

2D Theoretically Twistable Material Database

Yi Jiang,^{1,*} Urko Petralanda,^{2,*} Grigorii Skorupskii,^{3,*} Qiaoling Xu,^{4,5} Hanqi Pi,¹ Dumitru Călugăru,⁶ Haoyu Hu,^{1,7} Jiaze Xie,³ Rose Albu Mustaf,^{8,9,10} Peter Höhn,¹¹ Vicky Haase,¹¹ Maia G. Vergniory,^{12,1} Martin Claassen,¹³ Luis Elcoro,² Nicolas Regnault,^{14,6,15} Jie Shan,^{16,17,18} Kin Fai Mak,^{16,17,18} Dmitri K. Efetov,^{19,20} Emilia Morosan,^{8,9,10} Dante M. Kennes,^{21,22} Angel Rubio,^{22,14,23} Ledex Xian,^{5,24,22} Claudia Felser,¹¹ Leslie M. Schoop,³ and B. Andrei Bernevig^{6,1,25,†}

¹*Donostia International Physics Center (DIPC), Paseo Manuel de Lardizábal. 20018, San Sebastián, Spain*

²*Department of Physics, University of the Basque Country UPV/EHU, Apartado 644, 48080 Bilbao, Spain*

³*Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA*

⁴*College of Physics and Electronic Engineering, Center for Computational Sciences, Sichuan Normal University, Chengdu 610068, China*

⁵*Tsientang Institute for Advanced Study, Zhejiang 310024, China*

⁶*Department of Physics, Princeton University, Princeton, New Jersey 08544, USA*

⁷*Department of Physics, Princeton University, Princeton, NJ 08544, USA*

⁸*Department of Physics and Astronomy, Rice University, Houston, TX 77005, USA*

⁹*Rice Center for Quantum Materials (RCQM), Rice University, Houston, TX 77005, USA*

¹⁰*Smalley-Curl Institute, Rice University, Houston, TX 77005, USA*

¹¹*Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, Dresden 01187, Germany*

¹²*Département de Physique et Institut Quantique, Université de Sherbrooke, Sherbrooke, J1K 2R1 Québec, Canada*

¹³*Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104*

¹⁴*Center for Computational Quantum Physics, Flatiron Institute, 162 5th Avenue, New York, NY 10010, USA*

¹⁵*Laboratoire de Physique de l'Ecole normale supérieure, ENS, Université PSL, CNRS, Sorbonne Université, Université Paris-Diderot, Sorbonne Paris Cité, 75005 Paris, France*

¹⁶*School of Applied and Engineering Physics, Cornell University, Ithaca, NY 14850, USA*

¹⁷*Department of Physics, Cornell University, Ithaca, NY 14850, USA*

¹⁸*Kavli Institute at Cornell for Nanoscale Science, Ithaca, NY 14850, USA*

¹⁹*Faculty of Physics, Ludwig-Maximilians-University Munich, Munich 80799, Germany*

²⁰*Munich Center for Quantum Science and Technology (MCQST), Ludwig-Maximilians-University Munich, Munich 80799, Germany*

²¹*Institut für Theorie der Statistischen Physik, RWTH Aachen University and JARA-Fundamentals of Future Information Technology, 52056 Aachen, Germany*

²²*Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany*

²³*Nano-Bio Spectroscopy Group and ETSF, Universidad del País Vasco UPV/EHU- 20018 San Sebastián, Spain*

²⁴*Songshan-Lake Materials Laboratory, Dongguan, Guangdong 523808, China*

²⁵*IKERBASQUE, Basque Foundation for Science, Bilbao, Spain*

The study of twisted two-dimensional (2D) materials, where twisting layers create moiré superlattices, has opened new opportunities for investigating topological phases and strongly correlated physics. While systems such as twisted bilayer graphene (TBG) and twisted transition metal dichalcogenides (TMDs) have been extensively studied, the broader potential of a seemingly infinite set of other twistable 2D materials remains largely unexplored. In this paper, we define “theoretically twistable materials” as single- or multi-layer structures that allow for the construction of simple continuum models of their moiré structures. This excludes, for example, materials with a “spaghetti” of bands or those with numerous crossing points at the Fermi level, for which theoretical moiré modeling is unfeasible. We present a high-throughput algorithm that systematically searches for theoretically twistable semimetals and insulators based on the *Topological 2D Materials Database* (2D-TQCDB). By analyzing key electronic properties, we identify thousands of new candidate materials that could host rich topological and strongly correlated phenomena when twisted. We propose representative twistable materials for realizing different types of moiré systems, including materials with different Bravais lattices, valleys, and strength of spin-orbital coupling. We provide examples of crystal growth for several of these materials and showcase twisted bilayer band structures along with simplified twisted continuum models. Our results significantly broaden the scope of moiré heterostructures and provide a valuable resource for future experimental and theoretical studies on novel moiré systems.

I. INTRODUCTION

The discovery and study of two-dimensional (2D) materials have revolutionized condensed matter physics, opening new avenues for exploring quantum phenomena

* These authors contributed equally to this work.

† bernevig@princeton.edu

in reduced dimensions. One of the most exciting developments in the field is the concept of twistronics [1–4], where a small twist between layers of 2D materials leads to the formation of moiré superlattices, fundamentally altering the electronic structure and interaction landscape, giving rise to novel phenomena.

Twisting introduces periodic modulations and creates a moiré pattern that can drastically affect the low-energy electronic properties. The resulting moiré bands can become extremely flat due to the enlarged moiré unit cell, quenching the kinetic energy of electrons and thus enhancing the role of electron-electron interactions. These interactions can drive a wide range of topological and correlated phases, such as correlated insulating states [5], unconventional superconductivity [6], and fractional Chern insulators [7–9]. The prototypical example is twisted bilayer graphene (TBG) [10], where a “magic angle” twist between two graphene layers leads to the emergence of flat bands [5, 6, 11–30]. Beyond graphene, twisted transition metal dichalcogenides (TMDs), such as twisted MoTe_2 and WSe_2 , have also been shown to exhibit many different types of strongly correlated phases [31–54].

Despite the intense focus on TBG and TMD systems, many other potential moiré systems remain unexplored. Given the vast number of 2D materials with different crystal symmetries and electronic structures, there is a much larger space of twistable materials that could host rich correlated and topological physics [55–62]. The systematic exploration of this space is crucial to identifying new systems with novel properties that go beyond what has been observed in TBG and TMD moiré superlattices.

However, a systematic approach is hindered by the lack of theoretical predictions. Many single-, double-, and multilayer systems exhibit highly complex band structures, lacking simple effective models such as the Dirac cone in graphene or the quadratic band edge in TMD materials. Twisting an already complicated band structure leads to moiré bands that are theoretically intractable, making it difficult to predict the so-called “magic” angles [10]. In the case of TBG, the prediction of the magic angle was crucial in realizing superconductivity (SC) in the system. Therefore, we define “theoretically twistable” materials as 2D exfoliable materials with “clean” band structures. For metals, this means point or line Fermi surfaces that can be modeled theoretically. For insulators, we require clean band minima or maxima. We also impose experimentally relevant conditions, such as a gap smaller than 3 eV, as larger gaps would make forming good contacts difficult. Additional conditions, as described in the main text, are also applied.

With these conditions, we develop a high-throughput algorithm to screen the Topological 2D Materials Database (2D-TQCDB) [63] for twistable materials. Our algorithm identifies candidates based on their electronic structures, focusing on semimetals and insulators that exhibit clean band structures suitable for theoretically predictable moiré engineering. By applying the algo-

rithm, we have identified 61 clean twistable semimetals and 1568 twistable insulators, which we further classify into large classes based on their Bravais lattices, valley types, and spin-orbital coupling (SOC) splitting strength. We select representative materials for each universality class and present example twisted bilayer band structures alongside simplified moiré continuum models. We also offer experimental insights into the feasibility of realizing twistable materials, all these simple layers either exist or are predicted to exist. Complete data on the twisting properties of these materials are available on the 2D-TQCDB. This work not only provides a complete database of potential twistable materials but also broadens the scope of twistronics, paving the way for future experimental and theoretical investigations into novel 2D moiré systems.

II. CLASSIFICATION OF TWISTABLE MATERIALS

In twisted systems, the moiré potential breaks the translation symmetry of the monolayer and couples the electron states connected by the moiré reciprocal lattice vectors $\mathbf{G} \in \mathcal{Q} = \mathbb{Z}\mathbf{b}_{M_1} + \mathbb{Z}\mathbf{b}_{M_2}$, where $\mathbf{b}_{M_i} = 2 \sin(\frac{\theta}{2}) \mathbf{b}_i \times \hat{\mathbf{z}}$ are moiré reciprocal vectors, defined based on the monolayer reciprocal vectors $\mathbf{b}_{1,2}$ and twist angle θ . The single-particle Hamiltonian for moiré systems takes the form

$$\mathcal{H} = \sum_{\mathbf{k}, \mathbf{Q}, \mathbf{Q}', i, j} [h_{\mathbf{Q}, \mathbf{Q}'}]_{ij} \hat{c}_{\mathbf{k}, \mathbf{Q}, i}^\dagger \hat{c}_{\mathbf{k}, \mathbf{Q}', j} \quad (1)$$

where \mathbf{k} takes value in the first moiré Brillouin zone (BZ), i, j are composite indices for orbital, spin, and other degrees of freedom. \mathbf{Q} takes values in the moiré \mathbf{Q} lattice, *i.e.*, $\mathbf{K}_{\text{valley}} - \mathcal{Q}$, which is formed by the moiré plane wave components expanded around the valley momentum $\mathbf{K}_{\text{valley}}$. Depending on the Bravais lattice and valley types, moiré systems exhibit a diverse range of properties.

We classify twistable materials into two types. The first type includes semimetals with (approximately) zero-dimensional (0D) Fermi surfaces (FSs), such as graphene with a linear Dirac crossing. These semimetals may feature various crossing types at the Fermi level, including linear and quadratic degenerate points. The second type includes insulators with clean valence band maxima (VBM) or conduction band minima (CBM), exemplified by TMD materials. We refer to both the crossing points in semimetals and the clean VBM/CBM in insulators as the “twisting points”, which are not necessarily located at high-symmetry momentum points (HSPs). Each of the two types of twistable materials is further classified based on their (i) Bravais lattice, (ii) the momentum of the twisting point, and (iii) SOC splitting at the twisting point.

The four Bravais lattices corresponding to 80 layer groups (LGs) are hexagonal, square, rectangular (includ-

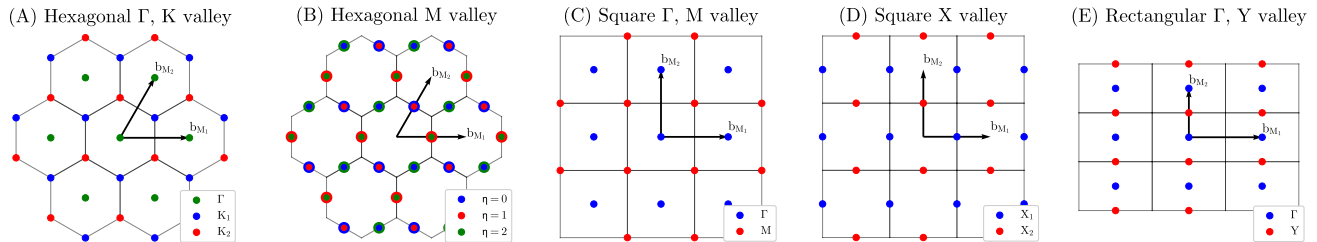


FIG. 1. **Moiré \mathbf{Q} lattices derived from different Bravais lattices and valleys.** (A) shows the \mathbf{Q} lattices corresponding to the Γ and K valley in the hexagonal lattice. The K valley generates two sets of \mathbf{Q} lattices from the two time-reversal symmetry (TRS)-related K points, K_1 and K_2 , forming a honeycomb lattice in momentum space. (B) depicts the \mathbf{Q} lattice from the M valley in the hexagonal lattice, which results in a kagome lattice in momentum space, with three sublattices corresponding to the three C_3 -symmetry-related M valleys. (C) presents the Γ and M valleys from the square lattice, both forming a square lattice in momentum space. (D) illustrates the \mathbf{Q} lattice generated by the X valley from the square lattice, forming two nested square lattices in momentum space given by the two C_4 -related valleys X_1 and X_2 . (E) shows the \mathbf{Q} lattices for the Γ and Y valleys from the rectangular lattice.

ing centered rectangular), and oblique. The valleys are labeled according to their momenta as follows: for hexagonal lattices, Γ , M , K , and non-HSPs; for square lattices, Γ , X , M , and non-HSPs; and for rectangular and oblique lattices, HSPs or non-HSPs for simplicity. The HSP labeling follows the conventions of the Bilbao Crystallographic Server [64–66]. For SOC classification, a numerical threshold of 50 meV energy splitting near the twisting point is used to identify materials with strong SOC. In practice, we evaluate the maximal SOC splitting within a specified momentum range relative to the twisting point—specifically, within the first moiré BZ at a chosen twist angle of 5° , an angle that covers the relevant momenta after twisting. This momentum range is particularly useful for time-reversal-invariant momenta (TRIM) such as the Γ and M points in the hexagonal lattice, where SOC splitting is zero (for a single band with two spins) at the TRIMs themselves but can be significant in their vicinity. The same moiré BZ is also used as the momentum resolution to determine whether a valley is located at an HSP. If the distance from the valley to an HSP falls within this first moiré BZ, we define the valley as being at the corresponding HSP.

In Fig. 1, we illustrate the moiré \mathbf{Q} lattices for various Bravais lattices and valley configurations. Fig. 1 (a) shows the Γ and K valleys within a hexagonal BZ. The \mathbf{Q} lattice associated with the Γ valley forms a triangular lattice, while that for the K valley forms a honeycomb lattice, with the two sublattices representing the two time-reversal symmetry (TRS)-related valleys, $K_{1,2}$. Fig. 1 (b) depicts the \mathbf{Q} lattice originating from the M valley, which forms a kagome lattice in the hexagonal BZ with three sublattices corresponding to the three C_3 -related M valleys. In [67], we introduced a new class of moiré materials based on the M -valley, specifically in SnSe_2 and ZrS_2 , which are representative materials from the current high-throughput results and can be exfoliated into single layers in experiments. These M -valley moiré materials exhibit unique non-symmorphic symme-

tries and a kagome \mathbf{Q} -lattice in momentum space, providing a novel platform for exploring flat-band physics, Luttinger liquid behavior, and interaction-driven phases. Fig. 1 (c) and (d) present the \mathbf{Q} lattices derived from the Γ , M , and X valleys of a square lattice. Both the Γ and M valleys form square lattices, while the X valley forms two nested square lattices representing the two C_4 -related $X_{1,2}$ valleys. Finally, Fig. 1 (e) illustrates the \mathbf{Q} lattices of the Γ and Y valleys in a rectangular lattice, which produce rectangular lattices in the BZ. In summary, the symmetry properties and valley configurations of the underlying Bravais lattice play a critical role in determining the structure of the moiré \mathbf{Q} lattices, offering diverse platforms for studying exotic electronic phenomena. We have already described the non-trivial physics of twisting the M point in the hexagonal lattice with negligible SOC [67]. This represents just one of the universality classes of twisted materials, with each class presented here likely to host novel physics.

III. HIGH-THROUGHPUT ALGORITHM

In this section, we outline the high-throughput screening algorithm used to identify twistable materials.

In the algorithm, we begin by excluding conventional metals with an odd number of valence electrons, as these generally cannot host 0D FSS or act as insulators. Next, we limit the selection to compounds with no more than 12 atoms or four distinct elements per monolayer unit cell; larger unit cells would be challenging to study both theoretically and experimentally upon twisting. We then introduce the concept of a “clean energy range” to quantify how well-isolated the bands are near the Fermi level, a necessary condition for obtaining clean twisted band structures. This range is defined as the energy window around the twisting point in which only one band is present without SOC, or two bands are present with SOC. In the following sections, we outline the specific cri-

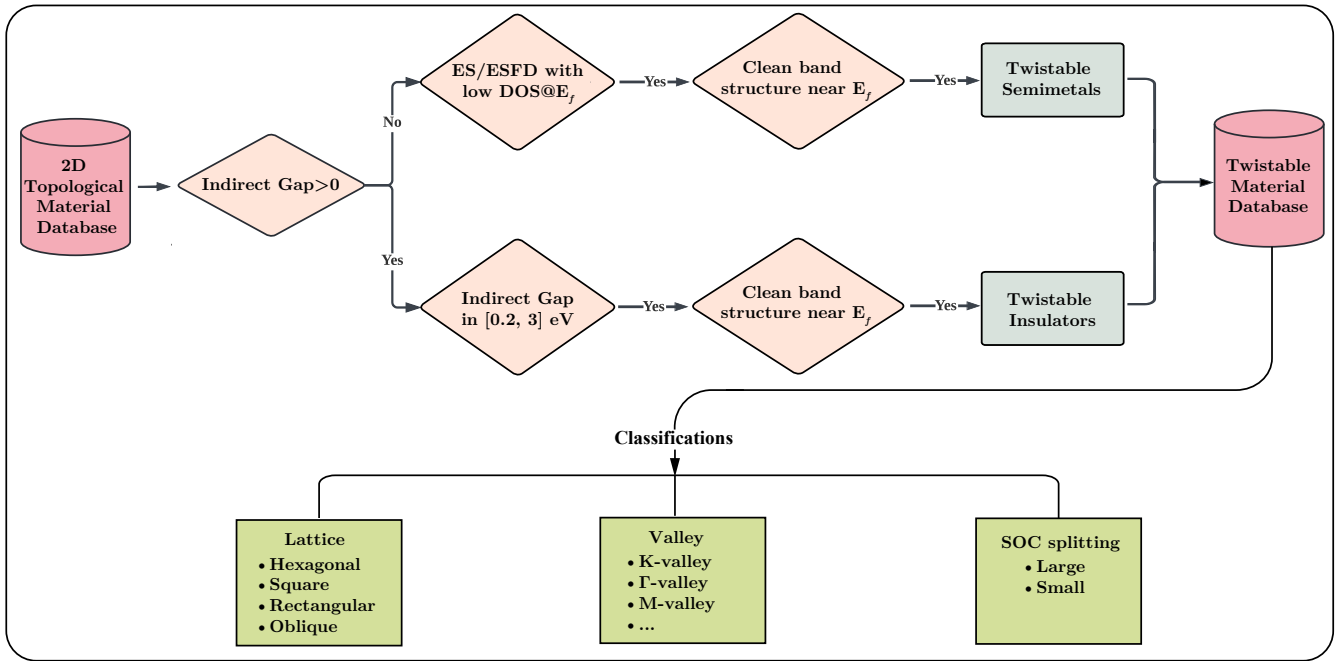


FIG. 2. **The high-throughput algorithm used to search for 2D twistable materials.** We start from all 2D materials in the 2D-TQCDB [63]. For a given material, if it has a zero indirect gap, we then determine whether it has a topological classification of ES or ESFD, a low DOS, and a clean band structure at the Fermi level. If these criteria are met, the material is classified as a theoretically twistable semimetal with symmetry-protected degeneracy at the Fermi level. Conversely, if the material has an indirect gap within the range of [0.2, 3] eV and a clean band edge in either the valence or conduction bands, it is considered a theoretically twistable insulator. The identified twistable semimetals and insulators are further categorized based on their Bravais lattice, valley momentum, and SOC splitting strength.

teria for identifying twistable semimetals and insulators.

For semimetals, the criteria are:

- (i) **Enforced-Semimetal Condition:** the topological classification of the material, either with or without SOC, must be either an enforced semimetal with Fermi degeneracy (ESFD), featuring crossings at high-symmetry points, or an enforced semimetal (ES) with crossings along high-symmetry lines, thereby ensuring a symmetry-protected crossing point between valence and conduction bands. We include semimetals in which SOC opens a small gap at the crossing points.
- (ii) **Density-of-States (DOS) Condition:** the DOS at the Fermi level E_f must be ≤ 2 states per unit cell per eV. This threshold takes an empirical value and is not strictly constrained, as it aims to account for significant DOS contributions from quadratic crossing points, small Fermi surface pockets from other bands, or multiple crossing points. For instance, the predicted material AuTe features several crossing points at E_f , resulting in a relatively large DOS of about 1 state per unit cell per eV. Nevertheless, the bands near E_f remain relatively clean, making it a viable twistable candidate.
- (iii) **Clear-Energy-Range Condition:** both the VBM

and CBM must exhibit a clean energy range of at least 200 meV. This energy range is on the order of the interlayer hopping in moiré systems, within which a reliable low-energy description can be achieved.

- (iv) **Band-Edge Condition:** the highest valence band edge and lowest conduction band edge should be within 0.1 eV from E_f . We note that even if the semimetal is gapped by SOC or other mechanisms, the gap is typically not large enough to fully separate the conduction and valence bands. As a result, the theoretical description must account for both bands together. We also allow small FS pockets within 0.1 eV from E_f , as they may be eliminated upon twisting.

For insulators, we apply the following criteria:

- (i) **Gap Condition:** a global band gap between 200 meV and 3 eV;
- (ii) **Clear-Energy-Range Condition:** a clean energy range of at least 200 meV in either the highest valence band or the lowest conduction band.
- (iii) **DOS condition:** we require the maximal DOS within 200 meV to the twisting point should be ≤ 4 states per unit cell per eV. This criterion

also takes an empirical threshold used to exclude extremely flat bands at the twisting point, which would generate a large DOS and are likely to produce spaghetti-like bands after twisting.

These conditions are applied to ensure well-isolated band structures. A maximum gap of 3 eV is chosen because a larger gap would be experimentally challenging for making electrical contacts and performing effective gating. Since *ab initio* calculations generally underestimate the band gap, compounds with large gaps will be ranked with low scores in the following. We note that multiple, symmetry-unrelated valleys may exist within the clean energy range. In practice, these valleys are typically either energetically distinct or effectively decoupled at the single-particle level after twisting. Therefore, they are included in our algorithm.

To rank the twistable materials identified by the algorithm, we have established a scoring system to quantify their suitability. The scores for semimetals and insulators are defined as follows:

$$\begin{aligned} \mathcal{S}_{\text{semimetal}} &= \frac{1}{5}(\mathcal{S}_{\text{DOS}} + \mathcal{S}_{\text{clean VB range}} + \mathcal{S}_{\text{clean CB range}} \\ &\quad + \mathcal{S}_{\text{symmetry}} + \mathcal{S}_{\text{atom number}}) \\ \mathcal{S}_{\text{insulator}}^{\text{VB/CB}} &= \frac{1}{4}(\mathcal{S}_{\text{gap}} + \mathcal{S}_{\text{clean VB/CB range}} \\ &\quad + \mathcal{S}_{\text{symmetry}} + \mathcal{S}_{\text{atom number}}) \end{aligned} \quad (2)$$

Here, the score for twistable insulators, *i.e.*, $\mathcal{S}_{\text{insulator}}^{\text{VB/CB}}$, is defined for the twisting point at VBM and CBM separately. The criteria for each component are as follows:

- **Gap Score (\mathcal{S}_{gap}):** This score assesses the indirect band gap Δ , aiming for an ideal range of 1 to 1.5 eV. The score decreases linearly with deviation from this range. Specifically, we set $\mathcal{S}_{\text{gap}} = 1$ for $\Delta \in [1, 1.5]$ eV, $\mathcal{S}_{\text{gap}} = 1 - |\Delta - 1|/0.8$ for $\Delta \in [0.2, 1]$ eV, and $\mathcal{S}_{\text{gap}} = 1 - |\Delta - 1.5|/1.5$ for $\Delta \in [1.5, 3]$ eV.
- **Clean-Range Score ($\mathcal{S}_{\text{clean VB/CB range}}$):** Measures the cleanliness of the energy range around the VBM or CBM. We define $\mathcal{S}_{\text{clean CB/VB range}} = 1 - |\max(\Delta E_{\text{VB/CB}}, 1) - 1|/0.8$, where $\Delta E_{\text{CB/VB}}$ is the clean range at the VB/CM, truncated at 1 eV since an excessively large energy range is not critical for twisting.
- **DOS Score (\mathcal{S}_{DOS}):** Derived from the density of states at the Fermi level, $D(E_f)$, in states per unit cell per eV. We define $\mathcal{S}_{\text{DOS}} = 1 - D(E_f)/2$, *i.e.*, a lower density of states results in a higher score.
- **Symmetry Score ($\mathcal{S}_{\text{symmetry}}$):** Defined as the number of point group (PG) symmetries divided by 24, which is the maximum number of PG operations in layer groups.

- **Atom Number Score ($\mathcal{S}_{\text{atom number}}$):** Inversely related to the number of atoms in the unit cell to favor simpler and more symmetrical compounds.

We can see that each component is normalized to ensure a maximum value of 1. The total scores for both semimetals and insulators range from 0 to 1, where higher scores indicate materials that are better candidates for experimental and theoretical exploration. We note that while these scores may involve a slight degree of arbitrariness, they are based on both theoretical and experimental facts. We intentionally applied less strict criteria to capture a broader range of potentially twistable materials. While adjusting the definition of the score would alter their rankings, the materials are already categorized into sub-classes of lattices, valleys, and SOC strength, and there are relatively few in each. This allows for the manual selection of candidates from each sub-class for further study, with the score serving as a reference rather than a strict determinant.

IV. RESULTS

We applied the algorithm to all materials in the Topological 2D Materials Database [63] and identified 61 candidates as twistable semimetals and 1568 as twistable insulators. The results are summarized in Table I, with materials further categorized as experimental, computationally exfoliable, computationally stable, and computationally unstable (see Appendix [IV] for more details). Computationally unstable materials are also included to ensure that potential twistable candidates are not overlooked. The significantly smaller number of twistable semimetals compared to insulators is due to the strict requirement for clean, symmetry-protected crossings at the Fermi level—a condition that is difficult to meet despite the relatively large number of 2D topological semimetals [63], which typically exhibit large FSSs. A comprehensive list of these materials is provided in Appendix [V] and Appendix [VI]. In the following, we discuss representative twistable semimetals and insulators across different classes.

A. Representative Twistable Semimetals

Twistable semimetals possess symmetry-protected crossing points near the Fermi level, which can be gapped in the presence of SOC. Table II presents representative twistable semimetals classified by type. From this list, we select three examples to examine their band structures and properties in the following.

Fig. 3 (A) shows the monolayer band structure of a predicted stable material $\text{Ta}_2\text{Te}_2\text{S}$ in LG 72 ($p\bar{3}m1$), which features a linear Dirac crossing at the K point without SOC. This crossing is gapped by SOC, resulting in a sizable gap of approximately 100 meV, much larger than

TABLE I. **Statistics of twistable materials.** The materials are classified by Bravais lattice, valley, and SOC strength. The number in parentheses indicates the number of corresponding twistable semimetals (omitted if zero), while the number without parentheses represents the number of twistable insulators. Valley types are based on the momentum at the twisting point. When the SOC splitting near the twisting point is significant, the valley is labeled as “valley-SOC.” Materials are further classified into experimental (Exp.), computationally exfoliable (Exfo.), computationally stable (Stab.), and computationally unstable (Unstab.). For insulators, we evaluate their VBM and CBM separately, meaning a single material could appear twice in the table.

Lattice	Valley	Exp.	Exfo.	Stab.	Unstab.
Hexagonal 1072 (48)	Γ	28	28	298	60 (2)
	Γ -SOC	13	10 (1)	124 (10)	20 (5)
	K	7 (3)	8	75	25 (9)
	K -SOC	7 (1)	2 (1)	43 (4)	12 (4)
	M	10	10	54	20
	M -SOC	1	0	3	2
	nHSP	10	8	79 (3)	18
	nHSP-SOC	1	3	65 (3)	28 (2)
Square 167 (3)	Γ	0	23	45	13
	Γ -SOC	0	3	14	0 (1)
	M	0	2	20	3
	M -SOC	0	0	3	1
	X	0	2	8	5
	X -SOC	0	0	0	1
	nHSP	0	1	3	9
	nHSP-SOC	0	0	7	4 (2)
Rectangular 710 (10)	HSP	4	96	290	85 (1)
	HSP-SOC	0	0	17	17
	nHSP	3	13 (1)	98 (1)	25
	nHSP-SOC	2 (2)	4 (2)	38 (2)	18 (1)
Oblique 38	HSP	0	6	10	3
	HSP-SOC	0	0	3	1
	nHSP	0	4	3	0
	nHSP-SOC	0	1	3	4

the negligible SOC gap in graphene. The large SOC in $\text{Ta}_2\text{Te}_2\text{S}$ leads to the formation of quantum spin Hall (QSH) states in both the valence and conduction bands, which are absent in graphene due to its negligible SOC. After twisting, the moiré band structure is expected to be markedly different from that of graphene and show distinct moiré physics.

