/3$, 1 , $4/3$, or $5/3$. In the absence of inversion, the corner charge $Q_{\text{c,no inv}}$ reads

$$Q_{\text{c,no inv}} = \frac{2}{3}K_{e^{i\pi/3}}^3 + \frac{2}{3}K_{-1}^3 \bmod 2. \quad (6)$$

This implies three equal corner charges with values $2/3$ or $4/3$. These formulas hold in the presence of spin-orbit coupling. For both the inversion-preserving and the inversion-breaking cases, the presence of spin-orbit coupling and time-reversal symmetry ensures that all states are at least twofold degenerate due to Kramers' theorem, which leads to the aforementioned allowed values for $Q_{\text{c,inv}}$ and $Q_{\text{c,no inv}}$ [38,39].

It is worthwhile to emphasize the non-uniqueness of the corner charge value [38], since the filling anomaly at the neutrality point can be overcome by either filling or depleting the Fermi level. In the following, we will work in units of the fundamental charge of the electron, and therefore assume that a corner charge of n/N indicates that each N -symmetric sector of the system would need n additional electrons for the states at the neutrality point to be completely filled. This convention has also been explicitly followed in previous works [89].

In this way, it is straightforward to predict the presence of corner charges $Q_{\text{c,inv}}$ and $Q_{\text{c,no inv}}$ in candidate materials from standard first-principles calculations. The existence of corner charges, which could be observed via STM measurements, is key for the experimental identification of novel types of topology such as HOTIs and fragile systems. The relevance of corner charges is further highlighted since, as discussed in the Introduction, realizations of fragile topology are elusive, but

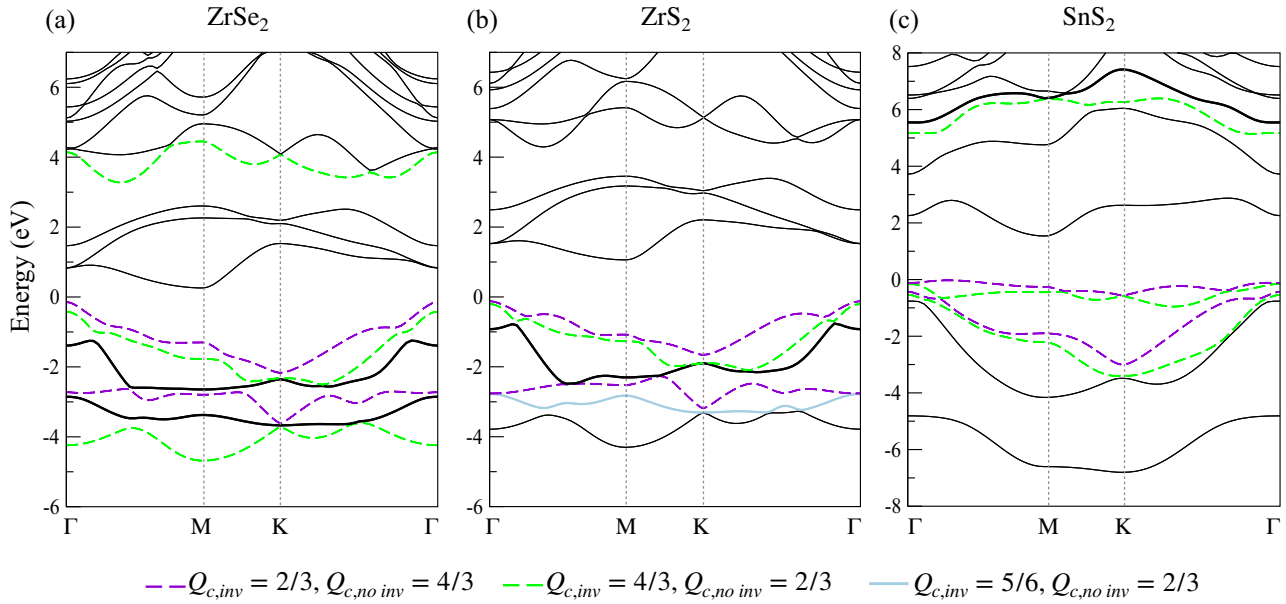


FIG. 3. Band structure of monolayer (a) ZrSe₂, (b) ZrS₂, and (c) SnS₂ with bands with nonzero partial corner charges colored in green and purple, respectively. Bands with ill-defined corner charges are colored gray. Fragile bands are represented with dashed lines, and stable topological bands are highlighted with thick lines.

nonzero $Q_{c,inv}$ or $Q_{c,no\ inv}$ would confirm that the fragility of these systems could be overcome in an open boundary setting.

However, as already commented in Refs. [38,39], symmetry-indicator invariants and corner charges are a shared property between second-order HOTIs, fragile systems, and obstructed atomic limits. In fact, besides stable and fragile bands, some SG 164 monolayers also show obstructed atomic insulator behavior [90,91]. Symmetry-indicator invariants $\nu_{c,inv}$ and $\nu_{c,no\ inv}$ do not distinguish between the aforementioned topological phases, since they are the same for all of them. Nevertheless, the presence of corner charges is mostly linked to HOTIs in the literature. Therefore, we aim to know whether the potential (well-defined) corner states are exclusively related to fragile topology in SG 164 monolayers or not. To this end, we follow two equivalent approaches. First, we compute a partial corner charge, which is the application of the above equations for $Q_{c,inv}$ and $Q_{c,no\ inv}$ to each set of doubly degenerate bands. Thus, we can identify which bands contribute to the total corner charge, and from the TQC analysis of Sec. III A, the type of topology they host. Second, we obtain the total value of the corner charges for the complete valence band set, which results from the addition (modulo 2) of the partial corner charges.

Application to case studies

We first present the result of the partial corner charge approach in panels (a), (b), and (c) of Fig. 3 for ZrSe₂, ZrS₂, and SnS₂, respectively. All three materials present fragile bands with well-defined nonzero corner charges $Q_{c,inv}$ and $Q_{c,no\ inv}$ near the Fermi level, which could be accessed individually in principle by doping processes. Analogous figures for semimetals ZrTe₂ and NiTe₂ can be found in the SM.

In Table I, we present a summary of the computed partial corner charges for the 16 types of basic band representations. It is readily observed that EBRs do not carry any partial corner charges, and that all the nonzero values stem from fragile and topologically stable bands. In particular, in the case with no inversion, as from Sec. III B, only fragile bands are present in SG 156, a nonzero total corner charge is exclusively associated with the presence of uncompensated (fragile) partial corner charges.

On the other hand, when inversion is present, fragile bands individually have a well-defined fractional corner charge according to the definition [38,39], whereas stable bands present corner charges that are not among the allowed values of Eq. 5 and thus could not give rise to the corresponding filling anomaly. This is the case, for example, of the fifth valence band of ZrS₂ in Fig. 3(b). However, the sum of an even number of stable topological bands (which will trivialize the $\mathbb{Z}_2$ invariant) results in a direct sum of EBRs and fragile bands, with a well-defined joint partial corner charge. For instance, the sum of the fifth and eighth stable bands in Table I, both present in ZrS₂, is

$$\begin{aligned}
 S5 + S8 &= (\bar{\Gamma}_9 \oplus \bar{M}_3\bar{M}_4 \oplus \bar{K}_6) \oplus (\bar{\Gamma}_8 \oplus \bar{M}_5\bar{M}_6 \oplus \bar{K}_4\bar{K}_5) \\
 &= (\bar{\Gamma}_9 \oplus \bar{M}_5\bar{M}_6 \oplus \bar{K}_6) \oplus (\bar{\Gamma}_8 \oplus \bar{M}_3\bar{M}_4 \oplus \bar{K}_4\bar{K}_5) \\
 &= \text{EBR} + \text{F3}.
 \end{aligned} \tag{7}$$

This set has a corner charge $Q_{c,inv} = 4/3$, which is a well-defined value and the same as that of fragile band F3. We have checked that this holds for all pairwise additions of strong bands in Table I. Moreover, even when partial corner charges stemming from fragile bands are trivialized mod 2 and the only contribution to $Q_{c,inv}$ is that of stable bands, these stable bands always come in pairs so that their joint contribution equals a sum of EBRs and fragile bands. Detailed calculations

TABLE III. List of all the materials studied in the database, sorted by the elements A and B in their formula AB_2 . The exemplary materials discussed in the main text and the SM are highlighted in bold text. Compounds highlighted in green have $Q_{c,inv} = 4/3$ and $Q_{c,no\,inv} = 2/3$, in gray, $Q_{c,inv}$ is not well defined, and the rest have no corner charges.