Fig. 3 (B) is for the computationally exfoliable material ZrBr in LG 72 ($p\bar{3}m1$), where a quadratic crossing is observed at Γ with an SOC gap of about 50 meV. The quadratic dispersion arises from the higher symmetry of the D_{3d} point group at Γ , which includes three in-plane C_2 rotations and the TRS in addition to the C_{3z} rotation. The effective $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian for the quadratic

TABLE II. **Representative twistable semimetals.** They are classified into different classes according to Bravais lattices, valleys, and SOC strength.

Lattice	SOC	Γ	K	nHSP
Hexagonal	Strong	ZrBr	$\text{Ta}_2\text{Te}_2\text{S}$	ZrTe
	Weak	Cu_2Se	Ge	IrPS_3
		HSP	nHSP	
Rectangular	Strong	/	MoS_2	
	Weak	/	Hg_3S_2	

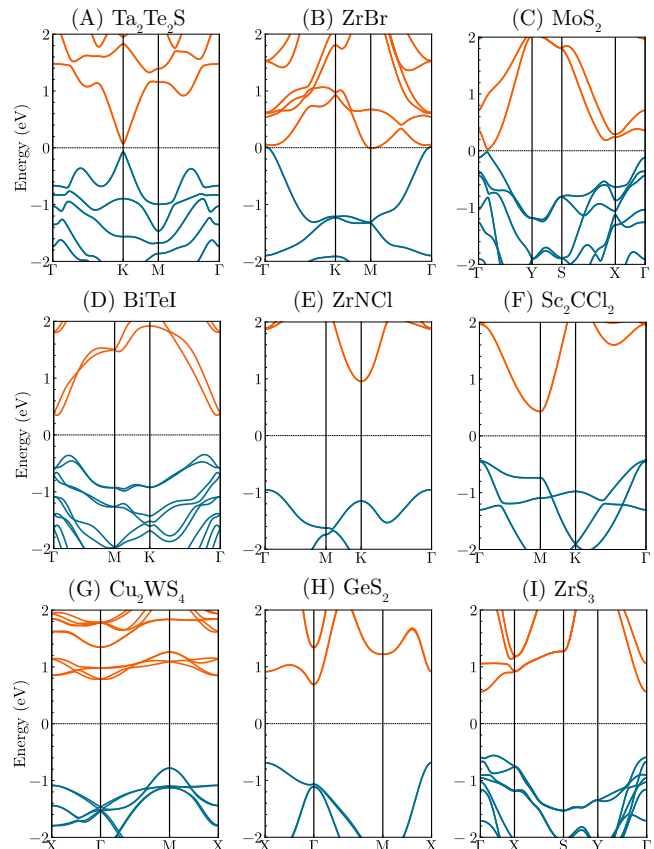


FIG. 3. **The monolayer band structures of representative twistable materials.** (A) Hexagonal $\text{Ta}_2\text{Te}_2\text{S}$ exhibits a Dirac cone at the K point, which is gapped by SOC with a gap of approximately 100 meV, placing it in a distinctly different universal class from TBG. (B) Hexagonal ZrBr features a quadratic crossing at the Γ point, further gapped by SOC with a gap of about 50 meV. (C) Rectangular MoS_2 displays a linear crossing along the $\Gamma - Y$ line, which opens a SOC gap of about 50 meV. (D) Hexagonal BiTeI hosts the CBM at the Γ point with strong Rashba SOC splitting. (E) Hexagonal ZrNCl features a clean K valley at the CBM with negligible SOC splitting. (F) Hexagonal Sc_2CCl_2 has the CBM at the M valley with negligible SOC splitting. (G) Square Cu_2WS_4 has the VBM at the M valley with negligible SOC splitting. (H) Square GeS_2 has the VBM at the X valley with negligible SOC splitting. (I) Rectangular ZrS_3 hosts the CBM at the Γ valley with negligible SOC splitting.

dispersion at Γ has the form:

$$h(\delta\mathbf{k}) \approx v_1 \delta\mathbf{k}^2 \sigma_0 + v_2 \begin{bmatrix} 0 & e^{i\frac{\pi}{3}} \delta k_+^2 \\ e^{-i\frac{\pi}{3}} \delta k_-^2 & 0 \end{bmatrix}, \quad (3)$$

where $\delta k_{\pm} = \delta k_x \pm i\delta k_y$, and $v_{1,2}$ are the parameters for the two terms. The quadratic dispersion leads to a quasi-flat segment of band near Γ and a large DOS at the Fermi level, which can result in flatter moiré bands after twisting. These flatter bands reduce the kinetic energy of electrons, enhancing correlation effects. As a result, ZrBr could exhibit strong interactions in its twisted form.

Fig. 3 (C) shows the experimental material MoS₂ [68] in LG 15 ($p2_1/m11$), featuring a linear crossing along the $\Gamma - Y$ high-symmetry line. MoS₂ adopts the $1T'$ structure, similar to $1T'$ -WTe₂ [69–72]. Note that $1T'$ -chMoS₂ is a meta-stable phase and is different from the common 2H-MoS₂ [73]. In $1T'$ -MoS₂, the linear crossing along the $\Gamma - Y$ line is protected by a C_2 rotation symmetry, where the two crossing bands have opposite C_2 eigenvalues, preventing hybridization. When SOC is introduced, this crossing point becomes gapped, with a gap of approximately 50 meV, and both the valence and conduction bands exhibit quantum spin Hall (QSH) states. Unlike WTe₂, where small Fermi surface pockets remain even with SOC, MoS₂ has a fully gapped band structure, potentially leading to much simpler moiré band structures and offering a cleaner platform for exploring correlated moiré phases. We note that the WS₂ in the same group exhibits similar gapped band structures and can be synthesized in this structure starting from K_xWS₂ [74].

Among all twistable semimetals, we note that only four candidates have a square lattice: CuCl₂, PtS, SnS, and RuCl₂. Of these, CuCl₂ is computationally exfoliable and has a twisting point at the X point, which is gapped by SOC with small magnetic moments developed on Cu. The others, however, are computationally unstable. For the hexagonal lattice, we note that the M valley has only 1D irreducible representations (IRREPs) in the absence of SOC, and therefore cannot host twistable semimetals.

B. Representative Twistable Insulators

Table III presents representative twistable insulators. From this list, we select six compounds with distinct properties, with their band structures shown in Fig. 3.

The first three compounds, BiTeI, Sc₂CCl₂, and ZrNCl, all possess a hexagonal lattice but have different valleys and SOC splitting strength.

Fig. 3 (D) shows the experimental material BiTeI in LG 69 ($p3m1$), with the CBM near the Γ point, characterized by strong Rashba-type SOC splitting. To model the spin splitting, we write down a $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian at Γ point with the first and second order terms:

$$h(\delta\mathbf{k}) \approx v\delta\mathbf{k} \cdot \boldsymbol{\sigma} + \frac{\delta k_x^2 + \delta k_y^2}{2m} \sigma_0, \quad (4)$$

TABLE III. **Representative twistable insulators.** They are classified into different types of lattices, valleys, and SOC strength.

Lattice	SOC	Γ	M	K	nHSP
Hexagonal	Strong	BiTeI	GaTe	GaSe	AsSb
	Weak	InSe	Sc ₂ CCl ₂	ZrNCl	PtSe ₂
		Γ	M	X	nHSP
Square	Strong	BiIO	HgH ₂	/	SnI ₂
	Weak	GeCl ₂	Cu ₂ WS ₄	GeS ₂	GeI
		HSP	nHSP		
Rectangular/ Oblique	Strong	Sb ₂ Te ₂ O	SnSe		
	Weak	ZrS ₃	SnPS ₃		

where v characterizes the strength of the linear SOC term and m is the effective mass. As the Γ valley has the time-reversal symmetry (TRS), the strong SOC effects could potentially induce QSH states in the moiré bands. At small twist angles where interactions become dominant, this non-trivial topology may give rise to fascinating correlated physical phenomena, including fractionalized topological states at non-integer fillings.

Fig. 3 (E) shows ZrNCl in LG 72 ($p\bar{3}m1$), with the CBM at the K valley and the VBM at the Γ valley, both of which exhibit negligible SOC splitting. The weak SOC splitting at the K valley contrasts sharply with that of the well-studied TMD materials such as MoTe₂ and WSe₂. In the literature, bulk ZrNCl and its Hf counterpart, HfNCl, have been shown to exhibit superconductivity at approximately 15 K and 25 K, respectively, upon doping into the conduction band [75–77]. Therefore, twisted ZrNCl may similarly exhibit superconducting properties upon doping.

Fig. 3 (F) features a predicted exfoliable material Sc₂CCl₂ in LG 72 ($p\bar{3}m1$), displaying a CBM at the M point. In contrast to the K valley in TMDs, there are three C_3 -related M valleys in the monolayer BZ. When mapped onto the moiré BZ, these M valleys form a kagome lattice in momentum space, which could lead to novel correlated physics enriched by the rich valley degrees of freedom [67].

The fourth and fifth compounds, Cu₂WS₄ and GeS₂, both have a square lattice. Although moiré systems with a square lattice have been theoretically proposed [59, 78, 79], they have not yet been realized in experiments. Here, we propose two twistable square lattice insulators Cu₂WS₄ and GeS₂, both are computationally exfoliable [80, 81] with bulk structures and exhibit different valley properties.

Fig. 3 (G) shows Cu₂WS₄ in LG 57 ($p\bar{4}2m$), featuring a VBM at the M point with negligible SOC splitting, and a flat CBM in the vicinity of Γ with strong SOC-splitting. Both the Γ and M valleys exhibit C_4 symmetry and form a square lattice in the moiré BZ upon twisting. Fig. 3 (H) presents GeS₂ in LG 59 ($p\bar{4}m2$), with the VBM at the X point and the CBM at the Γ point. The X point differs

from the Γ and M points, as it lacks C_4 symmetry. Upon twisting, the X valley forms two sets of staggered square lattices in the moiré BZ, related by the C_4 symmetry, as shown in Fig. 1 (d).

We note that the Γ , M , and X valleys from the square lattice all respect TRS, and could potentially give rise to quantum spin Hall (QSH) states in the presence of strong SOC. Moiré systems with a square lattice could serve as a platform for simulating the Hubbard model, particularly in relation to high-temperature SC in cuprates [82–84], and may also exhibit unconventional superconductivity.

Lastly, Fig. 3 (I) shows the band structure of ZrS_3 in LG 46 ($pmmn$), which has a rectangular lattice and is computationally exfoliable [80]. The CBM appears at Γ and VBM is located along the $\Gamma - X$ line. In the rectangular lattice, the two in-plane lattice constants differ, and this disparity is further amplified in the moiré unit cell at small twist angles [85, 86]. As a result, rectangular moiré systems are expected to exhibit quasi-1D characteristics, potentially acting as Luttinger liquid simulators [87]. In ZrS_3 , the two in-plane lattice constants have a ratio of approximately 1.5. Additionally, the bands near the VBM are relatively flat along the k_x direction, which could potentially lead to flat moiré bands and further enhance the potential for strongly correlated physics.

C. Band structures for twisted bilayer materials

The database of 2D theoretically twistable materials established in this work, identifies the most promising candidates for twist-engineering based on properties of the corresponding monolayers. The materials presented here exhibit a clean monolayer structure that will lead to clean twisted bands with simple theoretical continuum models. To show this, we exemplify the power of this approach by comparing its prediction to results obtained using a full density-functional characterization of the corresponding twisted bilayer materials. At small twist angles for the latter, huge unit cells with many thousands of atoms need to be considered posing a significant challenge, and limiting the number of materials that can be analyzed; for details see Appendix [III]. Fig. 4 summarizes results at moderate twist angle $\theta = 7.34^\circ$ for (A) SnSe_2 , (B) SnS_2 , (C) ZrS_2 , (D) HfS_2 , and (E) Sc_2CCl_2 which were identified as twistable materials by the database established in this work. All of them, as predicted, show the emergence of intriguing flat-band physics with a only few bands highlighting the twistable database’s utility. The insets complement these results obtained at moderate twist angles with those obtained at a smaller twist angle of 3.89° [67] for which we have already derived continuum models. This comparison illustrates that bandwidth control of few-flat-band physics can indeed be obtained by the twist angle while some main features are already present in the results obtained at the moderate twist angle. In a forthcoming publication, we will present a high-throughput algorithm to

establish a database for these moderate twist angle materials [88]. Combining the two databases, the one established in this work as well as in [88] will provide an even more holistic guide to future experiments on twisted two-dimensional materials and will hone in on the next generation of twist-engineering of correlated, emergent, and topological 2D quantum materials.

D. Simple moiré continuum model

In this section, we discuss a simple moiré continuum model for the M valley of the hexagonal lattice with negligible SOC, following Ref. [67].

The M valley of the hexagonal lattice has three C_3 -related subvalleys, forming a kagome \mathbf{Q} lattice in momentum space as shown in Fig. 1 (b). In valley $\eta = 0$, a simplified moiré Hamiltonian has the form

$$[h_{\mathbf{Q},\mathbf{Q}'}(\mathbf{k})]_{sl;s'l'} = \delta_{\mathbf{Q},\mathbf{Q}'}\delta_{ss'}\delta_{ll'} \left[\frac{(k_x - Q_x)^2}{2m_x} + \frac{(k_y - Q_y)^2}{2m_y} \right] + [T_{\mathbf{Q},\mathbf{Q}'}]_{sl;s'l'}, \quad \text{for } \mathbf{Q}^{(\prime)} \in \mathcal{Q}_{l^{(\prime)}}, \quad (5)$$

where m_x and m_y are two effective masses along the k_x and k_y directions, respectively, and s (l) is the spin (layer) index. The interlayer hopping terms have the form: $[T_{\mathbf{Q},\mathbf{Q}'}^{\text{AA}}]_{ls;(-l)s} = (\pm iw_1^{\text{AA}} + w_2^{\text{AA}})\delta_{\mathbf{Q}\pm\mathbf{q}_0,\mathbf{Q}'} + w_3^{\text{AA}}\delta_{\mathbf{Q}\pm(\mathbf{q}_1-\mathbf{q}_2),\mathbf{Q}'}$ and $[T_{\mathbf{Q},\mathbf{Q}'}^{\text{AB}}]_{ls;(-l)s} = w_2^{\text{AB}}\delta_{\mathbf{Q}\pm\mathbf{q}_0,\mathbf{Q}'} + w_4^{\text{AB}}\delta_{\mathbf{Q}\pm(\mathbf{q}_1-\mathbf{q}_2),\mathbf{Q}'}$. The superscript AA (AB) is for AA (AB) stacked bilayer, which has space group 149 (150) symmetry. Due to the negligible SOC, the model presents spin $\text{SU}(2)$ symmetry. In Ref.[67], we use this simplified M -valley model to fit the moiré bands of SnSe_2 and ZrS_2 , which gives good agreement in both dispersion and wavefunction. One key feature of this simplified M -valley moiré Hamiltonian is the emergence of an effective \tilde{M}_z symmetry, which acts non-symmetrically in momentum space by mapping \mathbf{k} to $\mathbf{k} + \frac{\mathbf{b}_{M_1}}{2}$. This momentum-space non-symmetric \tilde{M}_z symmetry has significant implications, including enforcing perfect nesting at $\mathbf{q}_0 = \frac{\mathbf{b}_{M_1}}{2}$ and making the system effectively 1D [67].

V. EXPERIMENTAL OBSERVATIONS

A key goal of this study was to select new twistable materials for immediate experimental study. Fabrication of moiré devices is most commonly done using exfoliated mono or few-layer materials[89]. As such, we focused on those systems where: 1) structures provided in the databases have bulk crystal analogs; 2) bulk crystals of sufficient size can be grown; 3) bulk crystals feature van der Waals gaps or have other pathways to exfoliation. Among the materials that fulfill all of those criteria, we additionally considered the following factors: a) stability of monolayers to brief air exposure; b) how clean the systems are expected to be in terms of defects, impurities,

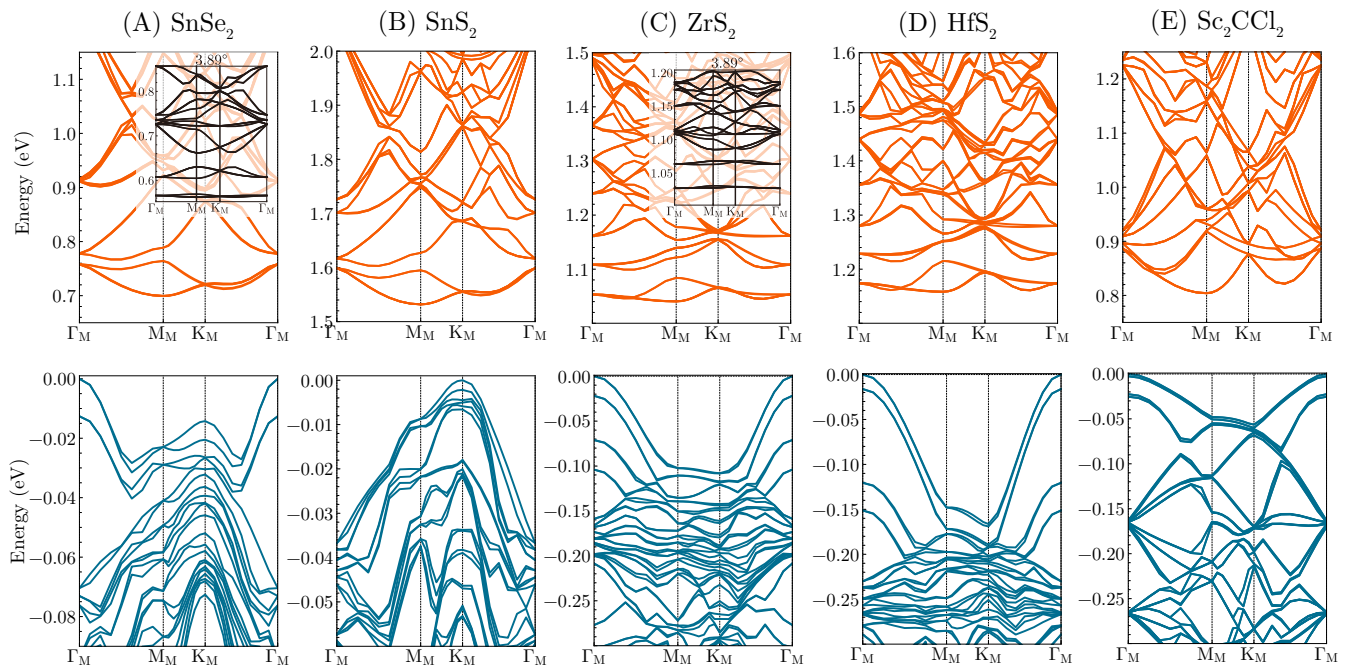


FIG. 4. **Band structures for twisted bilayer materials.** We consider (A) SnSe₂, (B) SnS₂, (C) ZrS₂, (D) HfS₂, and (E) Sc₂CCl₂, all with monolayer symmetry group LG 72 ($p\bar{3}m1$). The top row shows the conduction bands and the bottom row shows the valence bands, all computed at twist angle $\theta = 7.34^\circ$. In the inset of (A) and (C), we show the conduction band of SnSe₂ and ZrS₂ at $\theta = 3.89^\circ$ [67].

or disorder; c) reports of experimental exfoliation down to monolayers.

Generally, we can categorize experimental twistable materials matching our criteria of selection into six general classes:

TABLE IV. **Statistics of experimental twistable materials.** In the table, Ch denotes other chalcogenides than TMD, and Mixed P/C/H denotes mixed pnictides, chalcogenides, and halides.

Class	Element	TMD	Ch	Halide	Mixed P/C/H	Other
Semimetal	4	2	0	0	0	0
Insulator	6	14	24	3	7	6

1. **Elements:** Exfoliation of graphene to monolayers kickstarted the field of 2D electronics [90]. Yet, to this day, we have relatively few experimentally exfoliated elements to create moiré structures with. To the best of our knowledge, only phosphorus has been exfoliated to produce large crystalline flakes. Some studies report other elemental monolayers [91], but those either are produced as nanoscale particles, or are grown epitaxially on substrates [92–94]. Of promise is also elemental bismuth, which was recently obtained as high-quality 2D sheets by crystallization molded by van der Waals materials. Although monolayers have not been obtained so far, transport devices have been

made with few-layer bismuth grown in this fashion [95].

2. **TMDs:** TMDs have had an overwhelming influence on moiré research. Despite this, only a small subset of transition metals has been used to produce twisted moiré systems experimentally, or even theoretically. Materials including SnS₂¹, HfS₂, ZrS₂, and their selenium analogs, have all been exfoliated down to monolayers [96], however no twistrionic devices with them are reported to date. What makes them even more interesting is that they are all hexagonal M -valley systems, distinct from the well-studied moiré TMDs, which primarily involve the K valley. This distinction leads to significantly different physics [67].
3. **Other chalcogenides:** Chalcogenides are particularly likely to create van der Waals layered materials due to the chalcogen atoms' lone pairs. It is not surprising then that many candidate twistable materials belong to this class. Some standout materials here include group IIIA monochalcogenides,

¹ Note that, while Sn is not a transition metal, SnSe₂ and SnS₂ are metal dichalcogenides that adopt the same structure as traditional TMDs. For this reason, we categorize them within the TMD class.

such as GaSe. These are well established as exfoliable van der Waals systems [97], however few studies considered using them in heterostructure or twistrionic devices. Group IVB trichalcogenides such as ZrSe_3 and TiS_3 are another promising family here, representing well-established exfoliable systems [98, 99]. Lastly, tetradymite-type and related chalcogenides of antimony, bismuth, and group IVA metals comprise the last important family of twistable experimental chalcogenides. The materials, such as Bi_2Te_3 , are well known in the world of thermoelectrics and topological insulators [100]; optimized growth conditions have been established for a variety of compositions [101].

4. **Halides:** Similar to chalcogenides, van der Waals halides are fairly common. Not all of them, however, are stable to air or moisture, complicating exfoliation in some cases. The most promising systems according to our methodology are: PbI_2 , which has a 2H structure similar to many TMDs, and can be exfoliated mechanically [102]; BiI_3 , which has been exfoliated to yield small, but few-layer or even monolayer, flakes [103]; or, alternatively, can be grown on SiO_2/Si substrates to produce nanoplates with large lateral areas [104]; and CdI_2 , which can also be grown as nanoplates on substrates [105], but has no reports of experimental exfoliation to the best of our knowledge. Twisted magnetic CrI_3 has also been studied extensively [106–110], but it is not included in the current work as we do not consider magnetic orderings.
5. **Mixed pnictides, chalcogenides, and halides:** Both chalcogenides and halides are especially suitable to produce exfoliable materials; it is therefore unsurprising that combinations of halide and chalcogenide ions, or either of those with pnictides, also can produce materials good for exfoliation. Some key examples of materials in this class include ZrNCl , which has been exfoliated to monolayers [111], and is reported to be a superconductor when gated [112]; and bismuth chalcogenides such as BiTeI [113], which likewise form stable monolayers, so far unexplored in moiré research. Thiophosphates such as AgInP_2S_6 [114] have also recently been exfoliated experimentally, and can potentially produce clean twistable systems.
6. **Other materials:** Most experimental twistable materials fit into the five classes listed above. GeH is one of such unique candidates. Although bulk exfoliable crystals cannot be obtained directly, few- and monolayer samples can be obtained through topochemical reactions of CaGe_2 [115]. Its silicon analog has also been made, but is however less pure, with terminal hydrogens partially replaced by hydroxyl groups [116]. Several oxides also show

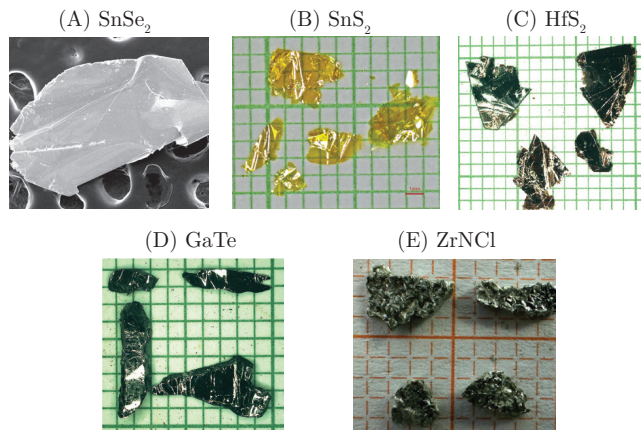


FIG. 5. **Samples of twistable materials.** (A) SnSe_2 , (B) SnS_2 , (C) HfS_2 (D) GaTe , and (E) ZrNCl .

promise for twisting theoretically, although experimental work may be somewhat challenging: TiO_2 and the MXene Ti_2CO_2 have been obtained as nanosheets, but only of small area [117, 118]. No large monolayers have been reported so far; both of these materials do not have exfoliable bulk crystals, and thus, similar to GeH , rely on wet chemistry to produce flakes, complicating the synthesis. Lastly, one of the highest twist scores for experimentally obtained materials we found in 2D-GaN. This phase of GaN was recently obtained by encapsulation between sheets of graphene [119]. Although currently, experimental twisting of this system would not appear possible, this could become an interesting material in the future, if synthetic strategies affording freestanding monolayers can be devised.

Among the experimentally twistable materials, we have successfully synthesized several of the most promising ones in bulk form, including TMDs SnSe_2 , SnS_2 , and HfS_2 , chalcogenide GaTe [120], and pnicto-halide ZrNCl , with images of the samples shown in Fig. 5. A more detailed description of the growth procedures is provided in Appendix [II 3]. These twistable materials can be exfoliated into monolayers, as our initial sample preparation has confirmed. They exhibit ideal band structures for theoretical modeling. As we found a huge phase-space for experimental-theory twistable materials, more detailed theoretical and experimental investigations of each of these materials separately will be presented in future works.

VI. DISCUSSION

In this study, we introduce a high-throughput algorithm to systematically explore twistable 2D materials, incorporating both theoretical and experimental aspects.

We identify 61 candidates as twistable semimetals and 1568 as twistable insulators, with electronic structures well-suited for moiré engineering. These materials are classified by their Bravais lattices, valley types, and SOC strengths, offering a diverse set of platforms for investigating novel topological and correlated phenomena in 2D moiré systems. Complete data on the twisting properties are accessible through the 2D-TQCDB, establishing a valuable foundation for both experimental investigations and theoretical predictions. This work advances the rapidly evolving field of moiré materials and their potential applications.

ACKNOWLEDGMENTS

Funding: Y.J. and H.H. were supported by the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation program (Grant Agreement No. 101020833), as well as by the IKUR Strategy under the collaboration agreement between Ikerbasque Foundation and DIPC on behalf of the Department of Education of the Basque Government. U.P. acknowledges funding from the European Union’s Next Generation EU plan through the María Zambrano Programme. U.P. and L.E. were supported by the Government of the Basque Country (Project No. IT1458-22). G.S. was supported by the Arnold and Mabel Beckman Foundation via an AOB postdoctoral fellowship (dx.doi.org/10.13039/100000997). D.C. acknowledges support from the DOE Grant No. DESC0016239 and the hospitality of the Donostia International Physics Center, at which this work was carried out. M.G.V and H.P. were supported by the Ministry for Digital Transformation and of Civil Service of the Spanish Government through the QUANTUM ENIA project call - Quantum Spain project, and by the European Union through the Recovery, Transformation and Resilience Plan - NextGenerationEU within the framework of the Digital Spain 2026 Agenda. M.G.V. thanks support to the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) GA 3314/1-1 – FOR 5249 (QUAST), the Spanish Ministerio de Ciencia e Innovación (PID2022-142008NB-I00) and the Canada Excellence Research Chairs Program for Topological Quantum Matter. L.M.S. was supported by the Gordon and Betty Moore Foundation’s EPIQS initiative through Grants GBMF9064, the David and Lucille Packard foundation, and NSF MRSEC through the Princeton Center for Complex Materials, DMR-2011750. D.K.E. acknowledges funding from the European Research Council (ERC) under the European Union’s Horizon 2020

research and innovation program (grant agreement No. 852927), the German Research Foundation (DFG) under the priority program SPP2244 (project No. 535146365), the EU EIC Pathfinder Grant “FLATS” (grant agreement No. 101099139) and the Keele Foundation. R.A.M. and E.M. and acknowledge support from the Robert A. Welch Foundation Grant C-2114 and the Department of Defense, Air Force Office of Scientific Research under Grant No. FA9550-21-1-0343. D.M.K. acknowledges support by the DFG via the Priority Program SPP 2244 “2DMP” — 443274199. L.X. and Q.X. acknowledge support by the Max Planck Partner group programme and Hangzhou Tsientang Education Foundation. A.R. acknowledges the support from the Max Planck-New York City Center for Non-Equilibrium Quantum Phenomena, the Cluster of Excellence ’CUI: Advanced Imaging of Matter’-EXC 2056 - project ID 390715994, SFB-925 "Light induced dynamics and control of correlated quantum systems" – project 170620586 of the Deutsche Forschungsgemeinschaft (DFG) and Grupos Consolidados (IT1453-22). The Flatiron Institute is a division of the Simons Foundation. B.A.B. was supported by the Gordon and Betty Moore Foundation through Grant No. GBMF8685 towards the Princeton theory program, the Gordon and Betty Moore Foundation’s EPIQS Initiative (Grant No. GBMF11070), the Office of Naval Research (ONR Grant No. N00014-20-1-2303), the Global Collaborative Network Grant at Princeton University, the Simons Investigator Grant No. 404513, the BSF Israel US foundation No. 2018226, the NSF-MERSEC (Grant No. MERSEC DMR 2011750), the Simons Collaboration on New Frontiers in Superconductivity, and the Schmidt Foundation at the Princeton University.

Author contributions: B.A.B. conceived of the study. Y.J., U.P., D.C., and H.H. developed the code and performed the high-throughput calculations. J.X., R.A.M., P.H., V.H., E.M., C.F., and L.M.S. synthesized the samples. N.R. built the Topological 2D materials Database with input data from U.P. and Y.J.. Q.X., M.C., D.M.K., A.R. and L.X. performed calculations and provided DFT results for moderate twist angles. Y.J., G.S., H.P., and B.A.B. wrote the original draft and supplementary materials. All authors contributed to the review and editing of the final draft.

Competing interests: The authors declare that they have no competing interests.

Data and materials availability: All data are available in the supplementary materials, through our public website Topological 2D Materials Database. Additional data, along with any code required for reproducing the figures, are available from the authors upon reasonable request.

[1] S. Carr, D. Massatt, S. Fang, P. Cazeaux, M. Luskin, and E. Kaxiras, *Physical Review B* **95**, 075420 (2017).

[2] E. Y. Andrei, D. K. Efetov, P. Jarillo-Herrero, A. H. MacDonald, K. F. Mak, T. Senthil, E. Tutuc, A. Yaz-

- dani, and A. F. Young, *Nat Rev Mater* **6**, 201 (2021).
- [3] D. M. Kennes, M. Claassen, L. Xian, A. Georges, A. J. Millis, J. Hone, C. R. Dean, D. N. Basov, A. N. Pasupathy, and A. Rubio, *Nat. Phys.* **17**, 155 (2021).
- [4] K. F. Mak and J. Shan, *Nature Nanotechnology* **17**, 686 (2022).
- [5] Y. Cao, V. Fatemi, A. Demir, S. Fang, S. L. Tomarken, J. Y. Luo, J. D. Sanchez-Yamagishi, K. Watanabe, T. Taniguchi, E. Kaxiras, R. C. Ashoori, and P. Jarillo-Herrero, *Nature* **556**, 80 (2018).
- [6] Y. Cao, V. Fatemi, S. Fang, K. Watanabe, T. Taniguchi, E. Kaxiras, and P. Jarillo-Herrero, *Nature* **556**, 43 (2018).
- [7] N. Regnault and B. A. Bernevig, *Physical Review X* **1**, 021014 (2011).
- [8] T. Neupert, L. Santos, C. Chamon, and C. Mudry, *Phys. Rev. Lett.* **106**, 236804 (2011).
- [9] D. N. Sheng, Z.-C. Gu, K. Sun, and L. Sheng, *Nature Communications* **2**, 389 (2011), arXiv:1102.2658 [cond-mat.str-el].
- [10] R. Bistritzer and A. H. MacDonald, *PNAS* **108**, 12233 (2011).
- [11] A. L. Sharpe, E. J. Fox, A. W. Barnard, J. Finney, K. Watanabe, T. Taniguchi, M. A. Kastner, and D. Goldhaber-Gordon, *Science* **365**, 605 (2019).
- [12] M. Serlin, C. L. Tschirhart, H. Polshyn, Y. Zhang, J. Zhu, K. Watanabe, T. Taniguchi, L. Balents, and A. F. Young, *Science* **367**, 900 (2020).
- [13] G. Chen, A. L. Sharpe, E. J. Fox, Y.-H. Zhang, S. Wang, L. Jiang, B. Lyu, H. Li, K. Watanabe, T. Taniguchi, Z. Shi, T. Senthil, D. Goldhaber-Gordon, Y. Zhang, and F. Wang, *Nature* **579**, 56 (2020).
- [14] Z.-D. Song and B. A. Bernevig, *Phys. Rev. Lett.* **129**, 047601 (2022).
- [15] A. Kerelsky, L. J. McGilly, D. M. Kennes, L. Xian, M. Yankowitz, S. Chen, K. Watanabe, T. Taniguchi, J. Hone, C. Dean, A. Rubio, and A. N. Pasupathy, *Nature* **572**, 95 (2019).
- [16] F. Wu, E. Hwang, and S. Das Sarma, *Physical Review B* **99**, 165112 (2019).
- [17] F. Wu and S. Das Sarma, *Phys. Rev. Lett.* **124**, 046403 (2020).
- [18] Y.-Z. Chou and S. Das Sarma, *Physical Review Letters* **131**, 026501 (2023).
- [19] Y. Saito, F. Yang, J. Ge, X. Liu, T. Taniguchi, K. Watanabe, J. I. A. Li, E. Berg, and A. F. Young, *Nature* **592**, 220 (2021).
- [20] Z. Lu, T. Han, Y. Yao, A. P. Reddy, J. Yang, J. Seo, K. Watanabe, T. Taniguchi, L. Fu, and L. Ju, *Nature* **626**, 759 (2024).
- [21] Z. Dong, A. S. Patri, and T. Senthil, arXiv:2311.03445 [cond-mat] 10.48550/arXiv.2311.03445 (2024), arXiv:2311.03445 [cond-mat].
- [22] J. Dong, T. Wang, T. Wang, T. Soejima, M. P. Zaletel, A. Vishwanath, and D. E. Parker, arXiv:2311.05568 [cond-mat] (2023), arXiv:2311.05568 [cond-mat].
- [23] J. Herzog-Arbeitman, Y. Wang, J. Liu, P. M. Tam, Z. Qi, Y. Jia, D. K. Efetov, O. Vafek, N. Regnault, H. Weng, Q. Wu, B. A. Bernevig, and J. Yu, *Phys. Rev. B* **109**, 205122 (2024).
- [24] M. Huang, Z. Wu, X. Zhang, X. Feng, Z. Zhou, S. Wang, Y. Chen, C. Cheng, K. Sun, Z. Y. Meng, *et al.*, *Physical Review Letters* **131**, 066301 (2023).
- [25] T. Zhang, N. Regnault, B. A. Bernevig, X. Dai, and H. Weng, *Phys. Rev. B* **105**, 125127 (2022).
- [26] Z. Song, Z. Wang, W. Shi, G. Li, C. Fang, and B. A. Bernevig, *Phys. Rev. Lett.* **123**, 036401 (2019).
- [27] Z. Zhu, S. Carr, D. Massatt, M. Luskin, and E. Kaxiras, *Physical review letters* **125**, 116404 (2020).
- [28] H. Yoo, R. Engelke, S. Carr, S. Fang, K. Zhang, P. Cazeaux, S. H. Sung, R. Hovden, A. W. Tsien, T. Taniguchi, *et al.*, *Nature materials* **18**, 448 (2019).
- [29] G. Tarnopolsky, A. J. Kruchkov, and A. Vishwanath, *Phys. Rev. Lett.* **122**, 106405 (2019).
- [30] F. Haddadi, Q. Wu, A. J. Kruchkov, and O. V. Yazyev, *Nano Lett.* **20**, 2410 (2020).
- [31] F. Wu, T. Lovorn, E. Tutuc, and A. H. MacDonald, *Phys. Rev. Lett.* **121**, 026402 (2018).
- [32] Y. Tang, L. Li, T. Li, Y. Xu, S. Liu, K. Barmak, K. Watanabe, T. Taniguchi, A. H. MacDonald, J. Shan, and K. F. Mak, *Nature* **579**, 353 (2020).
- [33] P. Wang, G. Yu, Y. H. Kwan, Y. Jia, S. Lei, S. Klemenzenz, F. A. Cevallos, R. Singha, T. Devakul, K. Watanabe, T. Taniguchi, S. L. Sondhi, R. J. Cava, L. M. Schoop, S. A. Parameswaran, and S. Wu, *Nature* **605**, 57 (2022).
- [34] T. Li, S. Jiang, B. Shen, Y. Zhang, L. Li, Z. Tao, T. Devakul, K. Watanabe, T. Taniguchi, L. Fu, J. Shan, and K. F. Mak, *Nature* **600**, 641 (2021).
- [35] F. Xu, Z. Sun, T. Jia, C. Liu, C. Xu, C. Li, Y. Gu, K. Watanabe, T. Taniguchi, B. Tong, J. Jia, Z. Shi, S. Jiang, Y. Zhang, X. Liu, and T. Li, *Phys. Rev. X* **13**, 031037 (2023).
- [36] H. Park, J. Cai, E. Anderson, Y. Zhang, J. Zhu, X. Liu, C. Wang, W. Holtzmann, C. Hu, Z. Liu, T. Taniguchi, K. Watanabe, J.-H. Chu, T. Cao, L. Fu, W. Yao, C.-Z. Chang, D. Cobden, D. Xiao, and X. Xu, *Nature* **622**, 74 (2023).
- [37] Y. Zeng, Z. Xia, K. Kang, J. Zhu, P. Knüppel, C. Vaswani, K. Watanabe, T. Taniguchi, K. F. Mak, and J. Shan, *Nature* **622**, 69 (2023).
- [38] J. Cai, E. Anderson, C. Wang, X. Zhang, X. Liu, W. Holtzmann, Y. Zhang, F. Fan, T. Taniguchi, K. Watanabe, Y. Ran, T. Cao, L. Fu, D. Xiao, W. Yao, and X. Xu, *Nature* **622**, 63 (2023).
- [39] C. Wang, X.-W. Zhang, X. Liu, Y. He, X. Xu, Y. Ran, T. Cao, and D. Xiao, *Phys. Rev. Lett.* **132**, 036501 (2024).
- [40] Y. Jia, J. Yu, J. Liu, J. Herzog-Arbeitman, Z. Qi, H. Pi, N. Regnault, H. Weng, B. A. Bernevig, and Q. Wu, *Phys. Rev. B* **109**, 205121 (2024).
- [41] J. Yu, J. Herzog-Arbeitman, M. Wang, O. Vafek, B. A. Bernevig, and N. Regnault, *Phys. Rev. B* **109**, 045147 (2024).
- [42] Y. Xia, Z. Han, K. Watanabe, T. Taniguchi, J. Shan, and K. F. Mak, *Nature*, 1 (2024).
- [43] Y. Guo, J. Pack, J. Swann, L. Holtzman, M. Cothrine, K. Watanabe, T. Taniguchi, D. Mandrus, K. Barmak, J. Hone, *et al.*, arXiv preprint arXiv:2406.03418 (2024).
- [44] T. Devakul, V. Crépel, Y. Zhang, and L. Fu, *Nat Commun* **12**, 6730 (2021).
- [45] F. Wu, T. Lovorn, E. Tutuc, I. Martin, and A. H. MacDonald, *Phys. Rev. Lett.* **122**, 086402 (2019).
- [46] M. Claassen, L. Xian, D. M. Kennes, and A. Rubio, *Nat Commun* **13**, 4915 (2022).
- [47] M. Angeli and A. H. MacDonald, *Proceedings of the National Academy of Sciences* **118**, e2021826118 (2021).

- [48] H. Li, Y. Su, Y. B. Kim, H.-Y. Kee, K. Sun, and S.-Z. Lin, *Physical Review B* **109**, 245131 (2024).
- [49] B. A. Foutty, C. R. Kometter, T. Devakul, A. P. Reddy, K. Watanabe, T. Taniguchi, L. Fu, and B. E. Feldman, *Science* **384**, 343 (2024).
- [50] D. Sheng, A. P. Reddy, A. Abouelkomsan, E. J. Bergholtz, and L. Fu, *Physical Review Letters* **133**, 066601 (2024).
- [51] D. Halbertal, N. R. Finney, S. S. Sunku, A. Kerelsky, C. Rubio-Verdú, S. Shabani, L. Xian, S. Carr, S. Chen, C. Zhang, *et al.*, *Nature communications* **12**, 242 (2021).
- [52] X.-W. Zhang, C. Wang, X. Liu, Y. Fan, T. Cao, and D. Xiao, *Nature Communications* **15**, 4223 (2024).
- [53] L. Wang, E.-M. Shih, A. Ghiotto, L. Xian, D. A. Rhodes, C. Tan, M. Claassen, D. M. Kennes, Y. Bai, B. Kim, *et al.*, *Nature materials* **19**, 861 (2020).
- [54] E. Anderson, F.-R. Fan, J. Cai, W. Holtzmann, T. Taniguchi, K. Watanabe, D. Xiao, W. Yao, and X. Xu, *Science* **381**, 325 (2023).
- [55] T. Song, Q.-C. Sun, E. Anderson, C. Wang, J. Qian, T. Taniguchi, K. Watanabe, M. A. McGuire, R. Stöhr, D. Xiao, *et al.*, *Science* **374**, 1140 (2021).
- [56] D. M. Kennes, L. Xian, M. Claassen, and A. Rubio, *Nat Commun* **11**, 1124 (2020).
- [57] L. Klebl, Q. Xu, A. Fischer, L. Xian, M. Claassen, A. Rubio, and D. M. Kennes, *Electronic Structure* **4**, 014004 (2022).
- [58] L. Xian, M. Claassen, D. Kiese, M. M. Scherer, S. Trebst, D. M. Kennes, and A. Rubio, *Nature communications* **12**, 5644 (2021).
- [59] Q. Xu, N. Tancogne-Dejean, E. V. Boström, D. M. Kennes, M. Claassen, A. Rubio, and L. Xian, arXiv preprint arXiv:2406.05626 (2024).
- [60] V. Crépel and J. Cano, arXiv preprint arXiv:2406.17843 (2024).
- [61] Y. Ye, J. Qian, X.-W. Zhang, C. Wang, D. Xiao, and T. Cao, *Nano Letters* **23**, 6536 (2023).
- [62] Q. Xu, Y. Guo, and L. Xian, *2D Materials* **9**, 014005 (2021).
- [63] U. Petralanda, Y. Jiang, B. A. Bernevig, N. Regnault, and L. Elcoro, Submitted (2024).
- [64] M. I. Aroyo, J. M. Perez-Mato, D. Orobengoa, E. Tasci, G. de la Flor, and A. Kirov, *Bulg. Chem. Commun* **43**, 183 (2011).
- [65] M. I. Aroyo, J. M. Perez-Mato, C. Capillas, E. Kroumova, S. Ivantchev, G. Madariaga, A. Kirov, and H. Wondratschek, *Zeitschrift für Kristallographie-Crystalline Materials* **221**, 15 (2006).
- [66] M. I. Aroyo, A. Kirov, C. Capillas, J. Perez-Mato, and H. Wondratschek, *Acta Crystallographica Section A: Foundations of Crystallography* **62**, 115 (2006).
- [67] D. Călugăru, Y. Jiang, H. Hu, H. Pi, M. G. Vergniory, J. Shan, C. Felser, L. M. Schoop, D. K. Efetov, K. F. Mak, and B. A. Bernevig, Submitted (2024).
- [68] X. Yin, Q. Wang, L. Cao, C. S. Tang, X. Luo, Y. Zheng, L. M. Wong, S. J. Wang, S. Y. Quek, W. Zhang, *et al.*, *Nature communications* **8**, 486 (2017).
- [69] S. Wu, V. Fatemi, Q. D. Gibson, K. Watanabe, T. Taniguchi, R. J. Cava, and P. Jarillo-Herrero, *Science* **359**, 76 (2018).
- [70] Z. He and H. Weng, *npj Quantum Materials* **6**, 101 (2021).
- [71] Y. Zhang, K. Kamiya, T. Yamamoto, M. Sakano, X. Yang, S. Masubuchi, S. Okazaki, K. Shinokita, T. Chen, K. Aso, *et al.*, *Nano Letters* **23**, 9280 (2023).
- [72] F. Yuan, Y. Jia, G. Cheng, R. Singha, S. Lei, N. Yao, S. Wu, and L. M. Schoop, *Nano Letters* **23**, 6868 (2023).
- [73] C. Backes, N. C. Berner, X. Chen, P. Lafargue, P. LaPlace, M. Freeley, G. S. Duesberg, J. N. Coleman, and A. R. McDonald, *Angewandte Chemie International Edition* **54**, 2638 (2015).
- [74] X. Song, B. Hoff, R. Singha, J. W. Stiles, G. Skorupskii, J. F. Khoury, G. Cheng, F. Kamm, A. J. Uzan, S. Dulovic, *et al.*, *Chemistry of Materials* **35**, 5487 (2023).
- [75] S. Yamanaka, K.-i. Hotehama, and H. Kawaji, *Nature* **392**, 580 (1998).
- [76] Y. Taguchi, A. Kitora, and Y. Iwasa, *Physical review letters* **97**, 107001 (2006).
- [77] Y. Kasahara, K. Kuroki, S. Yamanaka, and Y. Taguchi, *Physica C: Superconductivity and its Applications* **514**, 354 (2015).
- [78] T. Kariyado and A. Vishwanath, *Physical Review Research* **1**, 033076 (2019).
- [79] P. M. Eugenio, Z.-X. Luo, A. Vishwanath, and P. A. Volkov, arXiv preprint arXiv:2406.02448 (2024).
- [80] N. Mounet, M. Gibertini, P. Schwaller, D. Campi, A. Merkys, A. Marrazzo, T. Sohler, I. E. Castelli, A. Cepellotti, G. Pizzi, *et al.*, *Nature nanotechnology* **13**, 246 (2018).
- [81] D. Campi, N. Mounet, M. Gibertini, G. Pizzi, and N. Marzari, *ACS nano* **17**, 11268 (2023).
- [82] J. G. Bednorz and K. A. Müller, *Zeitschrift für Physik B Condensed Matter* **64**, 189 (1986).
- [83] J. Orenstein and A. Millis, *Science* **288**, 468 (2000).
- [84] A. Damascelli, Z. Hussain, and Z.-X. Shen, *Reviews of modern physics* **75**, 473 (2003).
- [85] P. Wang, G. Yu, Y. H. Kwan, Y. Jia, S. Lei, S. Klemenzt, F. A. Cevallos, R. Singha, T. Devakul, K. Watanabe, *et al.*, *Nature* **605**, 57 (2022).
- [86] G. Yu, P. Wang, A. J. Uzan-Narovlansky, Y. Jia, M. Onyszczak, R. Singha, X. Gui, T. Song, Y. Tang, K. Watanabe, *et al.*, *Nature communications* **14**, 7025 (2023).
- [87] D. M. Kennes, L. Xian, M. Claassen, and A. Rubio, *Nature communications* **11**, 1124 (2020).
- [88] X. Qiaoling *et al.*, in preparation. (2025).
- [89] Y. Huang, Y.-H. Pan, R. Yang, L.-H. Bao, L. Meng, H.-L. Luo, Y.-Q. Cai, G.-D. Liu, W.-J. Zhao, Z. Zhou, *et al.*, *Nature communications* **11**, 2453 (2020).
- [90] A. K. Geim and K. S. Novoselov, *Nature Mater* **6**, 183 (2007), publisher: Nature Publishing Group.
- [91] J. Shah, W. Wang, H. M. Sohail, and R. Uhrberg, *2D Materials* **7**, 025013 (2020).
- [92] N. Hussain, T. Liang, Q. Zhang, T. Anwar, Y. Huang, J. Lang, K. Huang, and H. Wu, *Small* **13**, 1701349 (2017).
- [93] Q.-Q. Yang, R.-T. Liu, C. Huang, Y.-F. Huang, L.-F. Gao, B. Sun, Z.-P. Huang, L. Zhang, C.-X. Hu, Z.-Q. Zhang, *et al.*, *Nanoscale* **10**, 21106 (2018).
- [94] Z. Lu, D. Yu, Y. Hong, G. Ma, F. Ru, T. Ge, G. Xi, L. Qin, M. Adilov, R. Ashurov, *et al.*, *Materials Today* (2024).
- [95] L. Chen, A. X. Wu, N. Tulu, J. Wang, A. Juanson, K. Watanabe, T. Taniguchi, M. T. Pettes, M. A. Campbell, M. Xu, C. A. Gadre, Y. Zhou, H. Chen, P. Cao, L. A. Jauregui, R. Wu, X. Pan, and J. D. Sanchez-Yamagishi, *Nat. Mater.* **23**, 741 (2024), publisher: Na-

- ture Publishing Group.
- [96] Y. Huang, Y.-H. Pan, R. Yang, L.-H. Bao, L. Meng, H.-L. Luo, Y.-Q. Cai, G.-D. Liu, W.-J. Zhao, Z. Zhou, L.-M. Wu, Z.-L. Zhu, M. Huang, L.-W. Liu, L. Liu, P. Cheng, K.-H. Wu, S.-B. Tian, C.-Z. Gu, Y.-G. Shi, Y.-F. Guo, Z. G. Cheng, J.-P. Hu, L. Zhao, G.-H. Yang, E. Sutter, P. Sutter, Y.-L. Wang, W. Ji, X.-J. Zhou, and H.-J. Gao, *Nat Commun* **11**, 2453 (2020), publisher: Nature Publishing Group.
- [97] D. Hlushchenko, A. Siudzinska, J. Cybinska, M. Guzik, A. Bachmatiuk, and R. Kudrawiec, *Sci Rep* **13**, 19114 (2023), publisher: Nature Publishing Group.
- [98] A. Lipatov, M. J. Loes, H. Lu, J. Dai, P. Patoka, N. S. Vorobeva, D. S. Muratov, G. Ulrich, B. Kästner, A. Hoehl, G. Ulm, X. C. Zeng, E. Rühl, A. Gruverman, P. A. Dowben, and A. Sinitiskii, *ACS Nano* **12**, 12713 (2018), publisher: American Chemical Society.
- [99] Y. Xu, S. Guo, and X. Chen, *Micromachines* **13**, 1994 (2022), number: 11 Publisher: Multidisciplinary Digital Publishing Institute.
- [100] J. P. Heremans, R. J. Cava, and N. Samarth, *Nat Rev Mater* **2**, 1 (2017), publisher: Nature Publishing Group.
- [101] D. Teweldebrhan and A. A. Balandin, *ECS Trans.* **33**, 103 (2010).
- [102] P. Wangyang, H. Sun, X. Zhu, D. Yang, and X. Gao, *Materials Letters* **168**, 68 (2016).
- [103] H. Wang, T. Song, X. Su, Z. Li, and J. Wang, *ACS Sustainable Chem. Eng.* **8**, 1262 (2020), publisher: American Chemical Society.
- [104] J. Li, X. Guan, C. Wang, H.-C. Cheng, R. Ai, K. Yao, P. Chen, Z. Zhang, X. Duan, and X. Duan, *Small* **13**, 1701034 (2017).
- [105] R. Ai, X. Guan, J. Li, K. Yao, P. Chen, Z. Zhang, X. Duan, and X. Duan, *ACS Nano* **11**, 3413 (2017), publisher: American Chemical Society.
- [106] B. Huang, G. Clark, E. Navarro-Moratalla, D. R. Klein, R. Cheng, K. L. Seyler, D. Zhong, E. Schmidgall, M. A. McGuire, D. H. Cobden, *et al.*, *Nature* **546**, 270 (2017).
- [107] Y. Xu, A. Ray, Y.-T. Shao, S. Jiang, K. Lee, D. Weber, J. E. Goldberger, K. Watanabe, T. Taniguchi, D. A. Muller, *et al.*, *Nature Nanotechnology* **17**, 143 (2022).
- [108] M. Akram, H. LaBollita, D. Dey, J. Kapeghian, O. Erten, and A. S. Botana, *Nano Letters* **21**, 6633 (2021).
- [109] H. Xie, X. Luo, G. Ye, Z. Ye, H. Ge, S. H. Sung, E. Rennie, S. Yan, Y. Fu, S. Tian, *et al.*, *Nature Physics* **18**, 30 (2022).
- [110] C. Wang, Y. Gao, H. Lv, X. Xu, and D. Xiao, *Physical Review Letters* **125**, 247201 (2020).
- [111] H. Nong, Q. Wu, J. Tan, Y. Sun, R. Zheng, R. Zhang, S. Zhao, and B. Liu, *Small* **18**, 2107490 (2022).
- [112] Y. Saito, Y. Kasahara, J. Ye, Y. Iwasa, and T. Nojima, *Science* **350**, 409 (2015), publisher: American Association for the Advancement of Science.
- [113] B. Fülöp, Z. Tajkov, J. Pető, P. Kun, J. Koltai, L. Oroszlány, E. Tóvári, H. Murakawa, Y. Tokura, S. Bordács, L. Tapasztó, and S. Csonka, *2D Mater.* **5**, 031013 (2018), publisher: IOP Publishing.
- [114] W. Gao, S. Li, H. He, X. Li, Z. Cheng, Y. Yang, J. Wang, Q. Shen, X. Wang, Y. Xiong, Y. Zhou, and Z. Zou, *Nat Commun* **12**, 4747 (2021), publisher: Nature Publishing Group.
- [115] E. Bianco, S. Butler, S. Jiang, O. D. Restrepo, W. Windl, and J. E. Goldberger, *ACS Nano* **7**, 4414 (2013), publisher: American Chemical Society.
- [116] B. J. Ryan, M. P. Hanrahan, Y. Wang, U. Ramesh, C. K. A. Nyamekye, R. D. Nelson, Z. Liu, C. Huang, B. Whitehead, J. Wang, L. T. Roling, E. A. Smith, A. J. Rossini, and M. G. Panthani, *Chem. Mater.* **32**, 795 (2020), publisher: American Chemical Society.
- [117] Z. Sun, T. Liao, Y. Dou, S. M. Hwang, M.-S. Park, L. Jiang, J. H. Kim, and S. X. Dou, *Nat Commun* **5**, 3813 (2014), publisher: Nature Publishing Group.
- [118] S. A. Melchior, K. Raju, I. S. Ike, R. M. Erasmus, G. Kabongo, I. Sigalas, S. E. Iyuke, and K. I. Ozoemena, *J. Electrochem. Soc.* **165**, A501 (2018), publisher: IOP Publishing.
- [119] Z. Y. Al Balushi, K. Wang, R. K. Ghosh, R. A. Vilá, S. M. Eichfeld, J. D. Caldwell, X. Qin, Y.-C. Lin, P. A. DeSario, G. Stone, S. Subramanian, D. F. Paul, R. M. Wallace, S. Datta, J. M. Redwing, and J. A. Robinson, *Nature Mater* **15**, 1166 (2016), publisher: Nature Publishing Group.
- [120] M. Jacobsen, Y. Meng, R. Kumar, and A. Cornelius, *Journal of Physics and Chemistry of Solids* **74**, 723 (2013).
- [121] B. Bradlyn, J. Cano, Z. Wang, M. Vergniory, C. Felser, R. J. Cava, and B. A. Bernevig, *Science* **353**, aaf5037 (2016).
- [122] Y. Jiang, Z. Fang, and C. Fang, *Chinese Physics Letters* **38**, 077104 (2021).
- [123] F. Tang and X. Wan, *Physical Review B* **104**, 085137 (2021).
- [124] G. Zhan, M. Shi, Z. Yang, and H. Zhang, *Chinese Physics Letters* **38**, 077105 (2021).
- [125] Z.-M. Yu, Z. Zhang, G.-B. Liu, W. Wu, X.-P. Li, R.-W. Zhang, S. A. Yang, and Y. Yao, *Science Bulletin* **67**, 375 (2022).
- [126] Z. Zhang, Z.-M. Yu, G.-B. Liu, Z. Li, S. A. Yang, and Y. Yao, *Computer Physics Communications* **290**, 108784 (2023).
- [127] S. Zhang, H. Sheng, Z.-D. Song, C. Liang, Y. Jiang, S. Sun, Q. Wu, H. Weng, Z. Fang, X. Dai, *et al.*, *Chinese Physics Letters* **40**, 127101 (2023).
- [128] C. Fang, H. Weng, X. Dai, and Z. Fang, *Chinese Physics B* **25**, 117106 (2016).
- [129] R. Yu, Z. Fang, X. Dai, and H. Weng, *Frontiers of Physics* **12**, 1 (2017).
- [130] J. Ahn, D. Kim, Y. Kim, and B.-J. Yang, *Physical review letters* **121**, 106403 (2018).
- [131] Z. Song, T. Zhang, and C. Fang, *Physical Review X* **8**, 031069 (2018).
- [132] L. A. Burton, D. Colombara, R. D. Abellon, F. C. Grozema, L. M. Peter, T. J. Savenije, G. Dennler, and A. Walsh, *Chemistry of Materials* **25**, 4908 (2013).
- [133] M. Ohashi, S. Yamanaka, M. Sumihara, and M. Hattori, *Journal of Solid State Chemistry* **75**, 99 (1988).
- [134] T. Bredow and M. Lerch, *Zeitschrift für anorganische und allgemeine Chemie* **633**, 2598 (2007).
- [135] J. Böhm, *Zeitschrift für anorganische und allgemeine Chemie* **149**, 217 (1925).
- [136] G. Kresse and J. Furthmüller, *Phys. Rev. B* **54**, 11169 (1996).
- [137] P. E. Blöchl, *Phys. Rev. B* **50**, 17953 (1994).
- [138] A. Tkatchenko and M. Scheffler, *Phys. Rev. Lett.* **102**, 073005 (2009).
- [139] O. Anatole von Lilienfeld and A. Tkatchenko, *J. Chem. Phys.* **132**, 234109 (2010).