A	B = Chalcogen			
Zr	ZrO ₂	ZrS₂	ZrSe₂	ZrTe₂
Sn	SnO ₂	SnS₂	SnSe ₂	
Ni	NiO ₂	NiS ₂		NiTe₂
Pt	PtO ₂	PtS ₂	PtSe ₂	PtTe ₂
Hf	HfO ₂	HfS ₂	HfSe ₂	
Pd	PdO ₂	PdS ₂	PdSe ₂	
Si			SiSe ₂	
Pb	PbO ₂	PbS ₂		
Ge	GeO ₂	GeS ₂		
A	B = Halogen			
Cd	CdI ₂	CdBr ₂	CdCl ₂	CdF ₂
Zn	ZnI ₂	ZnBr ₂	ZnCl ₂	ZnF ₂
Pb	PbI ₂	PbBr ₂	PbCl ₂	
Ru	RuI ₂	RuBr ₂	RuCl ₂	
Hg				HgF ₂
Mg	MgI ₂	MgBr ₂		
Ca	CaI ₂	CaBr ₂		
Sr	SrI ₂	SrBr ₂		
Ba	BaI ₂	BaBr ₂		
Os	OsI ₂	OsBr ₂		
Sn	SnI ₂			
Ge	GeI ₂			

that support this statement can be found in the SM for several materials.

It follows that the origin of the corner charges in this SG is related to fragile topology, even when $\mathbb{Z}_2 = 1$ bands are considered. Even when the whole valence band manifold is trivialized from a TQC perspective, corner states can appear.

We have verified that the sum of partial charges equals the corner charge obtained by applying Eqs. (5) and (6) for the whole set of valence bands for the five materials highlighted in this work. The results for all the valence bands for each material are gathered in Table III. For all materials in our database, well-defined corner charges $Q_{c,inv} = 4/3$ or $Q_{c,inv} = 0$, and $Q_{c,no\,inv} = 2/3$ or $Q_{c,no\,inv} = 0$ are found, except for ZrTe₂, that has an ill-defined $Q_{c,inv} = 5/6$. This is consistent with the fact that ZrTe₂ is stable topologically with $\mathbb{Z}_2 = 1$ and hosts Dirac cones, which hamper the presence of a filling anomaly at the neutrality point. Moreover, over 80% of the samples have nonzero corner charges.

However, we have found that all halogen-based materials show a mismatch between the computed $Q_{c,inv} = 4/3$, $Q_{c,no\,inv} = 2/3$ and the actual filling anomaly inferred from their flake eigenvalue spectra, as demonstrated in the SM for MgBr₂. Namely, by counting the number of filled states at the neutrality point, we find that flakes involving halogens should have $Q_{c,inv} = 5/3$ and $Q_{c,no\,inv} = 4/3$.

Even though chalcogen- and halogen-based SG 164 monolayers have identical crystalline symmetries, they do not host

the same number of filled states at the neutrality point. This difference in the filling anomaly value stems from the fact that the 2d WP in chalcogen-based materials has no atomic support in real space, whereas for halogen-based systems it has partial support [91]. In fact, the fractional corner charge of a system can be foreseen from symmetry arguments based on the real-space distribution of Wannier functions [22,38,39], and SG 164 monolayers also host a topological orbital-obstructed atomic insulator phase [90,91]. It follows that, unlike stable topological bands (whose effect on corner charges could be traced back to fragile bands), orbital-obstructed topology plays a major role along with fragile topology in the emergence of corner states in SG 164 monolayers. The trivialization of the fragile bands at the Fermi level, where obstructed atomic insulators are diagnosed, impedes the study of both topological phases separately. Since for chalcogen-based materials fractional corner charges can be determined solely from crystalline symmetry arguments, and a more detailed study of the number and disposition of the valence electrons is needed for halogen systems, in the following we will focus on the former and leave the latter for a different study [91]. Overall, for materials with no atomic support at the 2d WP, the arguments presented in this work are valid.

Besides the three highlighted systems, other materials with nonzero fractional charges are PdS₂, SnS₂, or PtS₂, which are synthesized in monolayer form and constitute interesting experimental candidates for STM measurements of corner charges.