- [140] B. Bradlyn, L. Elcoro, J. Cano, M. G. Vergniory, Z. Wang, C. Felser, M. I. Aroyo, and B. A. Bernevig, *Nature* **547**, 298 (2017).

Supplementary Information for ” 2D Theoretically Twistable Material Database“

CONTENTS

I. Introduction	1
II. Classification of twistable materials	2
III. High-throughput algorithm	3
IV. Results	5
A. Representative Twistable Semimetals	5
B. Representative Twistable Insulators	7
C. Band structures for twisted bilayer materials	8
D. Simple moiré continuum model	8
V. Experimental observations	8
VI. Discussion	10
Acknowledgments	11
I. Dispersion of Twistable Semimetals	18
a. Hexagonal lattice	18
b. Square lattice	18
c. Rectangular and Oblique lattice	18
II. Experimental twistable materials	19
1. Table of experimental twistable materials	19
2. Short-list of promising unexplored experimental twistable materials.	20
3. Experimental growth of twistable materials	21
a. SnSe ₂ and SnS ₂	21
b. HfS ₂	21
c. GaTe	21
d. ZrNCl	21
III. First-principles methods	22
IV. Introduction to the tables in the catalogue	22
V. Catalogue of twistable semimetals	24
1. Summary of results	24
2. Hexagonal lattice	24
a. Γ	24
b. Γ -SOC	24
c. K	25
d. K -SOC	25
e. nHSP	26
f. nHSP-SOC	26
3. Square lattice	27
a. Γ -SOC	27
b. nHSP-SOC	27
4. Rectangular lattice	27
a. HSP	27
b. nHSP	27
c. nHSP-SOC	27
VI. Catalogue of twistable insulators	29

1. Summary of results	29
2. Hexagonal lattice	29
a. Γ	29
b. Γ -SOC	38
c. K	41
d. K -SOC	44
e. M	46
f. M -SOC	48
g. nHSP	48
h. nHSP-SOC	51
3. Square lattice	53
a. Γ	53
b. Γ -SOC	55
c. M	56
d. M -SOC	57
e. X	57
f. X -SOC	58
g. nHSP	58
h. nHSP-SOC	58
4. Rectangular lattice	59
a. HSP	59
b. HSP-SOC	68
c. nHSP	69
d. nHSP-SOC	72
5. Oblique lattice	74
a. HSP	74
b. HSP-SOC	75
c. nHSP	75
d. nHSP-SOC	75

VII. Band Structures of Twistable Materials

Appendix I: Dispersion of Twistable Semimetals

In this section, we analyze the electronic dispersion characteristics of the twisting points of 2D twistable semimetals. These twistable semimetals host different types of dispersion. The nature of the dispersion, *i.e.*, whether linear or quadratic, at these crossing points is determined by the symmetry of the associated valley in the Brillouin zone (BZ). In the presence of certain symmetries, linear terms in the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian may be either allowed or forbidden, leading to distinct types of dispersion [121–127]. A linear dispersion appears when symmetry permits first-order terms, creating Dirac-like cones in the band structure. Conversely, quadratic dispersion emerges when the symmetry constraints eliminate the linear terms, resulting in parabolic band crossings. Note that crystalline symmetries and time-reversal symmetry (TRS) do not forbid all first- and second-order terms, meaning that cubic dispersion can only occur along specific directions, which we omit here for simplicity. Higher-dimensional (> 2) crossings are generally not allowed in the 80 layer groups (LGs) without SOC, except in rare cases involving non-symmorphic LGs, such as the $S = (\frac{1}{2}, \frac{1}{2})$ point in LG 33 ($pb2_1a$), which hosts a 4D irreducible representation (IRREP) S_1S_1 . However, in practice, we do not find twistable semimetals with such high-dimensional crossings. In the presence of SOC, crossing points are typically gapped.

We proceed by discussing the dispersion of semimetals based on the symmetries of the valley.

a. Hexagonal lattice

For semimetals in hexagonal lattices, quadratic dispersion can only appear at the Γ point. Γ valley of the hexagonal lattice exhibits C_3 and TRS symmetry, which lead to the 2D irreducible representation (IRREP) with C_3 eigenvalues $e^{\pm i \frac{2\pi}{3}}$ (without SOC). In this case, the presence of TRS symmetry forbids the linear $\mathbf{k} \cdot \mathbf{p}$ terms and leads to the quadratic dispersion.

The K valley, however, can only host linear crossings, *i.e.*, the Dirac cone. The K point possesses C_3 symmetry but lacks TRS. To host a Dirac cone at the K point, the system must also exhibit inversion or C_{2z} symmetry. In this case, a 2D IRREP with C_3 eigenvalues $e^{\pm i \frac{2\pi}{3}}$ (without SOC) is protected by C_3 and the space-time inversion symmetry $\mathcal{P} \cdot \mathcal{T}$ (or $C_{2z} \cdot \mathcal{T}$) with a linear dispersion.

The M valley of the hexagonal lattice can only host 1D IRREPs (without SOC) and is therefore omitted from consideration. Non-high-symmetry points (nHSPs), however, can host 2D degenerate points if the momentum possesses a twofold rotation C_2 or mirror symmetry. When two bands with opposite C_2 or mirror eigenvalues intersect, the crossing point is symmetry-protected, resulting in linear dispersion.

We note that in the presence of SOC, these degenerate points generally become gapped, leading to two quadratic band edges. However, since SOC is generally not large, a semimetal, even after the SOC-induced gap opens, will still require a model that includes both the valence and conduction bands around the formerly gapless point.

b. Square lattice

In the square lattice, quadratic dispersion at a crossing point can appear at the Γ and M points. These points possess C_4 symmetry and TRS, with TRS enforcing a two-dimensional irreducible representation (IRREP) characterized by C_4 eigenvalues of $\pm i$. In this case, TRS forbids linear terms in the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian, resulting in quadratic dispersion.

The X valley in the square lattice lacks C_4 symmetry but can still host 2D IRREPs (without SOC) when non-symmorphic symmetries are present. For example, in LG 63 ($p4/mbm$), there are two such IRREPs, X_1 and X_2 . However, linear $\mathbf{k} \cdot \mathbf{p}$ terms are allowed in this case. Similarly, symmetry-protected crossings at non-HSPs exhibit linear dispersion.

c. Rectangular and Oblique lattice

For rectangular and oblique lattices, the situation is similar to that of the X valley or non-HSPs in square lattices, which only have C_2 rotation, mirror symmetries, inversion, and TRS symmetries, but have no C_n ($n \leq 3$) symmetries. As a result, linear dispersion is generally allowed.

One semimetal with a rectangular lattice worth mentioning is AuCrO_4 in LG 41 ($pmma$). In the absence of SOC, it exhibits a twofold (or fourfold, if spin is considered) degenerate nodal line (NL) [128–131] along the $X - S$ line near the Fermi level. Upon introducing SOC, the nodal line is expected to be gapped, but the fourfold degenerate points at X and S should persist. However, our calculations show that AuCrO_4 develops spontaneous magnetic moments, breaking

the fourfold degeneracy at X and S . As Topological 2D Materials Database does not include magnetic materials, AuCrO_4 is thus not included in the current twistable material list. In contrast, a similar compound, AgCrO_4 , does not develop magnetic order and retains the fourfold degeneracies at X and S . However, the NL in AgCrO_4 leaves a large density of states (DOS) at the Fermi level, disqualifying it as a twistable semimetal.

Appendix II: Experimental twistable materials

1. Table of experimental twistable materials

In this section, we list the most promising materials that have either been experimentally exfoliated to mono- or few-layer flakes, or have been grown as mono- or few-layer thin films epitaxially on substrates. They are shown in Table S5 (semimetals) and Table S6 (insulators), sorted by the material class and twist score. The ‘‘Class’’ column designates each material as Element, TMD, Chalcogenide, Halide, Mixed P/C/H (mixed pnictides, chalcogenides, and halides), or Other, as introduced in the main text. The ‘‘Mat. Type’’ column reflects the experimental synthesis method, marked as ‘‘Exp.M.Exfo’’ for mechanical exfoliation, ‘‘Exp.W.Exfo’’ for wet exfoliation methods, ‘‘Exp.Substr’’ for materials grown on substrates, or ‘‘Other’’ for unique methods specific to the system or study. For insulators, the score is taken as the maximum of the VBM and CBM scores for simplicity.

TABLE S5: Experimental twistable semimetals.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Topology	Mat. type	Class
C	80	5.1.3	0.00	C2DB	hexagonal	K	0.00	0.90	AccidentalFermi	Exp.M.Exfo	Elements
Si	72	5.1.2	0.00	C2DB	hexagonal	K	0.00	0.80	SEBR	Exp.W.Exfo	Elements
Ge	72	1.1.15	0.02	C2DB	hexagonal	K	0.02	0.68	SEBR	Exp.W.Exfo	Elements
Sn	72	1.1.17	0.07	C2DB	hexagonal	K -SOC	0.07	0.66	SEBR	Exp.W.Exfo	Elements
WS_2	15	1.3.24	0.04	C2DB	rectangular	nHSP-SOC	0.15	0.29	NLC	Exp.W.Exfo	TMD
MoS_2	15	1.1.1	0.05	C2DB	rectangular	nHSP-SOC	0.05	0.28	NLC	Exp.M.Exfo	TMD

TABLE S6: Experimental twistable insulators.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Mat. type	Class
Sb	72	3.1.25	1.01	C2DB	hexagonal	Γ -SOC	nHSP	0.75	OAI	Exp.W.Exfo	Elements
As	72	3.1.11	1.48	C2DB	hexagonal	Γ -SOC	nHSP	0.75	OAI	Exp.W.Exfo	Elements
P	72	3.1.23	1.95	C2DB	hexagonal	/	nHSP	0.68	OAI	Exp.Substr	Elements
P	42	3.1.7	0.91	C2DB	rectangular	Γ	Γ	0.62	OAI	Exp.M.Exfo	Elements
Bi	72	1.1.10	0.53	MC2D	hexagonal	Γ -SOC	Γ	0.60	SEBR	Exp.Other	Elements
Bi	72	1.1.9	0.49	C2DB	hexagonal	/	Γ	0.59	SEBR	Exp.Other	Elements
WSe_2	78	3.1.46	1.26	C2DB	hexagonal	K -SOC	K -SOC	0.71	OAI	Exp.M.Exfo	TMD
WS_2	78	3.1.45	1.55	C2DB	hexagonal	K -SOC	K -SOC	0.70	OAI	Exp.M.Exfo	TMD
WTe_2	78	3.1.47	0.75	C2DB	hexagonal	K -SOC	K -SOC	0.61	OAI	Exp.W.Exfo	TMD
MoS_2	78	3.1.39	1.60	C2DB	hexagonal	K -SOC	K	0.68	OAI	Exp.M.Exfo	TMD
MoSe_2	78	3.1.41	1.34	C2DB	hexagonal	K -SOC	K	0.64	OAI	Exp.M.Exfo	TMD
MoSSe	69	3.1.10	1.48	C2DB	hexagonal	K -SOC	K	0.59	OAI	Exp.Substr	TMD
MoTe_2	78	3.1.43	0.96	C2DB	hexagonal	K -SOC	K	0.60	OAI	Exp.M.Exfo	TMD
SnS_2	72	6.1.75	1.58	C2DB	hexagonal	/	M	0.70	LCEBR	Exp.M.Exfo	TMD
SnSe_2	72	6.1.71	0.76	C2DB	hexagonal	Γ -SOC	M	0.63	LCEBR	Exp.M.Exfo	TMD
HfS_2	72	6.1.43	1.24	C2DB	hexagonal	/	M	0.64	LCEBR	Exp.M.Exfo	TMD
PtSe_2	72	6.1.58	1.18	C2DB	hexagonal	Γ -SOC	nHSP	0.53	LCEBR	Exp.M.Exfo	TMD
HfSe_2	72	6.1.44	0.45	C2DB	hexagonal	Γ -SOC	M	0.49	LCEBR	Exp.M.Exfo	TMD
ZrS_2	72	6.1.61	1.16	C2DB	hexagonal	/	M	0.55	LCEBR	Exp.M.Exfo	TMD
ZrSe_2	72	6.1.73	0.34	C2DB	hexagonal	Γ -SOC	M	0.39	LCEBR	Exp.M.Exfo	TMD
InSe	78	3.1.37	1.40	C2DB	hexagonal	nHSP	Γ	0.64	OAI	Exp.M.Exfo	Chalcogenide
GaSe	78	3.1.32	1.74	C2DB	hexagonal	nHSP	Γ	0.51	OAI	Exp.M.Exfo	Chalcogenide

GaTe	78	3.1.35	1.29	C2DB	hexagonal	/	M -SOC	0.58	OAI	Exp.M.Exfo	Chalcogenide
GaS	78	3.1.30	2.30	C2DB	hexagonal	nHSP	Γ	0.48	OAI	Exp.M.Exfo	Chalcogenide
Bi ₂ Se ₂ Te	72	6.1.23	0.37	C2DB	hexagonal	/	Γ	0.48	LCEBR	Exp.Substr	Chalcogenide
Bi ₂ Se ₂ Te	72	6.1.24	0.33	MC2D	hexagonal	Γ -SOC	Γ	0.46	LCEBR	Exp.Substr	Chalcogenide
Bi ₂ Se ₃	72	6.1.25	0.47	C2DB	hexagonal	/	Γ	0.51	LCEBR	Exp.M.Exfo	Chalcogenide
Bi ₂ SeTe ₂	72	6.1.27	0.31	C2DB	hexagonal	/	Γ	0.46	LCEBR	Exp.M.Exfo	Chalcogenide
Sb ₂ Se ₂ Te	72	6.1.63	0.61	C2DB	hexagonal	/	Γ	0.44	LCEBR	Exp.M.Exfo	Chalcogenide
SnS	32	6.1.2	1.43	C2DB	rectangular	nHSP	nHSP-SOC	0.40	LCEBR	Exp.M.Exfo	Chalcogenide
Sb ₂ SeTe ₂	72	6.1.67	0.44	C2DB	hexagonal	nHSP	Γ	0.41	LCEBR	Exp.M.Exfo	Chalcogenide
GeSe	32	6.1.1	1.12	C2DB	rectangular	nHSP	/	0.41	LCEBR	Exp.M.Exfo	Chalcogenide
SnSb ₂ Se ₄	72	6.1.66	0.39	C2DB	hexagonal	/	Γ	0.38	LCEBR	Exp.Substr	Chalcogenide
SnSe	32	6.1.4	0.89	C2DB	rectangular	nHSP	nHSP-SOC	0.37	LCEBR	Exp.M.Exfo	Chalcogenide
Bi ₂ PbSe ₄	72	6.1.18	0.51	C2DB	hexagonal	/	Γ	0.42	LCEBR	Exp.Substr	Chalcogenide
Bi ₂ Te ₃	72	6.1.30	0.27	C2DB	hexagonal	/	Γ	0.41	LCEBR	Exp.M.Exfo	Chalcogenide
GaGeTe	72	3.1.16	0.67	C2DB	hexagonal	/	Γ	0.44	OAI	Exp.M.Exfo	Chalcogenide
ZrS ₃	46	6.1.6	1.18	C2DB	rectangular	/	Γ	0.41	LCEBR	Exp.W.Exfo	Chalcogenide
Sb ₂ Te ₃	72	6.1.70	0.41	MC2D	hexagonal	/	Γ	0.36	LCEBR	Exp.M.Exfo	Chalcogenide
SnSb ₂ Te ₄	72	6.3.2582	0.42	C2DB	hexagonal	/	Γ	0.31	LCEBR	Exp.Substr	Chalcogenide
Bi ₂ SnTe ₄	72	6.1.29	0.20	C2DB	hexagonal	/	Γ	0.25	LCEBR	Exp.Substr	Chalcogenide
Bi ₂ PbTe ₄	72	6.1.19	0.34	C2DB	hexagonal	/	Γ	0.30	LCEBR	Exp.Substr	Chalcogenide
TiS ₃	46	6.1.8	0.29	C2DB	rectangular	/	Γ	0.18	LCEBR	Exp.M.Exfo	Chalcogenide
ZrSe ₃	46	6.1.7	0.41	C2DB	rectangular	Γ	/	0.18	LCEBR	Exp.M.Exfo	Chalcogenide
PbI ₂	72	6.1.54	1.87	C2DB	hexagonal	/	Γ	0.65	LCEBR	Exp.M.Exfo	Halide
CdI ₂	72	6.1.38	2.18	C2DB	hexagonal	Γ -SOC	M	0.60	LCEBR	Exp.Substr	Halide
BiI ₃	71	6.1.15	1.64	C2DB	hexagonal	/	Γ	0.49	LCEBR	Exp.Substr	Halide
ZrClN	72	6.3.2408	1.91	C2DB	hexagonal	Γ	K	0.58	LCEBR	Exp.M.Exfo	Mixed-P/C/H
BiClTe	69	6.3.1963	0.95	C2DB	hexagonal	Γ -SOC	Γ	0.63	LCEBR	Exp.M.Exfo	Mixed-P/C/H
ZrBrN	72	6.3.2323	1.62	C2DB	hexagonal	nHSP	K	0.65	LCEBR	Exp.W.Exfo	Mixed-P/C/H
BiBrTe	69	6.1.10	0.92	C2DB	hexagonal	Γ -SOC	Γ -SOC	0.62	LCEBR	Exp.M.Exfo	Mixed-P/C/H
BiClTe	69	6.1.11	0.94	C2DB	hexagonal	/	Γ	0.63	LCEBR	Exp.M.Exfo	Mixed-P/C/H
AgInP ₂ S ₆	67	3.3.222	1.33	C2DB	hexagonal	/	Γ	0.59	OAI	Exp.W.Exfo	Mixed-P/C/H
BiTe	69	6.1.13	0.70	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.55	LCEBR	Exp.M.Exfo	Mixed-P/C/H
GaN	78	6.1.78	1.82	C2DB	hexagonal	K	Γ	0.70	LCEBR	Exp.Other	Other
GeH	72	3.1.18	0.90	C2DB	hexagonal	/	Γ	0.66	OAI	Exp.M.Exfo	Other
C ₃ N	80	3.1.48	0.39	C2DB	hexagonal	M	/	0.59	OAI	Exp.Other	Other
HSi	72	3.1.19	2.18	C2DB	hexagonal	/	M	0.57	OAI	Exp.Other	Other
TiO ₂	72	6.1.49	2.66	C2DB	hexagonal	nHSP	/	0.27	LCEBR	Exp.Other	Other
Ti ₂ CO ₂	72	6.1.34	0.31	C2DB	hexagonal	/	M	0.24	LCEBR	Exp.Other	Other

2. Short-list of promising unexplored experimental twistable materials.

Based on the criteria specified in the main text, here we provide several families of materials that are especially likely to be immediately available for fabrication of moiré devices.

1. M -valley TMDs, such as SnSe₂ show much promise, and are well known to be exfoliable as large and high-quality monolayers [96].
2. Group IIIa monochalcogenides such as GaS likewise have been obtained as high-quality monolayer crystals [96], and feature fairly high twist scores according to our methodology.
3. Tetradymite-type chalcogenides such as Bi₂Te₃ have well-established procedures for crystal growth and exfoliation [96], and are some of the highest-scoring experimental twistable insulators.

4. ZrNCl has been exfoliated to monolayers [111], and can be gated to reach a superconducting state [112]. It remains to be seen what states can be achieved in twistrionic devices featuring the material.

3. Experimental growth of twistable materials

a. SnSe_2 and SnS_2

Both SnSe_2 and SnS_2 crystals were obtained by the iodine vapor transport technique and starting materials are commercial chemicals including Sn (Thermos Scientific Chemicals, 99.999%), S (Sigma-Aldrich, 99.999%), Se (Sigma-Aldrich, 99.99%) and I_2 (Sigma-Aldrich, 99.99%). While SnS_2 crystals were grown following the literature procedure [132] (5 mg/cm³ I_2 , 850-650 °C for 12 days), SnSe_2 crystals were synthesized with a modified method. Sn shots and Se shots were combined in a 1:2 molar ratio along with 250 mg I_2 and vacuum-sealed within a 15 cm-long quartz ampule. The ice bath was used during vacuum sealing to avoid iodine evaporation. After being placed in a tube furnace, the bottom of the ampule where the chemicals located was heated to 850 °C in 12h (temperature gradient is estimated about 850-650 °C), held at this temperature for 72h, and then cooled to room temperature in 12h. The metallic-looking crude products were collected close to the end of the cold zone, which contains extra selenides and iodine impurities. Therefore, a purification of evaporating impurities was performed. The crude products were vacuumed-sealed in a 7 cm-long quartz tube and moved into a tube furnace. The furnace was heated to 500 °C in 5h, held at this temperature for 12h, and cooled to room temperature in 5h. High-quality SnSe_2 crystals were collected at the hot zone and the middle of the tube except in the cold end. The pure phases of SnS_2 and SnSe_2 crystals were examined by powder-X-ray diffraction (PXRD) and elemental analysis of Inductively coupled plasma optical emission spectroscopy (ICP-OES) and Scanning Electron Microscopy (SEM) with Energy Dispersive X-ray (EDX).

The crystallinity and phase purity of bulk crystals were checked using pXRD patterns obtained from a STOE STADI P powder diffractometer with Mo $K\alpha_1$ radiation and a Dectris Mythen 2R 1K detector, in the 2θ range from 1° to 45°. SEM and EDX spectra were taken with a Verios 460 extreme high-resolution scanning electron microscope with an Oxford energy dispersive X-ray spectrometer. ICP-OES analysis was performed with Agilent 5800 ICP-OES spectrometer.

b. HfS_2

HfS_2 single crystals were synthesized using chemical vapor transport (CVT). Stoichiometric amounts of Hafnium (Alfa Aesar, 99.6%) and Sulfur (Alfa Aesar, 99.5%) powders were sealed in a quartz tube under vacuum along with iodine as a transport agent. The tube was heated with a temperature gradient of 800-900 °C and kept at that gradient for 10 days. The as-grown crystals were reddish and transparent layered plates with a typical dimension of $5 \times 5 \times 0.1$ mm³. Room-temperature powder X-ray diffraction (XRD) measurements were carried out in a Bruker diffractometer with Cu $K\alpha$ radiation and revealed the hexagonal crystal structure with lattice parameters $a = 3.632$ Å and $c = 5.847$ Å.

c. GaTe

GaTe single crystals were synthesized by a self-flux growth technique, using an excess amount of Ga. Elemental Ga (Sigma-Aldrich, 99.995%) and Te (Thermo Scientific, 99.999%) pieces in an atomic ratio of 0.57 : 0.43 were packed in an alumina crucible and sealed in a quartz ampoule under vacuum. The ampoule was heated up to 900 °C, kept at that temperature for 4 h, then slowly cooled down to 760 °C over 100 h, after which the excess flux was removed in a centrifuge. The as-grown crystals were layered plates with a typical dimension of $5 \times 2 \times 0.2$ mm³. Room-temperature powder X-ray diffraction (XRD) measurements were carried out in a Bruker diffractometer with Cu $K\alpha$ radiation. Rietveld analysis was performed and showed the monoclinic crystal structure with lattice parameters $a = 17.404$ Å, $b = 10.456$ Å, and $c = 4.077$ Å.

d. ZrNCl

Synthesis of ZrNCl was achieved via a two-step synthesis employing an approach slightly modified from literature [133].

Due to the sensitivity of the starting materials and reaction products to air and moisture, all work is carried out in a glove box or in a closed apparatus in the absence of air. To prepare the precursor, two alumina boats are prepared, one with a mixture of 1 g ZrH_2 (Alfa-Aesar, 99%) and 1 g NH_4Cl (Roth, 99%); a second alumina boat is charged with 1.6 g NH_4Cl . The two boats are placed in a quartz reaction tube and installed in a horizontal furnace. After purging with argon for five minutes, the apparatus is heated within 90 minutes to 650 °C in an ammonia stream (60 ml/min, Air Liquide 5.0) and held at this temperature for 30 minutes. It is then cooled down to room temperature in the ammonia stream within 120 minutes. After evacuation, the reaction tube is inserted into the glove box.

At the end of the reaction, the alumina boat originally filled with NH_4Cl is empty; the sample in the second alumina boat has changed its appearance considerably: with an increase in volume, a voluminous, microcrystalline green product with a mass of 0.88 g has formed in the ammonia/ammonium chloride mist. In the cooler area of the reaction tube towards the gas outlet, there is a clearly separated smaller area of an unidentifiable bright yellow precipitate as well as large, unspecified amounts of white fine crystalline powder, which is identified as $(\text{NH}_4)_2[\text{ZrCl}_6]$ and NH_4Cl .

In the second step, 710 mg of the above product together with 35 mg NH_4Cl and 60 mg PtCl_2 in a capillary as transport medium are placed in a quartz tube, evacuated and sealed. The chemical transport is carried out in a two-zone furnace with a temperature gradient of 750 – 850 °C; the starting material is placed in the temperature range of 750 °C, the transport takes place towards 850 °C. After a reaction time of 10 days, millimeter-sized green polycrystalline agglomerates of $\beta\text{-ZrNCl}$ are obtained in the hot area, whereas the small amount of grey, non-transported residue is identified as a mixture of $\text{Zr}_7\text{N}_4\text{O}_8$ [134] and ZrO_2 [135].

Appendix III: First-principles methods

The electronic properties calculations for the monolayer and twisted bilayer system were performed using density functional theory with the Vienna ab initio software package (VASP) [136]. The Perdew-Burke-Ernzerhof (PBE) exchange-correlation functionals [137] were employed. We use a 1.3 times larger cutoff value compared to the default value for the plane wave basis set. For the monolayer calculations, we use a Γ -centered k-mesh such that $n_{k_i} = \frac{75}{a_i}$, where n_{k_i} is the \mathbf{k} point amount in i direction and \mathbf{a}_i is the unit cell length in i direction in Å. For the twisted bilayer calculations, we use a Γ -centered k-mesh of $1 \times 1 \times 1$ for the geometry optimization and electronic structure calculations, with the Tkatchenko-Scheffler (TS) van der Waals corrections [138, 139], which have been shown to yield results consistent with experimental observations in our previous work [53]. The calculation is performed for periodic boundary conditions in all three spatial dimensions, including a vacuum thickness larger than 15 for the out-of-plane direction of the two-dimensional material. This is large enough to suppress artificial interactions between the periodic slab images and thus reflects the two-dimensional limit. All atoms were fully relaxed, ensuring a residual force less than 0.02 eV^{-1} per atom. While the internal atomic positions were fully optimized, the lattice constant for the moiré supercell was kept fixed at a value corresponding to the optimized lattice constant for a 1×1 unit cell in the monolayer to leverage the computational cost of the superlattice calculations. For all band structure calculations spin-orbit coupling was taken into account.

Appendix IV: Introduction to the tables in the catalogue

In the following two sections, we tabulate the twistable semimetals (Appendix [V]) and insulators (Appendix [VI]) found in the high-throughput search. The tables contain the relevant properties of each type of materials.

In each section, the twistable materials are classified based on their Bravais lattice, the valley of the twisting point, and SOC splitting strength. Within each type, we further separate materials into four groups, *i.e.*, experimental, computationally exfoliable, computationally stable, and computationally unstable, based on the following:

- *Experimentally existing*: materials that are already manually verified in the literature to have been experimentally fabricated, which could be reported as exfoliated (labeled in the table as “Exp.M.Exfo” for mechanical exfoliation, and “Exp.W.Exfo” for the various wet exfoliation methods), grown on a substrate (“Exp.Substr”), or other methods, unique to the system or study (“Other”).
- *Computationally exfoliable (MC2D)*: materials from the MC2D. In this database, all materials were computationally exfoliated from an experimentally existing material in 3D and then relaxed.
- *Stable (C2DB)*: materials that are marked as highly thermodynamically stable (the energy above the convex hull $< 0.2 \text{ eV/atom}$) or dynamically stable (all phonon frequencies are real) in the C2DB.