V. CORNER STATES IN FLAKES

In contrast to most materials hosting fragile topology, SG 164 does not have C_{2z} symmetry, so our fragile bands must be protected by other symmetry operations. Following our previous reasoning, we propose two flake geometries, a hexagonal one with C_3 symmetry and inversion, and a triangular one with C_3 but without inversion. The latter is the simplest approach since the triangular flake breaks not only the inversion but also the C_2 symmetries, having point group symmetry $3m$. For its part, the hexagonal flake preserves all monolayer symmetries, with point group symmetry $3m$.

For the triangular flake, a high electronic localization is observed via first-principles local density of states (LDOS) calculations at the three corners of Fig. 4 for the selected materials ZrSe₂, ZrS₂, and SnS₂. Since a band gap is necessary for well-defined corner charges, semimetals ZrTe₂ and NiTe₂ are not considered here.

In the bottom panel of Fig. 4, the flake eigenvalues depict a sixfold degeneracy at the Fermi level. Note that the states are not exactly localized at the Fermi level due to the absence of chiral symmetry [44]. DFT simulations also take into account potential interactions between corner states [92], which contribute to the elimination of degeneracy. This size effect is reduced by increasing the flake size; in fact, the number of degenerate states at the neutrality point can change depending on the system size, although the value of filled states is left unchanged (see SM). Such degeneracy is best observed the larger the band gap is, as verified by considering that SnS₂ has the largest gap of all three materials, and also comparing

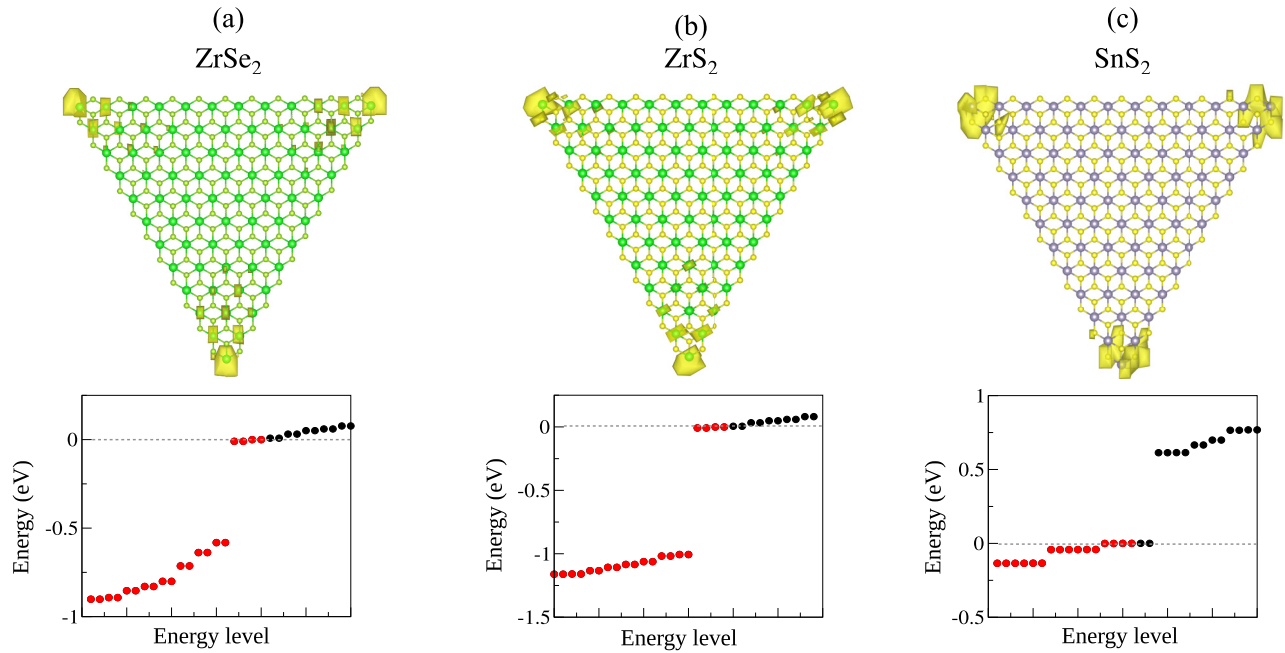


FIG. 4. LDOS (top panel) and eigenvalue spectra (bottom panel) for the (a) ZrSe₂, (b) ZrS₂, and (c) SnS₂ triangular flakes.

with Fig. 3 in the SM for MgBr₂ (with a gap over three times larger than SnS₂).