- *Not-stable (C2DB)*: materials that do not satisfy the conditions defined above from C2DB.

In each table, we list the following properties of each material:

- **Formula**: the chemical formula of the material.
- **LG**: the layer group.
- **ID**: the serial ID used in Topological 2D Materials Database, accompanied by the corresponding web link.
- **Gap**: the global (indirect) gap, given in eV.
- **Database**: the link of the material to the database where we obtain the crystal structure, including C2DB and MC2D.
- **Lattice**: the Bravais lattice of the material, *i.e.*, hexagonal, square, rectangular (including centered rectangular), and oblique.
- **Valley**: the momentum of the twisting point. For insulators, we give the VBM and CBM valley separately. When the SOC splitting near the valley is stronger than 50 meV, we add a “-SOC” suffix to the valley.
- **SOC gap**: the SOC splitting gap near the valley. In practice, we compute the SOC splitting within a specified momentum range relative to the twisting point — specifically, within the first moiré BZ at a chosen twist angle of 5° , an angle that covers the relevant momenta after twisting. This moiré BZ is also used as the momentum resolution to determine whether a valley is located at an HSP. If the distance from the valley to an HSP falls within this first moiré BZ, we define the valley as being at the corresponding HSP.
- **Twist Score**: the twisting score of the material, defined in Eq. (2). For insulators, since each table is for one specific valley type, the score of the corresponding valley is used. In case the VBM and CBM have the same valley, the twist score is taken as the larger one.
- **Dispersion**: The type of dispersion at the twisting point for twistable semimetals (without SOC), which can be either linear or quadratic.
- **Topology (SOC)**: the topological classification of the material with SOC, including LCEBR (linear combination of elementary band representations (EBR)), SEBR (split EBR), AccidentalFermi (accidental crossing point at Fermi level), ES (enforced semimetal), ESFD (enforced semimetal with Fermi degeneracy), OAI (obstructed atomic insulators), and OOAI (orbital-selective OAI) [140]. Among these classifications, the SEBR and NLC are topological insulators, the ES and ESFD are topological semimetals, the LCEBR are trivial insulators, the OAI are trivial insulators but have some electronic Wannier centers at empty sites, and the OOAI has Wannier centers at some atomic sites but can not form the outer-shell orbitals of those atoms.
- **Bulk**: If the material has an existing bulk structure, mark it as “Yes”; If it does not have or is unknown, mark it as “/”. Their bulk structures can be found in either C2DB or MC2D.
- **Mat. type**: the type of material, including experimental (Exp), computationally exfoliable (Comp.Exfo), computationally stable (Stable), and computationally unstable (Unstable).

Note that the 2D materials in Topological 2D Materials Database include structures from C2DB and MC2D, which contain some duplicate materials. We remove these duplicates based on the following criteria: (1) same chemical formula, (2) same layer group, (3) same topological classification with and without SOC, (4) same valley type at both the VBM and CBM, and (5) differences in the indirect gap and twist score within 0.2 (in the unit of eV for the gap).

Appendix V: Catalogue of twistable semimetals

1. Summary of results

Lattice	Valley	# of materials	Experimental	Comp. exfoliated	Comp. stable	Comp. unstable	Total #
Hexagonal	Γ	2	0	0	0	2	48
	Γ -SOC	16	0	1	10	5	
	K	12	3	0	0	9	
	K -SOC	10	1	1	4	4	
	M	0	0	0	0	0	
	M -SOC	0	0	0	0	0	
	nHSP	3	0	0	3	0	
	nHSP-SOC	5	0	0	3	2	
Square	Γ	0	0	0	0	0	3
	Γ -SOC	1	0	0	0	1	
	M	0	0	0	0	0	
	M -SOC	0	0	0	0	0	
	X	0	0	0	0	0	
	X -SOC	0	0	0	0	0	
	nHSP	0	0	0	0	0	
	nHSP-SOC	2	0	0	0	2	
Rectangular	HSP	1	0	0	0	1	10
	HSP-SOC	0	0	0	0	0	
	nHSP	2	0	1	1	0	
	nHSP-SOC	7	2	2	2	1	
Oblique	HSP	0	0	0	0	0	0
	HSP-SOC	0	0	0	0	0	
	nHSP	0	0	0	0	0	
	nHSP-SOC	0	0	0	0	0	

TABLE S7. Statistics of twistable semimetal, classified into Bravais lattice, valley, and strength of SOC. When the SOC splitting near the twisting point is strong, the valley is labeled as “valley-SOC” type. The materials are further grouped into four types, *i.e.*, experimental, computationally (Comp.) exfoliable, computationally stable, and computationally unstable.

2. Hexagonal lattice

a. Γ

TABLE S8: Computationally unstable materials with valley type: hexagonal- Γ .

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
Cu ₂ Se	80	1.4.326	0.00	C2DB	hexagonal	Γ	0.05	0.81	quadratic	SEBR	/	Unstable
NiZrH ₆	67	3.4.66	0.05	C2DB	hexagonal	Γ	0.05	0.40	quadratic	OAI	/	Unstable

b. Γ -SOC

TABLE S9: Computationally exfoliable materials with valley type: hexagonal- Γ -SOC.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
---------	----	----	-----	----------	---------	--------	---------	-------------	------------	----------	------	-----------

HfBr	72	1.2.104	0.06	MC2D	hexagonal	Γ -SOC	0.23	0.57	quadratic	SEBR	Yes	Comp.Exfo
------	----	---------	------	------	-----------	---------------	------	------	-----------	------	-----	-----------

TABLE S10: Computationally stable materials with valley type: hexagonal- Γ -SOC.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
Ag ₂ Te	80	1.3.420	0.14	C2DB	hexagonal	Γ -SOC	0.19	0.84	quadratic	SEBR	/	Stable
BrGe	72	1.3.209	0.16	C2DB	hexagonal	Γ -SOC	0.25	0.57	quadratic	SEBR	/	Stable
ZrBr	72	1.3.213	0.00	C2DB	hexagonal	Γ -SOC	0.06	0.54	quadratic	SEBR	Yes	Stable
BiMoAs	69	6.3.1923	0.00	C2DB	hexagonal	Γ -SOC	0.09	0.47	quadratic	LCEBR	/	Stable
Zr ₃ C ₂ Cl ₂	78	1.3.350	0.00	C2DB	hexagonal	Γ -SOC	0.61	0.47	quadratic	NLC	/	Stable
HgO	72	1.3.288	0.15	C2DB	hexagonal	Γ -SOC	0.15	0.41	quadratic	SEBR	/	Stable
GaSnTe	72	1.3.277	0.06	C2DB	hexagonal	Γ -SOC	0.44	0.40	quadratic	SEBR	/	Stable
HgTe	72	3.3.447	0.09	C2DB	hexagonal	Γ -SOC	0.23	0.39	quadratic	OAI	/	Stable
AlSnTe	72	1.3.192	0.09	C2DB	hexagonal	Γ -SOC	0.31	0.37	quadratic	SEBR	/	Stable
CdGa ₂ Se ₄	72	4.3.10	0.02	C2DB	hexagonal	Γ -SOC	0.12	0.28	quadratic	OOAI	/	Stable

TABLE S11: Computationally unstable materials with valley type: hexagonal- Γ -SOC.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
Cu ₂ S	80	1.4.325	0.00	C2DB	hexagonal	Γ -SOC	0.14	0.81	quadratic	SEBR	Yes	Unstable
Ag ₂ Se	80	1.4.314	0.00	C2DB	hexagonal	Γ -SOC	0.06	0.79	quadratic	SEBR	/	Unstable
Ag ₂ S	80	1.4.313	0.00	C2DB	hexagonal	Γ -SOC	0.21	0.79	quadratic	SEBR	/	Unstable
CrOS	69	6.4.547	0.00	C2DB	hexagonal	Γ -SOC	0.05	0.48	quadratic	LCEBR	/	Unstable
WTe	78	3.4.217	0.02	C2DB	hexagonal	Γ -SOC	0.25	0.39	quadratic	OAI	/	Unstable

c. K

TABLE S12: Experimental materials with valley type: hexagonal- K .

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
C	80	5.1.3	0.00	C2DB	hexagonal	K	0.00	0.90	linear	AccidentalFermi	Yes	Exp.M.Exfo
Si	72	5.1.2	0.00	C2DB	hexagonal	K	0.00	0.80	linear	SEBR	Yes	Exp.W.Exfo
Ge	72	1.1.15	0.02	C2DB	hexagonal	K	0.02	0.68	linear	SEBR	Yes	Exp.W.Exfo

TABLE S13: Computationally unstable materials with valley type: hexagonal- K .

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
FN	72	1.4.171	0.02	C2DB	hexagonal	K	0.02	0.70	linear	SEBR	/	Unstable
HN	72	1.4.177	0.01	C2DB	hexagonal	K	0.01	0.66	linear	SEBR	/	Unstable
ZrCl	72	1.4.162	0.04	C2DB	hexagonal	K	0.04	0.64	linear	SEBR	/	Unstable
ScSe	72	1.4.228	0.00	C2DB	hexagonal	K	0.01	0.59	linear	SEBR	/	Unstable
ScS	72	1.4.223	0.00	C2DB	hexagonal	K	0.01	0.59	linear	SEBR	/	Unstable
ScTe	72	1.4.229	0.00	C2DB	hexagonal	K	0.00	0.57	linear	SEBR	/	Unstable
VO	72	1.4.207	0.02	C2DB	hexagonal	K	0.02	0.55	linear	SEBR	/	Unstable
ZrBr	72	1.4.143	0.04	C2DB	hexagonal	K	0.04	0.53	linear	SEBR	/	Unstable
TiCl	72	1.4.159	0.01	C2DB	hexagonal	K	0.01	0.51	linear	SEBR	/	Unstable

d. K -SOC

TABLE S14: Experimental materials with valley type: hexagonal- K -SOC.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
Sn	72	1.1.17	0.07	C2DB	hexagonal	K -SOC	0.07	0.66	linear	SEBR	Yes	Exp.W.Exfo

TABLE S15: Computationally exfoliable materials with valley type: hexagonal- K -SOC.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
HgPt ₂ Se ₃	72	1.2.121	0.13	MC2D	hexagonal	K -SOC	0.17	0.45	linear	SEBR	Yes	Comp.Exfo

TABLE S16: Computationally stable materials with valley type: hexagonal- K -SOC.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
Ta ₂ STe ₂	72	1.3.321	0.15	C2DB	hexagonal	K -SOC	0.15	0.66	linear	SEBR	/	Stable
AsCl	72	1.3.193	0.19	C2DB	hexagonal	K -SOC	0.19	0.65	linear	SEBR	/	Stable
CdPt ₂ Se ₃	72	1.3.249	0.04	C2DB	hexagonal	K -SOC	0.16	0.47	linear	SEBR	/	Stable
CdPt ₂ Te ₃	72	1.3.250	0.05	C2DB	hexagonal	K -SOC	0.18	0.36	linear	SEBR	/	Stable

TABLE S17: Computationally unstable materials with valley type: hexagonal- K -SOC.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
HgCl	72	1.4.154	0.12	C2DB	hexagonal	K -SOC	0.12	0.75	linear	SEBR	/	Unstable
HgBr	72	1.4.136	0.18	C2DB	hexagonal	K -SOC	0.18	0.73	linear	SEBR	/	Unstable
InS	72	1.4.191	0.00	C2DB	hexagonal	K -SOC	0.17	0.67	linear	SEBR	/	Unstable
IrSe	72	1.4.195	0.14	C2DB	hexagonal	K -SOC	0.14	0.46	linear	SEBR	/	Unstable

e. nHSP

TABLE S18: Computationally stable materials with valley type: hexagonal-nHSP.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
TiH ₂	78	1.3.383	0.00	C2DB	hexagonal	nHSP	0.01	0.69	linear	NLC	/	Stable
IrPS ₃	71	1.3.186	0.00	C2DB	hexagonal	nHSP	0.01	0.59	linear	SEBR	/	Stable
RhPSe ₃	71	1.3.188	0.02	C2DB	hexagonal	nHSP	0.02	0.55	linear	SEBR	/	Stable

f. nHSP-SOC

TABLE S19: Computationally stable materials with valley type: hexagonal-nHSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
ZrH ₂	78	1.3.385	0.00	C2DB	hexagonal	nHSP-SOC	0.07	0.68	linear	NLC	/	Stable
ZrTe	72	1.3.333	0.11	C2DB	hexagonal	nHSP-SOC	0.11	0.43	linear	SEBR	/	Stable
AuTe	78	1.3.341	0.02	C2DB	hexagonal	nHSP-SOC	0.21	0.29	linear	NLC	/	Stable

TABLE S20: Computationally unstable materials with valley type: hexagonal-nHSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
MoO	78	1.4.277	0.00	C2DB	hexagonal	nHSP-SOC	0.19	0.48	linear	NLC	/	Unstable

HfSe	72	1.4.183	0.05	C2DB	hexagonal	nHSP-SOC	0.05	0.45	linear	SEBR	/	Unstable
------	----	---------	------	------	-----------	----------	------	------	--------	------	---	----------

3. Square lattice

a. Γ -SOC

TABLE S21: Computationally unstable materials with valley type: square- Γ -SOC.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
PtS	64	1.4.118	0.01	C2DB	square	Γ -SOC	0.38	0.33	quadratic	SEBR	/	Unstable

b. n HSP-SOC

TABLE S22: Computationally unstable materials with valley type: square- n HSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
SnS	61	1.4.63	0.03	C2DB	square	nHSP-SOC	0.22	0.78	linear	SEBR	/	Unstable
RuCl ₂	59	6.4.373	0.00	C2DB	square	nHSP-SOC	0.13	0.33	linear	LCEBR	/	Unstable

4. Rectangular lattice

a. HSP

TABLE S23: Computationally unstable materials with valley type: rectangular-HSP.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
TaF	18	1.4.14	0.00	C2DB	rectangular	Γ	0.04	0.45	linear	SEBR	/	Unstable

b. n HSP

TABLE S24: Computationally exfoliable materials with valley type: rectangular- n HSP.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
Hg ₃ S ₂	18	1.2.29	0.05	MC2D	rectangular	nHSP	0.05	0.44	linear	SEBR	Yes	Comp.Exfo

TABLE S25: Computationally stable materials with valley type: rectangular- n HSP.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
RhFS	46	1.3.81	0.01	C2DB	rectangular	nHSP	0.05	0.31	linear	SEBR	/	Stable

c. n HSP-SOC

TABLE S26: Experimental materials with valley type: rectangular- n HSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
WS ₂	15	1.3.24	0.04	C2DB	rectangular	nHSP-SOC	0.15	0.29	linear	NLC	Yes	Exp.W.Exfo
MoS ₂	15	1.1.1	0.05	C2DB	rectangular	nHSP-SOC	0.05	0.28	linear	NLC	Yes	Exp.M.Exfo

TABLE S27: Computationally exfoliable materials with valley type: rectangular-nHSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
Hg ₂ O	10	6.2.307	0.07	MC2D	rectangular	nHSP-SOC	0.07	0.63	linear	LCEBR	Yes	Comp.Exfo
Hg ₂ O	17	1.2.25	0.08	MC2D	rectangular	nHSP-SOC	0.08	0.33	linear	NLC	Yes	Comp.Exfo

TABLE S28: Computationally stable materials with valley type: rectangular-nHSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
AgGaSeTe	13	6.3.520	0.10	C2DB	rectangular	nHSP-SOC	0.11	0.64	linear	LCEBR	/	Stable
Ta ₂ Se ₃	18	1.3.50	0.03	C2DB	rectangular	nHSP-SOC	0.11	0.36	linear	SEBR	/	Stable

TABLE S29: Computationally unstable materials with valley type: rectangular-nHSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	valley	SOC gap	Twist score	Dispersion	Topology	Bulk	Mat. type
CrS ₂	15	1.4.5	0.00	C2DB	rectangular	nHSP-SOC	0.18	0.29	linear	NLC	/	Unstable

Appendix VI: Catalogue of twistable insulators

1. Summary of results

Lattice	Valley	# of materials	Experimental	Comp. exfoliated	Comp. stable	Comp. unstable	Total #
Hexagonal	Γ	414	28	28	298	60	1072
	Γ -SOC	167	13	10	124	20	
	K	115	7	8	75	25	
	K -SOC	64	7	2	43	12	
	M	94	10	10	54	20	
	M -SOC	6	1	0	3	2	
	nHSP	115	10	8	79	18	
	nHSP-SOC	97	1	3	65	28	
Square	Γ	81	0	23	45	13	167
	Γ -SOC	17	0	3	14	0	
	M	25	0	2	20	3	
	M -SOC	4	0	0	3	1	
	X	15	0	2	8	5	
	X -SOC	1	0	0	0	1	
	nHSP	13	0	1	3	9	
	nHSP-SOC	11	0	0	7	4	
Rectangular	HSP	475	4	96	290	85	710
	HSP-SOC	34	0	0	17	17	
	nHSP	139	3	13	98	25	
	nHSP-SOC	62	2	4	38	18	
Oblique	HSP	19	0	6	10	3	38
	HSP-SOC	4	0	0	3	1	
	nHSP	7	0	4	3	0	
	nHSP-SOC	8	0	1	3	4	

TABLE S30. Statistics of twistable insulator, classified into Bravais lattice, valley, and strength of SOC. When the SOC splitting near the twisting point is strong, the valley is labeled as “valley-SOC” type. The materials are further grouped into four types, *i.e.*, experimental, computationally (Comp.) exfoliable, computationally stable, and computationally unstable.

2. Hexagonal lattice

a. Γ

TABLE S31: Experimental materials with valley type: hexagonal- Γ .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
GaN	78	6.1.78	1.82	C2DB	hexagonal	K	Γ	0.70	LCEBR	Yes	Exp.
GeH	72	3.1.18	0.90	C2DB	hexagonal	/	Γ	0.66	OAI	Yes	Exp.M.Exfo
PbI ₂	72	6.1.54	1.87	C2DB	hexagonal	/	Γ	0.65	LCEBR	Yes	Exp.M.Exfo
InSe	78	3.1.37	1.40	C2DB	hexagonal	nHSP	Γ	0.64	OAI	Yes	Exp.M.Exfo
BiClTe	69	6.3.1963	0.95	C2DB	hexagonal	Γ -SOC	Γ	0.63	LCEBR	Yes	Exp.M.Exfo
BiClTe	69	6.1.11	0.94	C2DB	hexagonal	/	Γ	0.63	LCEBR	Yes	Exp.M.Exfo
BiClTe	69	6.1.12	0.94	MC2D	hexagonal	Γ -SOC	Γ	0.63	LCEBR	Yes	Exp.M.Exfo
Bi	72	1.1.10	0.53	MC2D	hexagonal	Γ -SOC	Γ	0.60	SEBR	Yes	Exp.
Bi	72	1.1.9	0.49	C2DB	hexagonal	/	Γ	0.59	SEBR	Yes	Exp.

AgInP ₂ S ₆	67	3.3.222	1.33	C2DB	hexagonal	/	Γ	0.59	OAI	Yes	Exp.W.Exfo
ZrClN	72	6.3.2408	1.91	C2DB	hexagonal	Γ	K	0.51	LCEBR	Yes	Exp.M.Exfo
GaSe	78	3.1.32	1.74	C2DB	hexagonal	nHSP	Γ	0.51	OAI	Yes	Exp.M.Exfo
Bi ₂ Se ₃	72	6.1.25	0.47	C2DB	hexagonal	/	Γ	0.51	LCEBR	Yes	Exp.M.Exfo
BiI ₃	71	6.1.15	1.64	C2DB	hexagonal	/	Γ	0.49	LCEBR	Yes	Exp.Substr
Bi ₂ Se ₂ Te	72	6.1.23	0.37	C2DB	hexagonal	/	Γ	0.48	LCEBR	Yes	Exp.Substr
Bi ₂ Se ₂ Te	72	6.1.24	0.33	MC2D	hexagonal	Γ -SOC	Γ	0.46	LCEBR	Yes	Exp.Substr
Bi ₂ SeTe ₂	72	6.1.27	0.31	C2DB	hexagonal	/	Γ	0.46	LCEBR	Yes	Exp.M.Exfo
Sb ₂ Se ₂ Te	72	6.1.63	0.61	C2DB	hexagonal	/	Γ	0.44	LCEBR	Yes	Exp.M.Exfo
GaGeTe	72	3.1.16	0.67	C2DB	hexagonal	/	Γ	0.44	OAI	Yes	Exp.M.Exfo
Bi ₂ PbSe ₄	72	6.1.18	0.51	C2DB	hexagonal	/	Γ	0.42	LCEBR	Yes	Exp.Substr
Bi ₂ Te ₃	72	6.1.30	0.27	C2DB	hexagonal	/	Γ	0.41	LCEBR	Yes	Exp.M.Exfo
Sb ₂ SeTe ₂	72	6.1.67	0.44	C2DB	hexagonal	nHSP	Γ	0.41	LCEBR	Yes	Exp.M.Exfo
SnSb ₂ Se ₄	72	6.1.66	0.39	C2DB	hexagonal	/	Γ	0.38	LCEBR	Yes	Exp.Substr
Sb ₂ Te ₃	72	6.1.70	0.41	MC2D	hexagonal	/	Γ	0.36	LCEBR	Yes	Exp.M.Exfo
GaS	78	3.1.30	2.30	C2DB	hexagonal	nHSP	Γ	0.34	OAI	Yes	Exp.M.Exfo
SnSb ₂ Te ₄	72	6.3.2582	0.42	C2DB	hexagonal	/	Γ	0.31	LCEBR	Yes	Exp.Substr
Bi ₂ PbTe ₄	72	6.1.19	0.34	C2DB	hexagonal	/	Γ	0.30	LCEBR	Yes	Exp.Substr
Bi ₂ SnTe ₄	72	6.1.29	0.20	C2DB	hexagonal	/	Γ	0.25	LCEBR	Yes	Exp.Substr

TABLE S32: Computationally exfoliable materials with valley type: hexagonal- Γ .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
PbTe	69	6.2.1129	1.14	MC2D	hexagonal	Γ -SOC	Γ	0.69	LCEBR	Yes	Comp.Exfo
Tl ₂ S	72	6.2.1302	1.27	MC2D	hexagonal	Γ	M	0.65	LCEBR	Yes	Comp.Exfo
NaSnP	69	6.2.1128	1.07	MC2D	hexagonal	nHSP-SOC	Γ	0.65	LCEBR	Yes	Comp.Exfo
TbBrH ₂	72	6.2.1255	1.58	MC2D	hexagonal	Γ	/	0.64	LCEBR	Yes	Comp.Exfo
Li ₃ As	78	6.2.1312	0.80	MC2D	hexagonal	/	Γ	0.63	LCEBR	Yes	Comp.Exfo
Li ₄ SrP ₂	72	6.2.1277	1.28	MC2D	hexagonal	/	Γ	0.62	LCEBR	Yes	Comp.Exfo
GaSe	69	6.2.1106	0.88	MC2D	hexagonal	K -SOC	Γ	0.59	LCEBR	Yes	Comp.Exfo
K ₂ SnAs ₂ S ₆	66	6.2.1064	1.12	MC2D	hexagonal	/	Γ	0.59	LCEBR	Yes	Comp.Exfo
K ₄ ZnAs ₂	72	6.2.1171	0.84	MC2D	hexagonal	/	Γ	0.51	LCEBR	Yes	Comp.Exfo
CdK ₄ As ₂	72	6.2.1168	0.80	MC2D	hexagonal	/	Γ	0.51	LCEBR	Yes	Comp.Exfo
ZnHN ₃ O	69	6.2.1114	2.18	MC2D	hexagonal	/	Γ	0.49	LCEBR	Yes	Comp.Exfo
CeH ₂ O ₆ P ₂	72	6.2.1246	1.21	MC2D	hexagonal	Γ	/	0.48	LCEBR	Yes	Comp.Exfo
HgK ₄ As ₂	72	6.2.1170	0.81	MC2D	hexagonal	/	Γ	0.47	LCEBR	Yes	Comp.Exfo
TlO ₃ Sb	71	6.2.1163	2.66	MC2D	hexagonal	/	Γ	0.46	LCEBR	Yes	Comp.Exfo
AgInP ₂ Se ₆	67	3.2.155	0.87	MC2D	hexagonal	/	Γ	0.45	OAI	Yes	Comp.Exfo
Pt ₂ TlS ₃	72	6.2.1293	1.33	MC2D	hexagonal	/	Γ	0.44	LCEBR	Yes	Comp.Exfo
Hg ₃ AsBrS ₄	69	6.2.1085	2.04	MC2D	hexagonal	/	Γ	0.43	LCEBR	Yes	Comp.Exfo
Hg ₃ AsClS ₄	69	6.2.1087	2.12	MC2D	hexagonal	/	Γ	0.43	LCEBR	Yes	Comp.Exfo
SSb ₂ Te ₂	72	6.2.1301	0.50	MC2D	hexagonal	nHSP	Γ	0.43	LCEBR	Yes	Comp.Exfo
SnP ₃	72	3.2.195	0.43	MC2D	hexagonal	/	Γ	0.42	OAI	Yes	Comp.Exfo
Hg ₃ AsBrSe ₄	69	6.2.1086	1.72	MC2D	hexagonal	/	Γ	0.40	LCEBR	Yes	Comp.Exfo
Hg ₃ AsISe ₄	69	6.2.1088	1.64	MC2D	hexagonal	/	Γ	0.40	LCEBR	Yes	Comp.Exfo
ZnFHO	69	6.2.1113	2.97	MC2D	hexagonal	/	Γ	0.38	LCEBR	Yes	Comp.Exfo
Bi ₂ Pb ₂ Se ₅	72	6.2.1177	0.34	MC2D	hexagonal	/	Γ	0.32	LCEBR	Yes	Comp.Exfo
GeSb ₂ Te ₄	72	6.2.1243	0.53	MC2D	hexagonal	/	Γ	0.31	LCEBR	Yes	Comp.Exfo
TlIO ₃	69	6.2.1118	2.84	MC2D	hexagonal	Γ	Γ	0.28	LCEBR	Yes	Comp.Exfo
Bi ₂ GeTe ₄	72	6.2.1176	0.43	MC2D	hexagonal	/	Γ	0.27	LCEBR	Yes	Comp.Exfo

$\text{Bi}_2\text{Pb}_2\text{Te}_5$	72	6.2.1178	0.27	MC2D	hexagonal	/	Γ	0.21	LCEBR	Yes	Comp.Exfo
-------------------------------------	----	----------	------	------	-----------	---	----------	------	-------	-----	-----------

TABLE S33: Computationally stable materials with valley type: hexagonal- Γ .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
CuI	78	6.3.2638	1.29	C2DB	hexagonal	/	Γ	0.75	LCEBR	/	Stable
CuBr	78	6.3.2619	1.02	C2DB	hexagonal	/	Γ	0.75	LCEBR	Yes	Stable
CuCl	78	6.3.2637	1.09	C2DB	hexagonal	/	Γ	0.75	LCEBR	/	Stable
AgI	78	6.3.2600	1.55	C2DB	hexagonal	Γ -SOC	Γ	0.74	LCEBR	/	Stable
AgBr	78	6.3.2598	1.58	C2DB	hexagonal	/	Γ	0.74	LCEBR	/	Stable
AgCl	78	6.3.2599	1.68	C2DB	hexagonal	Γ -SOC	Γ	0.72	LCEBR	/	Stable
PbO_2	72	6.3.2544	1.31	C2DB	hexagonal	/	Γ	0.71	LCEBR	/	Stable
WO_2	78	3.3.520	1.34	C2DB	hexagonal	Γ	K	0.71	OAI	/	Stable
HgF_2	78	6.3.2639	1.26	C2DB	hexagonal	K -SOC	Γ	0.71	LCEBR	/	Stable
HgBr_2	78	6.3.2614	1.52	C2DB	hexagonal	/	Γ	0.71	LCEBR	/	Stable
HgF_2	72	6.3.2423	1.62	C2DB	hexagonal	Γ -SOC	Γ	0.69	LCEBR	/	Stable
CuCl	72	6.3.2401	1.23	C2DB	hexagonal	/	Γ	0.69	LCEBR	/	Stable
HgI	72	3.3.445	1.27	C2DB	hexagonal	/	Γ	0.69	OAI	/	Stable
InSe	72	3.3.456	1.31	C2DB	hexagonal	nHSP	Γ	0.69	OAI	/	Stable
HgBr	72	3.3.384	1.50	C2DB	hexagonal	/	Γ	0.69	OAI	/	Stable
GaO	72	3.3.429	1.40	C2DB	hexagonal	/	Γ	0.69	OAI	/	Stable
ClSi	72	3.3.415	1.25	C2DB	hexagonal	/	Γ	0.69	OAI	/	Stable
ZnO	72	6.3.2548	1.40	C2DB	hexagonal	/	Γ	0.69	LCEBR	/	Stable
GaO	78	3.3.502	1.48	C2DB	hexagonal	/	Γ	0.69	OAI	/	Stable
PbTe	69	6.3.2143	1.15	C2DB	hexagonal	/	Γ	0.69	LCEBR	/	Stable
InP	69	6.3.2127	1.07	C2DB	hexagonal	K	Γ	0.69	LCEBR	/	Stable
MoO_2	78	3.3.512	0.92	C2DB	hexagonal	Γ	K	0.68	OAI	/	Stable
CuBr	72	6.3.2315	1.53	C2DB	hexagonal	/	Γ	0.68	LCEBR	/	Stable
GaP	69	6.3.2065	1.55	C2DB	hexagonal	K	Γ	0.68	LCEBR	/	Stable
$\text{Pb}_2\text{Br}_2\text{S}$	72	6.3.2326	1.38	C2DB	hexagonal	/	Γ	0.68	LCEBR	/	Stable
$\text{Sn}_2\text{Br}_2\text{Se}$	72	6.3.2330	1.06	C2DB	hexagonal	/	Γ	0.68	LCEBR	/	Stable
PbH_2S_2	72	6.3.2484	1.47	C2DB	hexagonal	K	Γ	0.68	LCEBR	/	Stable
SnH_2S_2	72	6.3.2485	1.00	C2DB	hexagonal	K	Γ	0.68	LCEBR	/	Stable
GeH_2S_2	72	6.3.2470	1.05	C2DB	hexagonal	K	Γ	0.68	LCEBR	/	Stable
PbSe	72	6.3.2559	1.21	C2DB	hexagonal	nHSP	Γ	0.67	LCEBR	/	Stable
AgCl	72	6.3.2259	1.59	C2DB	hexagonal	/	Γ	0.67	LCEBR	/	Stable
PbS	72	6.3.2558	1.54	C2DB	hexagonal	/	Γ	0.67	LCEBR	/	Stable
InS	72	3.3.454	1.61	C2DB	hexagonal	/	Γ	0.67	OAI	/	Stable
GaSe	72	3.3.434	1.61	C2DB	hexagonal	nHSP	Γ	0.67	OAI	/	Stable
PbS_2	78	3.3.521	1.71	C2DB	hexagonal	/	Γ	0.67	OAI	/	Stable
InTe	72	3.3.458	1.16	C2DB	hexagonal	nHSP	Γ	0.66	OAI	/	Stable
HgCl	72	3.3.412	1.66	C2DB	hexagonal	/	Γ	0.66	OAI	/	Stable
BiCl	72	1.3.200	0.91	C2DB	hexagonal	K	Γ	0.66	SEBR	/	Stable
PbSe	69	6.3.2142	1.68	C2DB	hexagonal	/	Γ	0.66	LCEBR	/	Stable
CdCl	72	3.3.408	1.68	C2DB	hexagonal	K	Γ	0.66	OAI	/	Stable
BiBr	72	1.3.199	0.88	C2DB	hexagonal	K	Γ	0.65	SEBR	/	Stable
AgBr	72	6.3.2258	1.74	C2DB	hexagonal	/	Γ	0.65	LCEBR	/	Stable
MoOS	69	3.3.283	1.09	C2DB	hexagonal	Γ	K	0.65	OAI	/	Stable
WSe	69	3.3.290	1.26	C2DB	hexagonal	Γ	K	0.65	OAI	/	Stable
PbPSe_3	71	3.3.348	1.07	C2DB	hexagonal	/	Γ	0.64	OAI	/	Stable

PbH ₂ O ₂	72	6.3.2479	1.68	C2DB	hexagonal	<i>K</i>	Γ	0.64	LCEBR	/	Stable
BiI	72	1.3.202	0.86	C2DB	hexagonal	<i>K</i>	Γ	0.64	SEBR	/	Stable
WOS	69	3.3.289	1.51	C2DB	hexagonal	Γ	<i>K</i>	0.64	OAI	/	Stable
HgBr ₂	72	6.3.2320	1.90	C2DB	hexagonal	/	Γ	0.64	LCEBR	Yes	Stable
InS	78	3.3.509	1.68	C2DB	hexagonal	/	Γ	0.64	OAI	/	Stable
BiFSe	69	6.3.1966	1.55	C2DB	hexagonal	/	Γ	0.64	LCEBR	/	Stable
AuI	72	6.3.2300	0.84	C2DB	hexagonal	/	Γ	0.64	LCEBR	/	Stable
AgI	72	6.1.17	1.81	C2DB	hexagonal	Γ -SOC	Γ	0.64	LCEBR	Yes	Stable
CdBr	72	3.3.380	1.84	C2DB	hexagonal	/	Γ	0.63	OAI	/	Stable
InN	78	6.3.2654	0.61	C2DB	hexagonal	/	Γ	0.63	LCEBR	/	Stable
BiFTe	69	6.3.1967	0.94	C2DB	hexagonal	Γ -SOC	Γ	0.63	LCEBR	/	Stable
HgBrHO	69	6.3.2074	1.17	C2DB	hexagonal	/	Γ	0.62	LCEBR	/	Stable
HgBrHS	69	6.3.2075	1.50	C2DB	hexagonal	/	Γ	0.62	LCEBR	/	Stable
HgClHS	69	6.3.2084	1.48	C2DB	hexagonal	/	Γ	0.62	LCEBR	/	Stable
HgFHO	69	6.3.2085	1.08	C2DB	hexagonal	Γ -SOC	Γ	0.62	LCEBR	/	Stable
HgHS	69	6.3.2087	1.09	C2DB	hexagonal	Γ -SOC	Γ	0.62	LCEBR	/	Stable
SrHIO	69	6.3.2088	1.47	C2DB	hexagonal	Γ -SOC	Γ	0.62	LCEBR	/	Stable
HgCl ₂	78	6.3.2632	2.02	C2DB	hexagonal	/	Γ	0.62	LCEBR	/	Stable
AsClSe	69	6.3.1933	1.36	C2DB	hexagonal	nHSP-SOC	Γ	0.62	LCEBR	/	Stable
GaInTe ₂	69	6.3.2064	0.98	C2DB	hexagonal	/	Γ	0.62	LCEBR	/	Stable
HgClHO	69	6.3.2083	1.54	C2DB	hexagonal	/	Γ	0.62	LCEBR	/	Stable
ClSbTe	69	6.3.2042	1.29	C2DB	hexagonal	nHSP-SOC	Γ	0.62	LCEBR	/	Stable
BiFS	69	6.3.1965	1.72	C2DB	hexagonal	/	Γ	0.61	LCEBR	/	Stable
PbS	69	6.3.2141	1.98	C2DB	hexagonal	/	Γ	0.61	LCEBR	/	Stable
CdI	72	3.3.409	1.95	C2DB	hexagonal	/	Γ	0.61	OAI	/	Stable
SnBr ₂	72	6.3.2331	2.12	C2DB	hexagonal	/	Γ	0.61	LCEBR	/	Stable
PbAsS ₃	71	3.3.311	1.25	C2DB	hexagonal	/	Γ	0.60	OAI	/	Stable
PbTe	72	6.3.2560	0.73	C2DB	hexagonal	<i>K</i> -SOC	Γ	0.60	LCEBR	/	Stable
InTe	78	3.3.510	1.25	C2DB	hexagonal	/	Γ	0.60	OAI	/	Stable
BrSbTe	69	6.3.2011	1.09	C2DB	hexagonal	nHSP-SOC	Γ	0.60	LCEBR	/	Stable
FSSb	69	6.3.2057	1.80	C2DB	hexagonal	/	Γ	0.60	LCEBR	/	Stable
CaCuClSe	69	6.3.2016	1.02	C2DB	hexagonal	/	Γ	0.59	LCEBR	/	Stable
Ag ₃ AsO ₄	69	6.3.1903	1.27	C2DB	hexagonal	/	Γ	0.59	LCEBR	/	Stable
FSbSe	69	6.3.2058	1.82	C2DB	hexagonal	/	Γ	0.59	LCEBR	/	Stable
PbI ₂	78	6.3.2651	2.03	C2DB	hexagonal	/	Γ	0.59	LCEBR	/	Stable
InAs	69	6.3.1946	0.68	C2DB	hexagonal	Γ -SOC	Γ	0.59	LCEBR	/	Stable
AgGaP ₂ S ₆	67	3.3.220	1.30	C2DB	hexagonal	/	Γ	0.59	OAI	/	Stable
CdBrHO	69	6.3.2072	1.73	C2DB	hexagonal	Γ -SOC	Γ	0.59	LCEBR	/	Stable
Bi ₂ S ₃	72	6.1.21	0.71	C2DB	hexagonal	/	Γ	0.58	LCEBR	/	Stable
FSi	72	3.3.422	0.67	C2DB	hexagonal	/	Γ	0.58	OAI	/	Stable
TIS	78	3.3.525	0.67	C2DB	hexagonal	nHSP	Γ	0.58	OAI	/	Stable
SnI ₂	72	6.3.2508	1.89	C2DB	hexagonal	/	Γ	0.58	LCEBR	/	Stable
MoSTe	69	3.3.286	1.03	C2DB	hexagonal	Γ	<i>K</i>	0.58	OAI	/	Stable
CuI	72	6.1.41	1.82	C2DB	hexagonal	Γ -SOC	Γ	0.58	LCEBR	Yes	Stable
GaInS ₂	69	6.3.2063	1.77	C2DB	hexagonal	nHSP	Γ	0.58	LCEBR	/	Stable
MoOSe	69	3.3.284	0.78	C2DB	hexagonal	Γ	<i>K</i>	0.58	OAI	/	Stable
HgH ₂ O ₂	72	6.3.2472	0.68	C2DB	hexagonal	/	Γ	0.58	LCEBR	/	Stable
Br ₂ Ge	72	6.3.2317	2.30	C2DB	hexagonal	/	Γ	0.57	LCEBR	/	Stable
PbBr ₂	72	6.3.2327	2.32	C2DB	hexagonal	/	Γ	0.57	LCEBR	/	Stable
ZnI	72	3.3.451	2.09	C2DB	hexagonal	/	Γ	0.57	OAI	/	Stable
TIS	72	3.3.470	0.62	C2DB	hexagonal	nHSP	Γ	0.57	OAI	/	Stable

Bi ₂ S ₂ Se	72	6.3.2307	0.66	C2DB	hexagonal	/	Γ	0.57	LCEBR	/	Stable
AsClTe	69	6.3.1935	1.50	C2DB	hexagonal	nHSP-SOC	Γ	0.57	LCEBR	/	Stable
PbSe ₂	78	3.3.522	1.32	C2DB	hexagonal	/	Γ	0.57	OAI	/	Stable
SnCl ₂	72	6.3.2415	2.34	C2DB	hexagonal	/	Γ	0.57	LCEBR	/	Stable
GaSSi	72	3.3.431	1.13	C2DB	hexagonal	/	Γ	0.57	OAI	/	Stable
SnF ₂	72	6.3.2432	2.36	C2DB	hexagonal	<i>K</i>	Γ	0.57	LCEBR	/	Stable
HgCl ₂	72	6.3.2405	2.36	C2DB	hexagonal	/	Γ	0.57	LCEBR	/	Stable
CdFHS	69	6.3.2080	1.87	C2DB	hexagonal	/	Γ	0.56	LCEBR	/	Stable
CdBr ₂	78	6.3.2612	2.37	C2DB	hexagonal	Γ -SOC	Γ	0.56	LCEBR	/	Stable
HgPS ₃	71	3.3.334	0.98	C2DB	hexagonal	<i>K</i>	Γ	0.56	OAI	Yes	Stable
CF ₂ Si	69	6.3.2014	1.91	C2DB	hexagonal	/	Γ	0.56	LCEBR	/	Stable
ZnTe	72	6.3.2590	0.57	C2DB	hexagonal	Γ -SOC	Γ	0.55	LCEBR	/	Stable
TlF ₃	80	6.3.2687	2.88	C2DB	hexagonal	/	Γ	0.55	LCEBR	/	Stable
CdH ₂ O ₂	72	6.3.2466	2.24	C2DB	hexagonal	/	Γ	0.55	LCEBR	Yes	Stable
OSb ₂ Se ₂	72	6.3.2551	0.60	C2DB	hexagonal	/	Γ	0.55	LCEBR	/	Stable
CdPS ₃	71	3.3.314	1.91	C2DB	hexagonal	<i>K</i>	Γ	0.55	OAI	Yes	Stable
AsFSe	69	6.3.1938	2.08	C2DB	hexagonal	/	Γ	0.55	LCEBR	/	Stable
CuInP ₂ S ₆	65	6.3.1837	1.56	C2DB	hexagonal	/	Γ	0.55	LCEBR	/	Stable
Hg ₃ B ₂ S ₆	79	6.3.2664	2.12	C2DB	hexagonal	/	Γ	0.54	LCEBR	/	Stable
In ₂ Se ₃	69	6.3.2123	0.78	C2DB	hexagonal	/	Γ	0.54	LCEBR	/	Stable
ZnBr	72	3.3.388	2.37	C2DB	hexagonal	/	Γ	0.54	OAI	/	Stable
AsFS	69	6.3.1937	2.12	C2DB	hexagonal	/	Γ	0.54	LCEBR	/	Stable
InGeSe ₃	71	3.3.329	1.20	C2DB	hexagonal	/	Γ	0.54	OAI	/	Stable
CdO	72	6.3.2392	0.53	C2DB	hexagonal	/	Γ	0.54	LCEBR	/	Stable
S ₃ Sb ₂	72	6.1.62	0.63	C2DB	hexagonal	/	Γ	0.54	LCEBR	/	Stable
PbAs ₂ S ₄	72	6.3.2285	0.95	C2DB	hexagonal	/	Γ	0.54	LCEBR	/	Stable
Bi ₂ SSe ₂	72	6.3.2310	0.55	C2DB	hexagonal	/	Γ	0.53	LCEBR	/	Stable
GaSeSi	72	3.3.433	1.39	C2DB	hexagonal	/	Γ	0.53	OAI	/	Stable
CdHIS	69	6.3.2082	2.06	C2DB	hexagonal	Γ -SOC	Γ	0.53	LCEBR	/	Stable
AuInP ₂ S ₆	67	3.3.239	0.81	C2DB	hexagonal	/	Γ	0.53	OAI	/	Stable
S ₂ Sb ₂ Se	72	6.3.2575	0.64	C2DB	hexagonal	/	Γ	0.53	LCEBR	/	Stable
CrO ₂	78	3.3.496	0.42	C2DB	hexagonal	Γ	<i>K</i>	0.53	OAI	/	Stable
TlSe	78	3.3.526	0.49	C2DB	hexagonal	nHSP	Γ	0.53	OAI	/	Stable
InGeS ₃	71	3.3.328	1.65	C2DB	hexagonal	/	Γ	0.53	OAI	/	Stable
CdBrI	69	6.3.1986	2.22	C2DB	hexagonal	Γ -SOC	Γ	0.53	LCEBR	/	Stable
InSb	69	6.3.2129	0.48	C2DB	hexagonal	Γ -SOC	Γ	0.52	LCEBR	/	Stable
S ₂ Sb ₂ Te	72	6.3.2576	0.87	C2DB	hexagonal	/	Γ	0.52	LCEBR	/	Stable
PtF	72	3.3.421	0.80	C2DB	hexagonal	Γ	/	0.52	OAI	/	Stable
PbAsSe ₃	71	3.3.312	0.71	C2DB	hexagonal	/	Γ	0.52	OAI	/	Stable
AuGaP ₂ S ₆	67	3.3.237	0.79	C2DB	hexagonal	/	Γ	0.52	OAI	/	Stable
Cl ₂ Ge	72	6.3.2402	2.62	C2DB	hexagonal	/	Γ	0.52	LCEBR	/	Stable
AlGeTe	72	3.3.372	0.85	C2DB	hexagonal	/	Γ	0.52	OAI	/	Stable
AlN	78	6.3.2602	2.88	C2DB	hexagonal	<i>K</i>	Γ	0.52	LCEBR	/	Stable
SnO ₂	72	6.3.2547	2.63	C2DB	hexagonal	/	Γ	0.52	LCEBR	/	Stable
SnPSe ₃	71	3.3.360	0.72	C2DB	hexagonal	/	Γ	0.52	OAI	/	Stable
F ₂ Ge	72	6.3.2420	2.64	C2DB	hexagonal	<i>K</i>	Γ	0.52	LCEBR	/	Stable
CdHIO	69	6.3.2081	0.66	C2DB	hexagonal	Γ -SOC	Γ	0.52	LCEBR	/	Stable
CuInP ₂ S ₆	67	3.3.249	0.97	C2DB	hexagonal	/	Γ	0.52	OAI	/	Stable
BiO	78	3.3.479	0.45	C2DB	hexagonal	Γ	<i>K</i> -SOC	0.52	OAI	/	Stable
GePSe ₃	71	3.3.332	0.98	C2DB	hexagonal	/	Γ	0.52	OAI	/	Stable
TlSe	72	3.3.471	0.44	C2DB	hexagonal	nHSP	Γ	0.51	OAI	/	Stable

In ₂ STe	69	6.3.2122	0.64	C2DB	hexagonal	Γ -SOC	Γ	0.51	LCEBR	/	Stable
CdPSe ₃	71	3.3.315	1.27	C2DB	hexagonal	K	Γ	0.51	OAI	Yes	Stable
AuP ₂ SbSe ₆	65	6.3.1833	0.85	C2DB	hexagonal	/	Γ	0.51	LCEBR	/	Stable
PbCl ₂	72	6.3.2411	2.69	C2DB	hexagonal	/	Γ	0.51	LCEBR	/	Stable
WO _{Te}	69	3.3.291	0.56	C2DB	hexagonal	Γ	nHSP-SOC	0.51	OAI	/	Stable
SnPS ₃	71	3.3.356	1.06	C2DB	hexagonal	Γ	K	0.51	OAI	Yes	Stable
AuBiP ₂ Se ₆	65	6.3.1831	0.94	C2DB	hexagonal	/	Γ	0.50	LCEBR	/	Stable
CdTe	72	6.3.2395	0.67	C2DB	hexagonal	Γ -SOC	Γ	0.50	LCEBR	/	Stable
BiI ₃	79	6.3.2666	1.29	C2DB	hexagonal	/	Γ	0.50	LCEBR	/	Stable
PbS ₄ Sb ₂	72	6.3.2562	0.71	C2DB	hexagonal	/	Γ	0.50	LCEBR	/	Stable
Bi ₂ PbS ₄	72	6.3.2306	0.74	C2DB	hexagonal	/	Γ	0.50	LCEBR	/	Stable
ZnH ₂ S ₂	72	6.3.2487	2.54	C2DB	hexagonal	/	Γ	0.50	LCEBR	/	Stable
ZnPSe ₃	71	3.3.362	1.30	C2DB	hexagonal	K	Γ	0.50	OAI	/	Stable
ZnSe	72	6.3.2586	1.61	C2DB	hexagonal	/	Γ	0.50	LCEBR	/	Stable
InSSi	72	3.3.453	1.53	C2DB	hexagonal	/	Γ	0.50	OAI	/	Stable
GeI ₂	72	6.3.2453	1.98	C2DB	hexagonal	nHSP	Γ	0.49	LCEBR	Yes	Stable
BiCl ₃	80	6.3.2682	2.51	C2DB	hexagonal	/	Γ	0.49	LCEBR	/	Stable
PbPS ₃	71	3.3.347	1.48	C2DB	hexagonal	Γ	K	0.49	OAI	/	Stable
AgGaP ₂ Se ₆	67	3.3.221	0.91	C2DB	hexagonal	/	Γ	0.49	OAI	Yes	Stable
AlAuP ₂ S ₆	67	3.3.228	1.27	C2DB	hexagonal	/	Γ	0.49	OAI	/	Stable
InO	78	3.3.508	0.37	C2DB	hexagonal	/	Γ	0.49	OAI	/	Stable
TlTe	78	3.3.529	0.37	C2DB	hexagonal	/	Γ	0.49	OAI	/	Stable
CdZnSeTe	69	6.3.2023	0.73	C2DB	hexagonal	Γ -SOC	Γ	0.48	LCEBR	/	Stable
BiCuAs ₂ S ₆	65	6.3.1827	1.09	C2DB	hexagonal	/	Γ	0.48	LCEBR	/	Stable
GaGeSe ₃	71	3.3.324	1.00	C2DB	hexagonal	/	Γ	0.48	OAI	/	Stable
As ₂ S ₃	72	6.3.2291	0.92	C2DB	hexagonal	nHSP	Γ	0.48	LCEBR	/	Stable
InGeS	72	3.3.437	0.42	C2DB	hexagonal	/	Γ	0.48	OAI	/	Stable
SSb ₂ Se ₂	72	6.3.2580	0.48	C2DB	hexagonal	/	Γ	0.48	LCEBR	/	Stable
TlTe	72	3.3.473	0.32	C2DB	hexagonal	/	Γ	0.48	OAI	/	Stable
Zr ₃ N ₂ O ₂	78	3.3.514	0.40	C2DB	hexagonal	Γ	M	0.47	OAI	/	Stable
Bi ₂ STe ₂	72	6.3.2311	0.36	C2DB	hexagonal	/	Γ	0.47	LCEBR	/	Stable
CuGaP ₂ S ₆	67	3.3.247	0.88	C2DB	hexagonal	/	Γ	0.47	OAI	/	Stable
CuP ₂ SbSe ₆	65	6.3.1840	1.05	C2DB	hexagonal	/	Γ	0.47	LCEBR	/	Stable
GaGeSe	72	3.3.427	0.38	C2DB	hexagonal	/	Γ	0.47	OAI	/	Stable
Bi ₂ S ₂ Te	72	6.3.2308	0.34	C2DB	hexagonal	Γ -SOC	Γ	0.47	LCEBR	/	Stable
ZnH ₂ O ₂	72	6.3.2482	2.29	C2DB	hexagonal	/	Γ	0.47	LCEBR	/	Stable
GaS	72	3.3.432	2.16	C2DB	hexagonal	nHSP	Γ	0.47	OAI	Yes	Stable
AgAs ₂ S ₆ Sb	65	6.3.1818	1.12	C2DB	hexagonal	/	Γ	0.47	LCEBR	/	Stable
AgBiAs ₂ S ₆	65	6.3.1815	1.34	C2DB	hexagonal	/	Γ	0.47	LCEBR	/	Stable
PbAs ₂ Se ₄	72	6.3.2286	0.63	C2DB	hexagonal	/	Γ	0.47	LCEBR	/	Stable
SnF	72	1.3.271	0.28	C2DB	hexagonal	nHSP	Γ	0.46	SEBR	/	Stable
GaGeS ₃	71	3.3.323	1.56	C2DB	hexagonal	/	Γ	0.46	OAI	/	Stable
As ₂ S ₂ Se	72	6.3.2290	0.82	C2DB	hexagonal	nHSP	Γ	0.46	LCEBR	/	Stable
Sb ₂ Se ₃	72	6.1.65	0.44	C2DB	hexagonal	nHSP	Γ	0.46	LCEBR	/	Stable
AgP ₂ SbSe ₆	65	6.3.1825	1.24	C2DB	hexagonal	/	Γ	0.46	LCEBR	/	Stable
HgHIO	69	6.3.2086	0.45	C2DB	hexagonal	Γ -SOC	Γ	0.45	LCEBR	/	Stable
ScBrF	72	3.3.381	0.31	C2DB	hexagonal	Γ	/	0.45	OAI	/	Stable
As ₂ STe ₂	72	6.3.2293	0.74	C2DB	hexagonal	nHSP	Γ	0.45	LCEBR	/	Stable
SnH	72	3.3.443	0.25	C2DB	hexagonal	Γ -SOC	Γ	0.45	OAI	/	Stable
InGeSe	72	3.3.438	0.54	C2DB	hexagonal	/	Γ	0.45	OAI	/	Stable
AgBiAs ₂ Se ₆	65	6.3.1816	0.65	C2DB	hexagonal	/	Γ	0.45	LCEBR	/	Stable

InSeSi	72	3.3.455	1.51	C2DB	hexagonal	nHSP	Γ	0.45	OAI	/	Stable
HgPSe ₃	71	3.3.335	0.56	C2DB	hexagonal	K	Γ	0.45	OAI	Yes	Stable
InSe ₃ Si	71	3.3.340	1.39	C2DB	hexagonal	/	Γ	0.45	OAI	/	Stable
ZnGeO ₃	71	6.3.2236	2.73	C2DB	hexagonal	/	Γ	0.45	LCEBR	Yes	Stable
AlCdGaS ₄	69	6.3.1914	0.72	C2DB	hexagonal	/	Γ	0.44	LCEBR	/	Stable
SnS ₄ Sb ₂	72	6.3.2579	0.56	C2DB	hexagonal	/	Γ	0.44	LCEBR	/	Stable
Cd ₂ SeTe	69	6.3.2017	0.42	C2DB	hexagonal	Γ -SOC	Γ	0.44	LCEBR	/	Stable
CdClHO	69	6.3.2077	2.61	C2DB	hexagonal	/	Γ	0.44	LCEBR	Yes	Stable
PbSb ₂ Se ₄	72	6.3.2563	0.49	C2DB	hexagonal	/	Γ	0.44	LCEBR	/	Stable
CdS	72	6.3.2393	1.81	C2DB	hexagonal	/	Γ	0.44	LCEBR	/	Stable
InSiTe	72	3.3.457	0.46	C2DB	hexagonal	/	Γ	0.43	OAI	/	Stable
As ₂ SSe ₂	72	6.3.2292	0.72	C2DB	hexagonal	nHSP	Γ	0.43	LCEBR	/	Stable
BiBr ₃	79	6.3.2665	2.03	C2DB	hexagonal	/	Γ	0.43	LCEBR	/	Stable
Br ₃ Sb	79	6.3.2669	2.08	C2DB	hexagonal	/	Γ	0.43	LCEBR	/	Stable
SSb ₂ Te ₂	72	6.3.2581	0.52	C2DB	hexagonal	/	Γ	0.43	LCEBR	/	Stable
Bi ₂ SnS ₄	72	6.3.2309	0.51	C2DB	hexagonal	/	Γ	0.43	LCEBR	/	Stable
MgH ₂ Se ₂	72	6.3.2475	2.75	C2DB	hexagonal	/	Γ	0.43	LCEBR	/	Stable
TlCl ₃	79	6.3.2676	1.66	C2DB	hexagonal	/	Γ	0.43	LCEBR	/	Stable
BiCuP ₂ Se ₆	65	6.3.1836	1.11	C2DB	hexagonal	/	Γ	0.43	LCEBR	Yes	Stable
IrS ₃ Sb	71	6.3.2249	0.28	C2DB	hexagonal	/	Γ	0.43	LCEBR	/	Stable
IrAsSe ₃	71	6.3.2200	0.30	C2DB	hexagonal	/	Γ	0.42	LCEBR	/	Stable
IrAsS ₃	71	6.3.2199	0.27	C2DB	hexagonal	/	Γ	0.42	LCEBR	/	Stable
CdFHO	69	6.3.2079	2.73	C2DB	hexagonal	/	Γ	0.42	LCEBR	/	Stable
In ₂ Mg ₂ S ₅	72	6.3.2512	1.31	C2DB	hexagonal	/	Γ	0.42	LCEBR	/	Stable
InI ₃	79	6.3.2677	0.70	C2DB	hexagonal	Γ -SOC	Γ	0.42	LCEBR	/	Stable
AgAlP ₂ Se ₆	67	3.3.214	1.37	C2DB	hexagonal	/	Γ	0.42	OAI	/	Stable
IrSbSe ₃	71	6.3.2250	0.30	C2DB	hexagonal	/	Γ	0.42	LCEBR	/	Stable
CuInP ₂ Se ₆	65	6.3.1838	0.91	C2DB	hexagonal	/	Γ	0.42	LCEBR	/	Stable
As ₂ SeTe ₂	72	6.3.2297	0.61	C2DB	hexagonal	/	Γ	0.42	LCEBR	/	Stable
AlGeSe ₃	71	3.3.299	1.63	C2DB	hexagonal	/	Γ	0.41	OAI	/	Stable
PbPTe ₃	71	3.3.349	0.75	C2DB	hexagonal	/	Γ	0.41	OAI	/	Stable
AuScP ₂ Se ₆	67	3.3.242	0.98	C2DB	hexagonal	/	Γ	0.41	OAI	/	Stable
CdBrHS	69	6.3.2073	2.78	C2DB	hexagonal	/	Γ	0.41	LCEBR	/	Stable
CdClHS	69	6.3.2078	2.78	C2DB	hexagonal	/	Γ	0.41	LCEBR	/	Stable
As ₂ Se ₃	72	6.3.2295	0.62	C2DB	hexagonal	nHSP	Γ	0.41	LCEBR	/	Stable
MgClI	69	6.3.2033	2.93	C2DB	hexagonal	Γ -SOC	Γ	0.41	LCEBR	/	Stable
ZnPS ₃	71	3.3.358	2.10	C2DB	hexagonal	K	Γ	0.40	OAI	Yes	Stable
HfClN	72	6.3.2403	2.33	C2DB	hexagonal	Γ	K	0.40	LCEBR	Yes	Stable
AlCdInS ₄	69	6.3.1916	0.93	C2DB	hexagonal	/	Γ	0.40	LCEBR	/	Stable
MoOTe	69	3.3.285	0.21	C2DB	hexagonal	Γ	/	0.40	OAI	/	Stable
PbAs ₂ Te ₄	72	6.3.2287	0.58	C2DB	hexagonal	/	Γ	0.40	LCEBR	/	Stable
AlAuP ₂ Se ₆	67	3.3.229	0.77	C2DB	hexagonal	/	Γ	0.39	OAI	/	Stable
SnTe	72	6.3.2588	0.72	C2DB	hexagonal	nHSP	Γ	0.39	LCEBR	/	Stable
MgH ₂ Te ₂	72	6.3.2476	2.22	C2DB	hexagonal	/	Γ	0.39	LCEBR	/	Stable
MgF ₂ O ₂	72	6.3.2425	2.83	C2DB	hexagonal	/	Γ	0.38	LCEBR	/	Stable
AgAs ₂ SbSe ₆	65	6.3.1819	0.60	C2DB	hexagonal	/	Γ	0.38	LCEBR	/	Stable
CrSTe	69	3.3.277	0.29	C2DB	hexagonal	Γ	K	0.38	OAI	/	Stable
BiCuAs ₂ Se ₆	65	6.3.1828	0.42	C2DB	hexagonal	/	Γ	0.38	LCEBR	/	Stable
TlBr ₃	79	6.3.2671	0.89	C2DB	hexagonal	/	Γ	0.38	LCEBR	/	Stable
Bi ₂ SnSe ₄	72	6.3.2312	0.35	C2DB	hexagonal	/	Γ	0.37	LCEBR	/	Stable
P ₂ STe ₂	72	6.3.2554	0.66	C2DB	hexagonal	nHSP	Γ	0.37	LCEBR	/	Stable