To fill this sixfold degeneracy, two additional electrons are needed for each material; therefore, each corner of the triangle should contribute $2/3$ (in units of the electron charge). From Table III, both ZrS₂ and SnS₂ have a corner charge without inversion $Q_{c, \text{no inv}} = 2/3$, in agreement with the value obtained by inspection of the eigenvalue spectra. The only exception is ZrSe₂, whose eigenvalue spectra yields $Q_{c, \text{no inv}} = 2/3$ but has a computed $Q_{c, \text{no inv}} = 0$ from Table III. This is due to the trivialization of partial corner charges by the extra low-lying valence bands that are considered within our DFT framework for Se-based alloys, and that are absent in other different DFT approaches [32].

Figure 5 shows the LDOS and energy spectra of hexagonal flakes with $C_3 + I$ symmetry. As in Fig. 4, there are four filled states at the neutrality point; however, now degeneracies are increased due to the presence of inversion symmetry. Namely, the spectrum is 12-fold degenerate at the Fermi level; this is best seen for flakes with larger band gaps whose edge states sit higher in energy, such as SnS₂ in panel (c). In fact, panels (a), (b), and (c) are ordered by increasing band gap. In order to fill the Fermi level, eight extra electrons would be needed, yielding $Q_{c, \text{inv}} = 4/3$ per corner of the flake. This value is in agreement with our previous calculations of the corner charge in Table III. Additional hexagonal flake figures are shown in the SM for smaller systems, emphasizing the need for sizable flakes in order to obtain robust degeneracies.

VI. CONCLUSIONS

SG 164 monolayer systems span a great variety of structures, which motivates a thorough search for nontrivial topological properties in this family. A comprehensive selection of compounds with AB₂ formula was surveyed, and

the case studies ZrSe₂, ZrS₂, and SnS₂ were selected for a detailed description. Our general results indicate the presence of stable ($\mathbb{Z}_2 = 1$) and fragile topological bands. Thus, SG 164 is an interesting platform to study the interplay between fragile and stable topology and its experimental implications, and where other topological phases, such as orbital-obstructed atomic insulator behavior, have also been reported.

Using first-principles calculations, we have analyzed the symmetry eigenvalues of the topologically nontrivial bands in these materials and computed their corner charges and related invariants. We have found nonzero topological indices for more than 80% of the screened materials. A detailed analysis of partial corner charges, computed for each band, has proven fundamental in clarifying the role of stable topological and fragile bands. Whereas these fractional charges are usually related to higher-order topology, we show that, in many SG 164 monolayers, corner charges are closely related to fragile bands. Moreover, via irrep subduction to the SG 156, we demonstrate that the nontrivial character of the fragility-induced topological invariants must be preserved in configurations where inversion is explicitly broken. Halogen-based monolayers are an exception, since the predicted corner charges are not in agreement with subsequent flake calculations. For these materials, a real-space analysis following an orbital-obstructed study can correctly foresee corner charges, and fragile topology plays a secondary role.

These findings were therefore tested mainly on nonhalogen compounds and using triangular and hexagonal geometries. For triangular flakes, a filling anomaly was identified for the three exemplary materials, resulting in a corner charge value of $2/3$. Regarding hexagonal structures, we find a corner charge of $4/3$. Both values agree with our previous analytical calculations.