AgAlP ₂ S ₆	67	3.3.213	1.96	C2DB	hexagonal	/	Γ	0.36	OAI	/	Stable
SnAs ₂ Se ₄	72	6.3.2296	0.38	C2DB	hexagonal	/	Γ	0.36	LCEBR	/	Stable
CdIn ₂ S ₄	72	6.3.2398	0.62	C2DB	hexagonal	/	Γ	0.36	LCEBR	/	Stable
Sb ₂ Te ₃	72	6.3.2583	0.40	C2DB	hexagonal	nHSP	Γ	0.36	LCEBR	/	Stable
AuGaP ₂ Se ₆	67	3.3.238	0.46	C2DB	hexagonal	/	Γ	0.36	OAI	/	Stable
AlGeSe	72	3.3.371	0.62	C2DB	hexagonal	/	Γ	0.35	OAI	/	Stable
PbSb ₂ Te ₄	72	6.3.2564	0.43	C2DB	hexagonal	/	Γ	0.35	LCEBR	Yes	Stable
AlCuP ₂ Se ₆	67	3.3.230	1.54	C2DB	hexagonal	/	Γ	0.35	OAI	/	Stable
AgTlP ₂ Se ₆	67	3.3.227	0.25	C2DB	hexagonal	/	Γ	0.35	OAI	/	Stable
CuAs ₂ SbSe ₆	65	6.3.1829	0.50	C2DB	hexagonal	/	Γ	0.35	LCEBR	/	Stable
TlO ₃ Sb	67	6.3.1902	2.84	C2DB	hexagonal	/	Γ	0.35	LCEBR	Yes	Stable
As ₂ Te ₃	72	6.3.2299	0.56	C2DB	hexagonal	/	Γ	0.34	LCEBR	/	Stable
In ₂ Mg ₂ Se ₅	72	6.3.2513	0.71	C2DB	hexagonal	Γ -SOC	Γ	0.34	LCEBR	/	Stable
AlCuP ₂ Se ₆	67	3.3.231	0.95	C2DB	hexagonal	/	Γ	0.34	OAI	/	Stable
In ₂ MgSe ₄	72	6.3.2515	0.59	C2DB	hexagonal	Γ -SOC	Γ	0.34	LCEBR	/	Stable
BiCl ₃	71	6.3.2205	2.69	C2DB	hexagonal	/	Γ	0.34	LCEBR	/	Stable
P ₂ SeTe ₂	72	6.3.2556	0.51	C2DB	hexagonal	nHSP	Γ	0.33	LCEBR	/	Stable
Cl ₃ Sb	71	6.3.2221	2.68	C2DB	hexagonal	/	Γ	0.33	LCEBR	/	Stable
Nb ₃ I ₇ S	69	6.3.2103	0.56	C2DB	hexagonal	/	Γ	0.33	LCEBR	/	Stable
AuInP ₂ Se ₆	67	3.3.240	0.42	C2DB	hexagonal	/	Γ	0.32	OAI	/	Stable
AlSe ₃ Si	71	3.3.303	2.14	C2DB	hexagonal	/	Γ	0.32	OAI	/	Stable
IrAsTe ₃	71	6.3.2201	0.34	C2DB	hexagonal	/	Γ	0.32	LCEBR	/	Stable
IrSbTe ₃	71	6.3.2251	0.33	C2DB	hexagonal	/	Γ	0.31	LCEBR	/	Stable
CuInP ₂ Se ₆	67	3.3.250	0.49	C2DB	hexagonal	/	Γ	0.31	OAI	Yes	Stable
CdGaInS ₄	69	6.3.2018	0.42	C2DB	hexagonal	/	Γ	0.30	LCEBR	Yes	Stable
CdGa ₂ S ₄	72	6.3.2397	0.51	C2DB	hexagonal	/	Γ	0.30	LCEBR	/	Stable
SnAs ₂ Te ₄	72	6.3.2298	0.39	C2DB	hexagonal	nHSP	Γ	0.29	LCEBR	/	Stable
Al ₂ MgO ₄	72	6.3.2268	2.64	C2DB	hexagonal	/	Γ	0.28	LCEBR	/	Stable
RuH ₂ O ₂	72	6.3.2480	0.49	C2DB	hexagonal	/	Γ	0.27	LCEBR	/	Stable
CuGaP ₂ Se ₆	67	3.3.248	0.46	C2DB	hexagonal	/	Γ	0.27	OAI	/	Stable
P ₂ Se ₃	72	6.3.2555	0.42	C2DB	hexagonal	nHSP	Γ	0.26	LCEBR	/	Stable
Al ₂ MgTe ₄	72	6.3.2271	0.49	C2DB	hexagonal	Γ -SOC	Γ	0.26	LCEBR	/	Stable
RhAsTe ₃	71	6.3.2204	0.26	C2DB	hexagonal	Γ	Γ	0.26	LCEBR	/	Stable
HgPTe ₃	71	3.3.336	0.35	C2DB	hexagonal	/	Γ	0.26	OAI	/	Stable
SnPTe ₃	71	3.3.363	0.43	C2DB	hexagonal	/	Γ	0.26	OAI	/	Stable
WBr ₃	79	3.3.531	0.23	C2DB	hexagonal	Γ -SOC	Γ	0.26	OAI	/	Stable
IrPTe ₃	71	6.3.2248	0.23	C2DB	hexagonal	/	Γ	0.25	LCEBR	/	Stable
Ga ₂ MgSe ₄	72	6.3.2443	0.33	C2DB	hexagonal	Γ -SOC	Γ	0.24	LCEBR	/	Stable
In ₂ Mg ₂ Te ₅	72	6.3.2514	0.42	C2DB	hexagonal	Γ -SOC	Γ	0.24	LCEBR	/	Stable
Ga ₂ Mg ₂ Se ₅	72	6.3.2442	0.44	C2DB	hexagonal	Γ -SOC	Γ	0.24	LCEBR	/	Stable
CdInTlS ₄	69	6.3.2021	0.33	C2DB	hexagonal	/	Γ	0.23	LCEBR	/	Stable
AlPSe ₃	70	6.3.2167	0.61	C2DB	hexagonal	nHSP-SOC	Γ	0.23	LCEBR	/	Stable
In ₂ MgTe ₄	72	6.3.2516	0.29	C2DB	hexagonal	Γ -SOC	Γ	0.22	LCEBR	/	Stable
InCl ₃	79	6.3.2674	2.87	C2DB	hexagonal	/	Γ	0.21	LCEBR	/	Stable
RhSbTe ₃	71	6.3.2257	0.24	C2DB	hexagonal	Γ	Γ	0.20	LCEBR	/	Stable
AlCdInSe ₄	69	6.3.1917	0.31	C2DB	hexagonal	/	Γ	0.20	LCEBR	/	Stable
CoSbSe ₃	71	6.3.2228	0.23	C2DB	hexagonal	Γ	Γ	0.19	LCEBR	/	Stable
AlGeS	72	3.3.370	0.20	C2DB	hexagonal	/	Γ	0.19	OAI	/	Stable
TlAsO ₃	67	6.3.1885	2.89	C2DB	hexagonal	/	Γ	0.18	LCEBR	/	Stable

TABLE S34: Computationally unstable materials with valley type: hexagonal- Γ .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
AlAs	78	6.4.691	1.24	C2DB	hexagonal	K	Γ	0.75	LCEBR	/	Unstable
CdS	78	6.4.702	1.63	C2DB	hexagonal	/	Γ	0.73	LCEBR	/	Unstable
SrO	78	6.4.725	1.75	C2DB	hexagonal	K -SOC	Γ	0.71	LCEBR	/	Unstable
GeO ₂	78	6.4.712	1.39	C2DB	hexagonal	/	Γ	0.71	LCEBR	/	Unstable
CdSe	69	6.4.528	1.11	C2DB	hexagonal	Γ -SOC	Γ	0.69	LCEBR	/	Unstable
CdTe	69	6.4.529	1.01	C2DB	hexagonal	Γ -SOC	Γ	0.69	LCEBR	/	Unstable
CdO	78	6.4.701	0.76	C2DB	hexagonal	/	Γ	0.68	LCEBR	/	Unstable
GeH ₂ O ₂	72	6.4.655	1.09	C2DB	hexagonal	K	Γ	0.68	LCEBR	/	Unstable
PbH	72	1.4.179	0.96	C2DB	hexagonal	nHSP	Γ	0.67	SEBR	/	Unstable
CdF ₂ O ₂	72	6.4.623	1.51	C2DB	hexagonal	/	Γ	0.67	LCEBR	/	Unstable
As ₂ OS ₂	72	6.4.603	0.99	C2DB	hexagonal	/	Γ	0.67	LCEBR	/	Unstable
F ₂ Si	72	6.4.646	1.78	C2DB	hexagonal	K	Γ	0.66	LCEBR	/	Unstable
Br ₂ Si	72	6.4.613	1.82	C2DB	hexagonal	/	Γ	0.66	LCEBR	/	Unstable
FOP	69	6.4.557	1.07	C2DB	hexagonal	K	Γ	0.65	LCEBR	/	Unstable
SnH ₂ O ₂	72	6.4.659	0.88	C2DB	hexagonal	K	Γ	0.64	LCEBR	/	Unstable
AsFO	69	6.4.484	1.55	C2DB	hexagonal	K	Γ	0.64	LCEBR	/	Unstable
ZnF ₂ O ₂	72	6.4.641	1.76	C2DB	hexagonal	/	Γ	0.63	LCEBR	/	Unstable
GaTlS ₂	69	6.4.562	1.10	C2DB	hexagonal	/	Γ	0.62	LCEBR	/	Unstable
HgClFO	69	6.4.531	1.28	C2DB	hexagonal	/	Γ	0.62	LCEBR	/	Unstable
HgBrFO	69	6.4.502	1.26	C2DB	hexagonal	/	Γ	0.62	LCEBR	/	Unstable
PbF ₂ O ₂	72	6.4.638	1.61	C2DB	hexagonal	/	Γ	0.62	LCEBR	/	Unstable
Cl ₂ Si	72	6.4.627	2.08	C2DB	hexagonal	/	Γ	0.61	LCEBR	/	Unstable
HgFHS	69	6.4.564	0.94	C2DB	hexagonal	/	Γ	0.61	LCEBR	/	Unstable
CdClFS	69	6.4.520	1.68	C2DB	hexagonal	/	Γ	0.60	LCEBR	/	Unstable
SnO ₂	78	6.4.722	0.62	C2DB	hexagonal	/	Γ	0.59	LCEBR	/	Unstable
PbCl ₂ O	78	6.4.703	0.67	C2DB	hexagonal	/	Γ	0.58	LCEBR	/	Unstable
CdGeS ₂	69	6.4.524	0.83	C2DB	hexagonal	/	Γ	0.57	LCEBR	/	Unstable
SnF ₂ O ₂	72	6.4.639	1.08	C2DB	hexagonal	K	Γ	0.57	LCEBR	/	Unstable
HgClFS	69	6.4.532	0.82	C2DB	hexagonal	/	Γ	0.57	LCEBR	/	Unstable
CF ₂ Ge	69	6.4.517	1.85	C2DB	hexagonal	/	Γ	0.57	LCEBR	/	Unstable
CdBrFS	69	6.4.498	1.89	C2DB	hexagonal	/	Γ	0.56	LCEBR	/	Unstable
FPS	69	6.4.559	2.04	C2DB	hexagonal	/	Γ	0.56	LCEBR	/	Unstable
ZnBr ₂	78	6.4.698	2.41	C2DB	hexagonal	Γ -SOC	Γ	0.56	LCEBR	/	Unstable
OS ₂ Sb ₂	72	6.4.680	0.61	C2DB	hexagonal	/	Γ	0.55	LCEBR	/	Unstable
I ₂ Si	72	6.4.669	1.60	C2DB	hexagonal	nHSP	Γ	0.55	LCEBR	/	Unstable
CdF ₂ S ₂	72	6.4.624	1.08	C2DB	hexagonal	M	Γ	0.53	LCEBR	/	Unstable
HgO	78	1.4.265	0.30	C2DB	hexagonal	nHSP-SOC	Γ	0.53	NLC	/	Unstable
AuCl	78	1.4.247	0.29	C2DB	hexagonal	nHSP-SOC	Γ	0.53	NLC	/	Unstable
AuBr	72	6.4.604	0.49	C2DB	hexagonal	/	Γ	0.53	LCEBR	/	Unstable
HfF ₂	78	3.4.181	1.14	C2DB	hexagonal	K	Γ	0.52	OAI	/	Unstable
CdF ₂ S	69	6.4.521	0.65	C2DB	hexagonal	/	Γ	0.52	LCEBR	/	Unstable
AuBr	78	1.4.246	0.24	C2DB	hexagonal	/	Γ	0.51	NLC	/	Unstable
ZnF ₂ S ₂	72	6.4.645	1.07	C2DB	hexagonal	M	Γ	0.51	LCEBR	/	Unstable
CdFIO	69	6.4.522	1.36	C2DB	hexagonal	Γ -SOC	Γ	0.51	LCEBR	/	Unstable
CdSe	72	6.4.621	0.96	C2DB	hexagonal	/	Γ	0.50	LCEBR	/	Unstable
InO	72	3.4.155	0.35	C2DB	hexagonal	/	Γ	0.48	OAI	/	Unstable
CCl	72	3.4.135	1.47	C2DB	hexagonal	/	Γ	0.47	OAI	/	Unstable
CdF ₂	78	6.4.700	2.99	C2DB	hexagonal	/	Γ	0.46	LCEBR	/	Unstable
CdBrFO	69	6.4.497	2.30	C2DB	hexagonal	/	Γ	0.45	LCEBR	/	Unstable

HgF ₂ O	69	6.4.552	0.43	C2DB	hexagonal	/	Γ	0.45	LCEBR	/	Unstable
CdClFO	69	6.4.519	2.75	C2DB	hexagonal	/	Γ	0.42	LCEBR	/	Unstable
SrSe	72	6.4.690	2.94	C2DB	hexagonal	/	Γ	0.42	LCEBR	/	Unstable
CdTe	72	6.4.622	0.88	C2DB	hexagonal	/	Γ	0.41	LCEBR	/	Unstable
AIP	78	6.4.692	2.29	C2DB	hexagonal	K	Γ	0.41	LCEBR	/	Unstable
MgF ₂ S ₂	72	6.4.637	1.79	C2DB	hexagonal	/	Γ	0.41	LCEBR	/	Unstable
BiSe	72	3.1.13	0.38	C2DB	hexagonal	Γ	K	0.37	OAI	/	Unstable
BiTe	72	3.4.129	0.37	C2DB	hexagonal	Γ	Γ	0.34	OAI	/	Unstable
CaF ₂ O ₂	72	6.4.620	2.78	C2DB	hexagonal	/	Γ	0.31	LCEBR	/	Unstable
SbSe	72	3.4.169	0.45	C2DB	hexagonal	/	Γ	0.31	OAI	/	Unstable
SrF ₂ O ₂	72	6.4.640	2.76	C2DB	hexagonal	/	Γ	0.28	LCEBR	/	Unstable

b. Γ -SOC

TABLE S35: Experimental materials with valley type: hexagonal- Γ -SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
BiTe	69	6.1.13	0.70	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.55	LCEBR	Yes	Exp.M.Exfo
Sb	72	3.1.25	1.01	C2DB	hexagonal	Γ -SOC	nHSP	0.54	OAI	Yes	Exp.W.Exfo
As	72	3.1.11	1.48	C2DB	hexagonal	Γ -SOC	nHSP	0.50	OAI	Yes	Exp.W.Exfo
PtSe ₂	72	6.1.58	1.18	C2DB	hexagonal	Γ -SOC	nHSP	0.48	LCEBR	Yes	Exp.M.Exfo
BiClTe	69	6.3.1963	0.95	C2DB	hexagonal	Γ -SOC	Γ	0.44	LCEBR	Yes	Exp.M.Exfo
BiBrTe	69	6.1.10	0.92	C2DB	hexagonal	Γ -SOC	Γ -SOC	0.41	LCEBR	Yes	Exp.M.Exfo
SnSe ₂	72	6.1.71	0.76	C2DB	hexagonal	Γ -SOC	M	0.39	LCEBR	Yes	Exp.M.Exfo
BiClTe	69	6.1.12	0.94	MC2D	hexagonal	Γ -SOC	Γ	0.38	LCEBR	Yes	Exp.M.Exfo
Bi	72	1.1.10	0.53	MC2D	hexagonal	Γ -SOC	Γ	0.36	SEBR	Yes	Exp.
CdI ₂	72	6.1.38	2.18	C2DB	hexagonal	Γ -SOC	M	0.35	LCEBR	Yes	Exp.Substr
HfSe ₂	72	6.1.44	0.45	C2DB	hexagonal	Γ -SOC	M	0.32	LCEBR	Yes	Exp.M.Exfo
ZrSe ₂	72	6.1.73	0.34	C2DB	hexagonal	Γ -SOC	M	0.28	LCEBR	Yes	Exp.M.Exfo
Bi ₂ Se ₂ Te	72	6.1.24	0.33	MC2D	hexagonal	Γ -SOC	Γ	0.25	LCEBR	Yes	Exp.Substr

TABLE S36: Computationally exfoliable materials with valley type: hexagonal- Γ -SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
GeTe	69	6.2.1108	1.25	MC2D	hexagonal	Γ -SOC	nHSP	0.50	LCEBR	Yes	Comp.Exfo
PbTe	69	6.2.1129	1.14	MC2D	hexagonal	Γ -SOC	Γ	0.48	LCEBR	Yes	Comp.Exfo
AsSb	69	6.2.1090	1.18	MC2D	hexagonal	Γ -SOC	nHSP-SOC	0.46	LCEBR	Yes	Comp.Exfo
Bi ₂ STe ₂	69	6.2.1092	0.36	MC2D	hexagonal	nHSP-SOC	Γ -SOC	0.36	LCEBR	Yes	Comp.Exfo
AlLiTe ₂	69	6.2.1084	0.67	MC2D	hexagonal	Γ -SOC	Γ -SOC	0.36	LCEBR	Yes	Comp.Exfo
BiCuP ₂ Se ₆	67	3.2.159	0.65	MC2D	hexagonal	/	Γ -SOC	0.34	OAI	Yes	Comp.Exfo
ZrBrN	69	6.2.1099	2.59	MC2D	hexagonal	Γ -SOC	K -SOC	0.26	LCEBR	Yes	Comp.Exfo
Y ₂ Cl ₂	72	6.2.1201	0.24	MC2D	hexagonal	Γ -SOC	M	0.26	LCEBR	Yes	Comp.Exfo
TmI ₃	71	6.2.1159	2.75	MC2D	hexagonal	Γ -SOC	/	0.24	LCEBR	Yes	Comp.Exfo
LuI ₃	71	6.2.1154	2.84	MC2D	hexagonal	Γ -SOC	/	0.24	LCEBR	Yes	Comp.Exfo

TABLE S37: Computationally stable materials with valley type: hexagonal- Γ -SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
GaAs	69	6.3.1940	1.07	C2DB	hexagonal	K	Γ -SOC	0.69	LCEBR	/	Stable

BiBrS	69	6.3.1954	1.23	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.65	LCEBR	/	Stable
BiBrSe	69	6.3.1957	1.38	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.65	LCEBR	/	Stable
BiBrSe	69	6.3.1956	1.03	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.65	LCEBR	/	Stable
BiIS	69	6.3.1969	1.14	C2DB	hexagonal	/	Γ -SOC	0.65	LCEBR	/	Stable
BrSSb	69	6.3.2007	1.23	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.65	LCEBR	/	Stable
BrSbSe	69	6.3.2009	1.07	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.65	LCEBR	/	Stable
ClSSb	69	6.3.2038	1.33	C2DB	hexagonal	nHSP	Γ -SOC	0.65	LCEBR	/	Stable
ClSbSe	69	6.3.2040	1.18	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.65	LCEBR	/	Stable
BiClS	69	6.3.1959	1.33	C2DB	hexagonal	/	Γ -SOC	0.65	LCEBR	/	Stable
BiClSe	69	6.3.1961	1.14	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.65	LCEBR	/	Stable
PbO	69	6.3.2134	1.81	C2DB	hexagonal	/	Γ -SOC	0.64	LCEBR	/	Stable
BiBrS	69	6.3.1955	1.59	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.63	LCEBR	/	Stable
BiClSe	69	6.3.1962	1.60	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.63	LCEBR	/	Stable
BiISe	69	6.3.1971	0.93	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.62	LCEBR	/	Stable
WSTe	69	3.3.293	1.17	C2DB	hexagonal	Γ -SOC	K -SOC	0.61	OAI	/	Stable
BiBrTe	69	6.3.1958	0.88	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.61	LCEBR	/	Stable
AsClS	69	6.3.1932	1.53	C2DB	hexagonal	nHSP	Γ -SOC	0.60	LCEBR	/	Stable
Sn ₂ BrIS	69	6.3.2001	0.93	C2DB	hexagonal	K -SOC	Γ -SOC	0.59	LCEBR	/	Stable
AsBrSe	69	6.3.1928	1.21	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.59	LCEBR	/	Stable
BiClS	69	6.3.1960	1.84	C2DB	hexagonal	nHSP	Γ -SOC	0.59	LCEBR	/	Stable
SnBrHO	69	6.3.2076	1.74	C2DB	hexagonal	K -SOC	Γ -SOC	0.58	LCEBR	/	Stable
ISbSe	69	6.3.2113	1.06	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.58	LCEBR	/	Stable
ISSb	69	6.3.2110	1.28	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.57	LCEBR	/	Stable
AsBrS	69	6.3.1926	1.38	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.57	LCEBR	/	Stable
AgPbISe	69	6.3.1906	0.79	C2DB	hexagonal	/	Γ -SOC	0.56	LCEBR	/	Stable
AsBrTe	69	6.3.1930	1.25	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.55	LCEBR	/	Stable
HgI ₂	72	6.3.2498	1.15	C2DB	hexagonal	Γ -SOC	M	0.53	LCEBR	/	Stable
ISbTe	69	6.3.2115	0.89	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.53	LCEBR	/	Stable
AsISe	69	6.3.1942	1.16	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.52	LCEBR	/	Stable
AsITe	69	6.3.1944	1.01	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.52	LCEBR	/	Stable
AgPbITe	69	6.3.1907	0.62	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.51	LCEBR	/	Stable
CdI ₂	78	6.3.2630	1.52	C2DB	hexagonal	Γ -SOC	M	0.50	LCEBR	/	Stable
AgI	78	6.3.2600	1.55	C2DB	hexagonal	Γ -SOC	Γ	0.50	LCEBR	/	Stable
AlISe	69	6.3.1921	1.47	C2DB	hexagonal	Γ -SOC	M	0.50	LCEBR	/	Stable
SrHIO	69	6.3.2088	1.47	C2DB	hexagonal	Γ -SOC	Γ	0.49	LCEBR	/	Stable
Cd ₂ BrIS	69	6.3.1985	0.97	C2DB	hexagonal	Γ -SOC	M	0.49	LCEBR	/	Stable
AgCl	78	6.3.2599	1.68	C2DB	hexagonal	Γ -SOC	Γ	0.48	LCEBR	/	Stable
HgF ₂	72	6.3.2423	1.62	C2DB	hexagonal	Γ -SOC	Γ	0.47	LCEBR	/	Stable
BiIS	69	6.3.1970	0.85	C2DB	hexagonal	Γ -SOC	Γ -SOC	0.47	LCEBR	/	Stable
GeTe	69	6.3.2069	1.49	C2DB	hexagonal	Γ -SOC	nHSP	0.46	LCEBR	/	Stable
HgHIS	69	6.3.2087	1.09	C2DB	hexagonal	Γ -SOC	Γ	0.46	LCEBR	/	Stable
BiFTe	69	6.3.1967	0.94	C2DB	hexagonal	Γ -SOC	Γ	0.44	LCEBR	/	Stable
CdHIO	69	6.3.2081	0.66	C2DB	hexagonal	Γ -SOC	Γ	0.44	LCEBR	/	Stable
CuI	72	6.1.41	1.82	C2DB	hexagonal	Γ -SOC	Γ	0.44	LCEBR	Yes	Stable
FSbTe	69	6.3.2059	1.57	C2DB	hexagonal	Γ -SOC	nHSP-SOC	0.44	LCEBR	/	Stable
ISSb	69	6.3.2111	0.87	C2DB	hexagonal	Γ -SOC	M	0.43	LCEBR	/	Stable
AsIS	69	6.3.1941	1.39	C2DB	hexagonal	Γ -SOC	Γ -SOC	0.43	LCEBR	/	Stable
AsBrTe	69	6.3.1931	1.10	C2DB	hexagonal	Γ -SOC	K -SOC	0.43	LCEBR	/	Stable
SnTe	69	6.3.2164	1.59	C2DB	hexagonal	Γ -SOC	nHSP	0.43	LCEBR	/	Stable
AsClTe	69	6.3.1936	1.32	C2DB	hexagonal	Γ -SOC	K -SOC	0.43	LCEBR	/	Stable
ISbSe	69	6.3.2114	1.08	C2DB	hexagonal	Γ -SOC	M	0.43	LCEBR	/	Stable