It can also be noted that, as the nontrivial results depend on the $3m1$ symmetry, materials with a bulk structure described

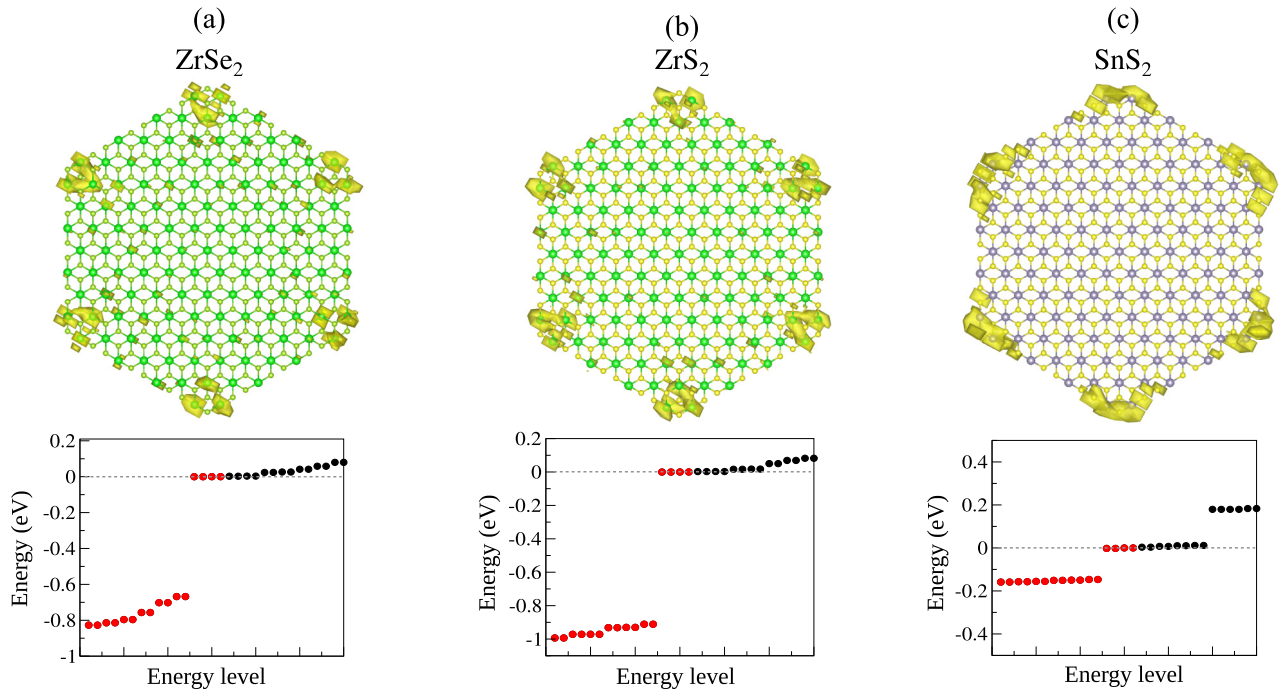


FIG. 5. LDOS (top panel) and eigenvalue spectra (bottom panel) for the (a) ZrSe_2 , (b) ZrS_2 , and (c) SnS_2 hexagonal flakes.

by SG 156 are likely to present the same effects. Examples of this are Janus TMDs, which are seen as an attractive platform for extending and applying the results achieved in this work. In summary, a direct link was established between C_3 symmetry-protected corner charges and fragile topology in a wide set of two-dimensional materials. The universality of our findings among SG 164, and possibly other SGs sharing the relevant threefold symmetry, encourages the experimental realization of responses bound to fragile topology in real materials.

ACKNOWLEDGMENTS

The authors thank J. D. Correa for helpful discussions. We acknowledge the financial support of the Agencia Estatal de Investigación of Spain under Grant No. PID2022-136285NB-C31 and from the Comunidad de Madrid through the (MAD2D-CM)-UCM5 project, funded by the Recovery, Transformation and Resilience Plan, and by NextGenerationEU from the European Union. O.A.G.

acknowledges the support of Grant No. PRE2019-088874 funded by MCIN/AEI/10.13039/501100011033 and by “ESF Investing in your future,” and of European Union NextGenerationEU/PRTR project Consolidación Investigadora (Project No. CNS2022-136025), as well as Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC) and Universidad Complutense de Madrid, where this project was initiated. S.B. acknowledges the support of the Postdoctoral Grant from the Universidad Técnica Federico Santa María. M.P. acknowledges the financial support of Chilean FONDECYT by Grant No. 1211913. Finally, we thank the Centro de Supercomputación de Galicia, CESGA, (Santiago de Compostela, Spain) and Supercomputación Castilla y León (SCAYLE) for providing access to their supercomputing facilities.

DATA AVAILABILITY

The data supporting this study’s findings are available within the article. Additional Supplemental Material can be found in Ref. [83].

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