AsFTe	69	6.3.1939	1.65	C2DB	hexagonal	Γ -SOC	nHSP-SOC	0.42	LCEBR	/	Stable
ClSbTe	69	6.3.2043	1.44	C2DB	hexagonal	Γ -SOC	/	0.42	LCEBR	/	Stable
GaClSe	69	6.3.2032	1.27	C2DB	hexagonal	Γ -SOC	M	0.42	LCEBR	/	Stable
AgI	72	6.1.17	1.81	C2DB	hexagonal	Γ -SOC	Γ	0.42	LCEBR	Yes	Stable
AlSiTe ₃	71	3.3.304	1.13	C2DB	hexagonal	Γ -SOC	/	0.42	OAI	Yes	Stable
ZrBr ₂ O	69	6.3.1978	1.07	C2DB	hexagonal	Γ -SOC	K	0.41	LCEBR	/	Stable
AlGeTe ₃	71	3.3.300	0.96	C2DB	hexagonal	Γ -SOC	/	0.41	OAI	/	Stable
Al ₂ Mg ₂ Se ₅	72	6.3.2266	1.12	C2DB	hexagonal	Γ -SOC	/	0.41	LCEBR	Yes	Stable
BiISe	69	6.3.1972	0.84	C2DB	hexagonal	Γ -SOC	Γ -SOC	0.41	LCEBR	/	Stable
CdHIS	69	6.3.2082	2.06	C2DB	hexagonal	Γ -SOC	Γ	0.41	LCEBR	/	Stable
CdBrI	69	6.3.1986	2.22	C2DB	hexagonal	Γ -SOC	Γ	0.40	LCEBR	/	Stable
BiBrISb	69	6.3.1953	0.69	C2DB	hexagonal	Γ -SOC	nHSP-SOC	0.39	LCEBR	/	Stable
HgFHO	69	6.3.2085	1.08	C2DB	hexagonal	Γ -SOC	Γ	0.39	LCEBR	/	Stable
CaH ₂ Te ₂	72	6.3.2465	2.34	C2DB	hexagonal	Γ -SOC	M	0.39	LCEBR	/	Stable
InZnITe	69	6.3.2107	1.30	C2DB	hexagonal	Γ -SOC	Γ -SOC	0.39	LCEBR	/	Stable
ScClTe	69	6.3.2044	0.82	C2DB	hexagonal	Γ -SOC	M	0.39	LCEBR	/	Stable
AsISe	69	6.3.1943	0.52	C2DB	hexagonal	Γ -SOC	M	0.39	LCEBR	/	Stable
ScI ₃	71	6.3.2243	1.91	C2DB	hexagonal	Γ -SOC	/	0.39	LCEBR	/	Stable
HgI ₂	78	6.3.2649	0.66	C2DB	hexagonal	Γ -SOC	M -SOC	0.39	LCEBR	/	Stable
AgBiP ₂ Se ₆	65	6.3.1822	1.23	C2DB	hexagonal	/	Γ -SOC	0.38	LCEBR	Yes	Stable
InI ₃	79	6.3.2677	0.70	C2DB	hexagonal	Γ -SOC	Γ	0.38	LCEBR	/	Stable
CdBrHO	69	6.3.2072	1.73	C2DB	hexagonal	Γ -SOC	Γ	0.38	LCEBR	/	Stable
ZnTe	72	6.3.2590	0.57	C2DB	hexagonal	Γ -SOC	Γ	0.37	LCEBR	/	Stable
InSiTe ₃	71	3.3.341	0.71	C2DB	hexagonal	Γ -SOC	/	0.37	OAI	Yes	Stable
BaH ₂ Te ₂	72	6.3.2461	2.46	C2DB	hexagonal	Γ -SOC	/	0.37	LCEBR	/	Stable
ZrOSe	69	6.3.2138	0.86	C2DB	hexagonal	Γ -SOC	/	0.37	LCEBR	/	Stable
WCl ₃	79	3.3.533	0.74	C2DB	hexagonal	Γ -SOC	/	0.37	OAI	/	Stable
SnSSe	69	6.3.2148	0.84	C2DB	hexagonal	Γ -SOC	M	0.37	LCEBR	/	Stable
MgI ₂	78	6.3.2650	2.59	C2DB	hexagonal	Γ -SOC	M	0.36	LCEBR	/	Stable
CdTe	72	6.3.2395	0.67	C2DB	hexagonal	Γ -SOC	Γ	0.36	LCEBR	/	Stable
HgHIO	69	6.3.2086	0.45	C2DB	hexagonal	Γ -SOC	Γ	0.36	LCEBR	/	Stable
InSb	69	6.3.2129	0.48	C2DB	hexagonal	Γ -SOC	Γ	0.36	LCEBR	/	Stable
PtSeTe	69	6.3.2146	0.75	C2DB	hexagonal	Γ -SOC	nHSP	0.36	LCEBR	/	Stable
InGeTe ₃	71	3.3.330	0.67	C2DB	hexagonal	Γ -SOC	/	0.36	OAI	/	Stable
InAs	69	6.3.1946	0.68	C2DB	hexagonal	Γ -SOC	Γ	0.35	LCEBR	/	Stable
ZnPTe ₃	71	3.3.365	0.61	C2DB	hexagonal	Γ -SOC	/	0.35	OAI	/	Stable
PtTe ₂	72	6.3.2574	0.37	C2DB	hexagonal	Γ -SOC	/	0.35	LCEBR	Yes	Stable
SrH ₂ Te ₂	72	6.3.2489	2.56	C2DB	hexagonal	Γ -SOC	M	0.35	LCEBR	/	Stable
In ₂ STe	69	6.3.2122	0.64	C2DB	hexagonal	Γ -SOC	Γ	0.35	LCEBR	/	Stable
AsITe	69	6.3.1945	0.42	C2DB	hexagonal	Γ -SOC	K -SOC	0.34	LCEBR	/	Stable
CdZnSeTe	69	6.3.2023	0.73	C2DB	hexagonal	Γ -SOC	Γ	0.34	LCEBR	/	Stable
CdBr ₂	78	6.3.2612	2.37	C2DB	hexagonal	Γ -SOC	Γ	0.34	LCEBR	/	Stable
PdSe ₂	72	6.3.2570	0.53	C2DB	hexagonal	Γ -SOC	nHSP	0.34	LCEBR	/	Stable
BiITe	69	6.3.1973	0.69	C2DB	hexagonal	Γ -SOC	Γ -SOC	0.33	LCEBR	/	Stable
CuBrGeTe	69	6.3.1994	0.66	C2DB	hexagonal	Γ -SOC	Γ -SOC	0.32	LCEBR	/	Stable
In ₂ Mg ₂ Se ₅	72	6.3.2513	0.71	C2DB	hexagonal	Γ -SOC	Γ	0.32	LCEBR	/	Stable
HfSSe	69	6.3.2094	0.71	C2DB	hexagonal	Γ -SOC	M	0.32	LCEBR	/	Stable
Al ₂ MgTe ₄	72	6.3.2271	0.49	C2DB	hexagonal	Γ -SOC	Γ	0.31	LCEBR	/	Stable
Bi ₂ S ₂ Te	72	6.3.2308	0.34	C2DB	hexagonal	Γ -SOC	Γ	0.30	LCEBR	/	Stable
MgClI	69	6.3.2033	2.93	C2DB	hexagonal	Γ -SOC	Γ	0.30	LCEBR	/	Stable
In ₂ MgSe ₄	72	6.3.2515	0.59	C2DB	hexagonal	Γ -SOC	Γ	0.30	LCEBR	/	Stable

ZrTe ₂	78	6.1.81	0.28	C2DB	hexagonal	Γ -SOC	nHSP	0.29	LCEBR	/	Stable
WCl ₃	71	3.3.317	0.51	C2DB	hexagonal	Γ -SOC	/	0.28	OAI	/	Stable
ZrSSe	69	6.3.2151	0.62	C2DB	hexagonal	Γ -SOC	M	0.28	LCEBR	/	Stable
Al ₂ Mg ₂ Te ₅	72	6.3.2267	0.54	C2DB	hexagonal	Γ -SOC	/	0.27	LCEBR	/	Stable
SnH	72	3.3.443	0.25	C2DB	hexagonal	Γ -SOC	Γ	0.27	OAI	/	Stable
GaSiTe ₃	71	3.3.327	0.32	C2DB	hexagonal	Γ -SOC	/	0.26	OAI	/	Stable
Cd ₂ SeTe	69	6.3.2017	0.42	C2DB	hexagonal	Γ -SOC	Γ	0.25	LCEBR	/	Stable
CaI ₂	78	6.3.2628	2.99	C2DB	hexagonal	Γ -SOC	M	0.25	LCEBR	/	Stable
In ₂ MgTe ₄	72	6.3.2516	0.29	C2DB	hexagonal	Γ -SOC	Γ	0.25	LCEBR	/	Stable
HfZrSe ₆	71	6.3.2237	0.40	C2DB	hexagonal	Γ -SOC	/	0.25	LCEBR	/	Stable
CoITe	69	6.3.2048	0.43	C2DB	hexagonal	Γ -SOC	nHSP	0.25	LCEBR	/	Stable
AgAlP ₂ Te ₆	67	3.3.215	0.52	C2DB	hexagonal	Γ -SOC	K -SOC	0.25	OAI	/	Stable
In ₂ Mg ₂ Te ₅	72	6.3.2514	0.42	C2DB	hexagonal	Γ -SOC	Γ	0.24	LCEBR	/	Stable
Ga ₂ Mg ₂ Se ₅	72	6.3.2442	0.44	C2DB	hexagonal	Γ -SOC	Γ	0.24	LCEBR	/	Stable
YIS	69	6.3.2112	2.92	C2DB	hexagonal	Γ -SOC	/	0.23	LCEBR	/	Stable
Ga ₂ MgSe ₄	72	6.3.2443	0.33	C2DB	hexagonal	Γ -SOC	Γ	0.22	LCEBR	/	Stable
WBr ₃	79	3.3.531	0.23	C2DB	hexagonal	Γ -SOC	Γ	0.19	OAI	/	Stable
ZrSeTe	69	6.3.2163	0.28	C2DB	hexagonal	Γ -SOC	nHSP	0.19	LCEBR	/	Stable
AgBiP ₂ Te ₆	65	6.3.1823	0.48	C2DB	hexagonal	Γ -SOC	Γ -SOC	0.16	LCEBR	/	Stable
ZrSTe	69	6.3.2157	0.22	C2DB	hexagonal	Γ -SOC	/	0.16	LCEBR	/	Stable
AgP ₂ SbTe ₆	65	6.3.1826	0.50	C2DB	hexagonal	Γ -SOC	Γ -SOC	0.16	LCEBR	/	Stable

TABLE S38: Computationally unstable materials with valley type: hexagonal- Γ -SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
FOsb	69	6.4.558	1.32	C2DB	hexagonal	K	Γ -SOC	0.65	LCEBR	/	Unstable
HgBrFS	69	6.4.503	1.01	C2DB	hexagonal	/	Γ -SOC	0.62	LCEBR	/	Unstable
AlSb	69	6.4.478	1.45	C2DB	hexagonal	K	Γ -SOC	0.59	LCEBR	/	Unstable
BiFO	69	6.4.492	1.85	C2DB	hexagonal	K	Γ -SOC	0.59	LCEBR	/	Unstable
HgFIS	69	6.4.554	0.98	C2DB	hexagonal	/	Γ -SOC	0.57	LCEBR	/	Unstable
CdFIO	69	6.4.522	1.36	C2DB	hexagonal	Γ -SOC	Γ	0.54	LCEBR	/	Unstable
ZnI ₂	78	6.4.720	0.93	C2DB	hexagonal	Γ -SOC	M	0.53	LCEBR	/	Unstable
CdTe	69	6.4.529	1.01	C2DB	hexagonal	Γ -SOC	Γ	0.52	LCEBR	/	Unstable
SiTe	69	6.4.596	1.53	C2DB	hexagonal	Γ -SOC	nHSP-SOC	0.45	LCEBR	/	Unstable
BrOSb	69	6.4.511	1.21	C2DB	hexagonal	Γ -SOC	M -SOC	0.44	LCEBR	/	Unstable
CdSe	69	6.4.528	1.11	C2DB	hexagonal	Γ -SOC	Γ	0.44	LCEBR	/	Unstable
AsIO	69	6.4.486	0.63	C2DB	hexagonal	Γ -SOC	nHSP-SOC	0.44	LCEBR	/	Unstable
BiBrO	69	6.4.490	1.54	C2DB	hexagonal	Γ -SOC	nHSP-SOC	0.43	LCEBR	/	Unstable
HgFIO	69	6.4.553	0.73	C2DB	hexagonal	Γ -SOC	Γ -SOC	0.42	LCEBR	/	Unstable
IOP	69	6.4.574	0.65	C2DB	hexagonal	Γ -SOC	nHSP-SOC	0.42	LCEBR	/	Unstable
HfOSe	69	6.4.569	0.97	C2DB	hexagonal	Γ -SOC	nHSP-SOC	0.42	LCEBR	/	Unstable
CdFIS	69	6.4.523	1.80	C2DB	hexagonal	/	Γ -SOC	0.41	LCEBR	/	Unstable
ZnBr ₂	78	6.4.698	2.41	C2DB	hexagonal	Γ -SOC	Γ	0.37	LCEBR	/	Unstable
AsBrO	69	6.4.481	2.04	C2DB	hexagonal	Γ -SOC	nHSP-SOC	0.35	LCEBR	/	Unstable
AsIS	69	6.4.487	0.29	C2DB	hexagonal	Γ -SOC	M	0.32	LCEBR	/	Unstable

c. K

TABLE S39: Experimental materials with valley type: hexagonal- K .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
---------	----	----	-----	----------	---------	------------	------------	-------------	----------	------	-----------

ZrBrN	72	6.3.2323	1.62	C2DB	hexagonal	nHSP	K	0.65	LCEBR	Yes	Exp.W.Exfo
ZrClN	72	6.3.2408	1.91	C2DB	hexagonal	Γ	K	0.58	LCEBR	Yes	Exp.M.Exfo
MoS ₂	78	3.1.39	1.60	C2DB	hexagonal	K -SOC	K	0.57	OAI	Yes	Exp.M.Exfo
MoSe ₂	78	3.1.41	1.34	C2DB	hexagonal	K -SOC	K	0.57	OAI	Yes	Exp.M.Exfo
MoTe ₂	78	3.1.43	0.96	C2DB	hexagonal	K -SOC	K	0.54	OAI	Yes	Exp.M.Exfo
GaN	78	6.1.78	1.82	C2DB	hexagonal	K	Γ	0.52	LCEBR	Yes	Exp.
MoSSe	69	3.1.10	1.48	C2DB	hexagonal	K -SOC	K	0.51	OAI	Yes	Exp.Substr

TABLE S40: Computationally exfoliable materials with valley type: hexagonal- K .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
PbO ₆ Se ₂	72	6.2.1287	0.49	MC2D	hexagonal	/	K	0.49	LCEBR	Yes	Comp.Exfo
SnPS ₃	66	3.2.152	1.59	MC2D	hexagonal	/	K	0.49	OAI	Yes	Comp.Exfo
AgErP ₂ Se ₆	67	3.2.153	1.50	MC2D	hexagonal	/	K	0.37	OAI	Yes	Comp.Exfo
AgTmP ₂ Se ₆	67	3.2.158	1.50	MC2D	hexagonal	/	K	0.36	OAI	Yes	Comp.Exfo
YFSe	72	6.2.1225	2.57	MC2D	hexagonal	/	K	0.33	LCEBR	Yes	Comp.Exfo
PrIS	72	6.2.1268	2.47	MC2D	hexagonal	nHSP	K	0.28	LCEBR	Yes	Comp.Exfo
NdIS	72	6.2.1266	2.47	MC2D	hexagonal	nHSP	K	0.28	LCEBR	Yes	Comp.Exfo
GdIS	72	6.2.1238	2.57	MC2D	hexagonal	nHSP	K	0.26	LCEBR	Yes	Comp.Exfo

TABLE S41: Computationally stable materials with valley type: hexagonal- K .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
BP	78	6.3.2606	0.91	C2DB	hexagonal	K	K	0.72	LCEBR	/	Stable
TiF ₂	78	3.3.500	1.28	C2DB	hexagonal	K	/	0.71	OAI	/	Stable
ZrCl ₂	78	3.3.495	0.99	C2DB	hexagonal	K	nHSP	0.70	OAI	Yes	Stable
InBr	72	6.3.2321	1.34	C2DB	hexagonal	nHSP	K	0.69	LCEBR	/	Stable
InI	72	6.3.2500	1.01	C2DB	hexagonal	nHSP	K	0.69	LCEBR	/	Stable
AlO	78	3.3.475	1.32	C2DB	hexagonal	K	M	0.69	OAI	/	Stable
TiCl ₂	78	3.3.494	0.90	C2DB	hexagonal	K	/	0.68	OAI	/	Stable
InCl	72	6.3.2406	1.55	C2DB	hexagonal	/	K	0.68	LCEBR	/	Stable
SnH ₂ S ₂	72	6.3.2485	1.00	C2DB	hexagonal	K	Γ	0.68	LCEBR	/	Stable
GeH ₂ S ₂	72	6.3.2470	1.05	C2DB	hexagonal	K	Γ	0.68	LCEBR	/	Stable
AsB	78	6.3.2603	0.75	C2DB	hexagonal	K	K	0.67	LCEBR	/	Stable
BiCl	72	1.3.200	0.91	C2DB	hexagonal	K	Γ	0.66	SEBR	/	Stable
CdCl	72	3.3.408	1.68	C2DB	hexagonal	K	Γ	0.66	OAI	/	Stable
SnO	69	6.3.2139	1.68	C2DB	hexagonal	K	M	0.66	LCEBR	/	Stable
BiBr	72	1.3.199	0.88	C2DB	hexagonal	K	Γ	0.65	SEBR	/	Stable
SnPS ₃	71	3.3.356	1.06	C2DB	hexagonal	Γ	K	0.65	OAI	Yes	Stable
MoO ₂	78	3.3.512	0.92	C2DB	hexagonal	Γ	K	0.65	OAI	/	Stable
TiClF	69	3.3.271	1.13	C2DB	hexagonal	K	/	0.65	OAI	/	Stable
ZrClF	69	3.3.272	1.25	C2DB	hexagonal	K	nHSP	0.65	OAI	/	Stable
PbH ₂ O ₂	72	6.3.2479	1.68	C2DB	hexagonal	K	Γ	0.64	LCEBR	/	Stable
WO ₂	78	3.3.520	1.34	C2DB	hexagonal	Γ	K	0.64	OAI	/	Stable
GePS ₃	71	3.3.331	1.42	C2DB	hexagonal	/	K	0.64	OAI	/	Stable
ZrBr ₂ O	69	6.3.1978	1.07	C2DB	hexagonal	Γ -SOC	K	0.62	LCEBR	/	Stable
PbPS ₃	71	3.3.347	1.48	C2DB	hexagonal	Γ	K	0.62	OAI	/	Stable
PbH ₂ S ₂	72	6.3.2484	1.47	C2DB	hexagonal	K	Γ	0.61	LCEBR	/	Stable
YIO	72	6.3.2503	1.87	C2DB	hexagonal	/	K	0.61	LCEBR	/	Stable

MoOS	69	3.3.283	1.09	C2DB	hexagonal	Γ	K	0.60	OAI	/	Stable
WSe	69	3.3.290	1.26	C2DB	hexagonal	Γ	K	0.59	OAI	/	Stable
TiBrCl	69	3.3.266	0.83	C2DB	hexagonal	K	/	0.59	OAI	/	Stable
HfBrN	72	6.3.2318	1.97	C2DB	hexagonal	nHSP	K	0.59	LCEBR	Yes	Stable
GeO	69	6.3.2066	2.09	C2DB	hexagonal	K	M	0.59	LCEBR	/	Stable
ISbTe	69	6.3.2116	1.03	C2DB	hexagonal	nHSP-SOC	K	0.57	LCEBR	/	Stable
MoOSe	69	3.3.284	0.78	C2DB	hexagonal	Γ	K	0.57	OAI	/	Stable
BiI	72	1.3.202	0.86	C2DB	hexagonal	K	Γ	0.57	SEBR	/	Stable
SnF ₂	72	6.3.2432	2.36	C2DB	hexagonal	K	Γ	0.57	LCEBR	/	Stable
Nb ₃ F ₇ S	69	6.3.2051	0.96	C2DB	hexagonal	/	K	0.56	LCEBR	/	Stable
HfIN	72	6.3.2492	0.62	C2DB	hexagonal	/	K	0.55	LCEBR	Yes	Stable
BSb	78	6.3.2607	0.30	C2DB	hexagonal	K	K	0.53	LCEBR	/	Stable
HfClN	72	6.3.2403	2.33	C2DB	hexagonal	Γ	K	0.53	LCEBR	Yes	Stable
CrS ₂	78	3.3.497	0.90	C2DB	hexagonal	K -SOC	K	0.52	OAI	/	Stable
WOS	69	3.3.289	1.51	C2DB	hexagonal	Γ	K	0.52	OAI	/	Stable
MoSTe	69	3.3.286	1.03	C2DB	hexagonal	Γ	K	0.52	OAI	/	Stable
F ₂ Ge	72	6.3.2420	2.64	C2DB	hexagonal	K	Γ	0.52	LCEBR	/	Stable
GaP	69	6.3.2065	1.55	C2DB	hexagonal	K	Γ	0.50	LCEBR	/	Stable
BrSb	72	1.3.212	0.39	C2DB	hexagonal	K	K	0.50	SEBR	/	Stable
ClSb	72	1.3.254	0.39	C2DB	hexagonal	K	K	0.50	SEBR	/	Stable
MoSeTe	69	3.3.287	1.16	C2DB	hexagonal	K -SOC	K	0.49	OAI	/	Stable
CrO ₂	78	3.3.496	0.42	C2DB	hexagonal	Γ	K	0.49	OAI	/	Stable
CdPSe ₃	71	3.3.315	1.27	C2DB	hexagonal	K	Γ	0.47	OAI	Yes	Stable
ZrIN	72	6.3.2502	0.36	C2DB	hexagonal	/	K	0.47	LCEBR	Yes	Stable
ZnPSe ₃	71	3.3.362	1.30	C2DB	hexagonal	K	Γ	0.46	OAI	/	Stable
ZrFN	72	6.3.2427	2.32	C2DB	hexagonal	K	K	0.46	LCEBR	/	Stable
InP	69	6.3.2127	1.07	C2DB	hexagonal	K	Γ	0.45	LCEBR	/	Stable
GaAs	69	6.3.1940	1.07	C2DB	hexagonal	K	Γ -SOC	0.44	LCEBR	/	Stable
HgPS ₃	71	3.3.334	0.98	C2DB	hexagonal	K	Γ	0.44	OAI	Yes	Stable
CrSe ₂	78	3.3.498	0.70	C2DB	hexagonal	K -SOC	K	0.44	OAI	/	Stable
AlN	78	6.3.2602	2.88	C2DB	hexagonal	K	Γ	0.44	LCEBR	/	Stable
MgAsSe ₃	71	3.3.308	1.28	C2DB	hexagonal	/	K	0.42	OAI	/	Stable
CrSSe	69	3.3.276	0.80	C2DB	hexagonal	K -SOC	K	0.41	OAI	/	Stable
CdPS ₃	71	3.3.314	1.91	C2DB	hexagonal	K	Γ	0.40	OAI	Yes	Stable
ZnPS ₃	71	3.3.358	2.10	C2DB	hexagonal	K	Γ	0.37	OAI	Yes	Stable
MgPSe ₃	71	3.3.343	2.01	C2DB	hexagonal	K	/	0.37	OAI	Yes	Stable
HfFN	72	6.3.2421	2.70	C2DB	hexagonal	K	K	0.37	LCEBR	/	Stable
CrTe ₂	78	3.3.499	0.47	C2DB	hexagonal	K -SOC	K	0.35	OAI	/	Stable
AlGeS ₃	71	3.3.298	2.02	C2DB	hexagonal	/	K	0.34	OAI	/	Stable
InPt ₂ Te ₃	72	6.3.2526	0.66	C2DB	hexagonal	/	K	0.33	LCEBR	/	Stable
MgAsS ₃	71	3.3.307	2.01	C2DB	hexagonal	/	K	0.33	OAI	/	Stable
HgPSe ₃	71	3.3.335	0.56	C2DB	hexagonal	K	Γ	0.33	OAI	Yes	Stable
CrSeTe	69	3.3.278	0.59	C2DB	hexagonal	/	K	0.32	OAI	/	Stable
YIS	72	6.3.2506	2.56	C2DB	hexagonal	nHSP	K	0.26	LCEBR	/	Stable
InPd ₂ Te ₃	72	6.3.2522	0.37	C2DB	hexagonal	/	K	0.26	LCEBR	/	Stable
CrSTe	69	3.3.277	0.29	C2DB	hexagonal	Γ	K	0.24	OAI	/	Stable
MgPS ₃	71	3.3.342	2.81	C2DB	hexagonal	K	K	0.24	OAI	Yes	Stable
Pd ₂ TlTe ₃	72	6.3.2568	0.37	C2DB	hexagonal	/	K	0.24	LCEBR	/	Stable
ReS	72	1.3.310	0.24	C2DB	hexagonal	K	/	0.22	SEBR	/	Stable

TABLE S42: Computationally unstable materials with valley type: hexagonal- K .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
AlAs	78	6.4.691	1.24	C2DB	hexagonal	K	Γ	0.75	LCEBR	/	Unstable
HfF ₂	78	3.4.181	1.14	C2DB	hexagonal	K	Γ	0.71	OAI	/	Unstable
ZrF ₂	78	3.4.184	1.52	C2DB	hexagonal	K	/	0.71	OAI	/	Unstable
AlO	72	3.4.124	1.18	C2DB	hexagonal	K	M	0.69	OAI	/	Unstable
SnF ₂ O ₂	72	6.4.639	1.08	C2DB	hexagonal	K	Γ	0.68	LCEBR	/	Unstable
F ₂ GeO ₂	72	6.4.634	1.09	C2DB	hexagonal	K	M	0.68	LCEBR	/	Unstable
GeH ₂ O ₂	72	6.4.655	1.09	C2DB	hexagonal	K	Γ	0.68	LCEBR	/	Unstable
F ₂ Si	72	6.4.646	1.78	C2DB	hexagonal	K	Γ	0.66	LCEBR	/	Unstable
TiBrF	69	3.4.89	1.03	C2DB	hexagonal	K	/	0.65	OAI	/	Unstable
ZrBrF	69	3.4.90	1.16	C2DB	hexagonal	K	nHSP	0.65	OAI	/	Unstable
FOP	69	6.4.557	1.07	C2DB	hexagonal	K	Γ	0.65	LCEBR	/	Unstable
FOSb	69	6.4.558	1.32	C2DB	hexagonal	K	Γ -SOC	0.65	LCEBR	/	Unstable
SnH ₂ O ₂	72	6.4.659	0.88	C2DB	hexagonal	K	Γ	0.64	LCEBR	/	Unstable
AsFO	69	6.4.484	1.55	C2DB	hexagonal	K	Γ	0.64	LCEBR	/	Unstable
AIP	78	6.4.692	2.29	C2DB	hexagonal	K	Γ	0.61	LCEBR	/	Unstable
ClOSb	69	6.4.541	1.53	C2DB	hexagonal	K	M	0.59	LCEBR	/	Unstable
BiFO	69	6.4.492	1.85	C2DB	hexagonal	K	Γ -SOC	0.59	LCEBR	/	Unstable
SnF ₂	78	6.4.709	2.31	C2DB	hexagonal	K	M	0.57	LCEBR	/	Unstable
ClOP	69	6.4.540	1.95	C2DB	hexagonal	K	nHSP	0.57	LCEBR	/	Unstable
F ₂ Si	78	3.4.183	0.51	C2DB	hexagonal	K	K	0.56	OAI	/	Unstable
AlSb	69	6.4.478	1.45	C2DB	hexagonal	K	Γ -SOC	0.53	LCEBR	/	Unstable
AsClO	69	6.4.482	2.25	C2DB	hexagonal	K	nHSP-SOC	0.52	LCEBR	/	Unstable
OSi	69	6.4.587	0.39	C2DB	hexagonal	K	M	0.50	LCEBR	/	Unstable
F ₂ Ge	78	6.4.706	2.80	C2DB	hexagonal	K	M	0.49	LCEBR	/	Unstable
BiSe	72	3.1.13	0.38	C2DB	hexagonal	Γ	K	0.47	OAI	/	Unstable

d. K -SOC

TABLE S43: Experimental materials with valley type: hexagonal- K -SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
WSe ₂	78	3.1.46	1.26	C2DB	hexagonal	K -SOC	K -SOC	0.71	OAI	Yes	Exp.M.Exfo
WS ₂	78	3.1.45	1.55	C2DB	hexagonal	K -SOC	K -SOC	0.70	OAI	Yes	Exp.M.Exfo
MoS ₂	78	3.1.39	1.60	C2DB	hexagonal	K -SOC	K	0.68	OAI	Yes	Exp.M.Exfo
MoSe ₂	78	3.1.41	1.34	C2DB	hexagonal	K -SOC	K	0.64	OAI	Yes	Exp.M.Exfo
WTe ₂	78	3.1.47	0.75	C2DB	hexagonal	K -SOC	K -SOC	0.61	OAI	Yes	Exp.W.Exfo
MoTe ₂	78	3.1.43	0.96	C2DB	hexagonal	K -SOC	K	0.60	OAI	Yes	Exp.M.Exfo
MoSSe	69	3.1.10	1.48	C2DB	hexagonal	K -SOC	K	0.59	OAI	Yes	Exp.Substr

TABLE S44: Computationally exfoliable materials with valley type: hexagonal- K -SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
GaSe	69	6.2.1106	0.88	MC2D	hexagonal	K -SOC	Γ	0.45	LCEBR	Yes	Comp.Exfo
ZrBrN	69	6.2.1099	2.59	MC2D	hexagonal	Γ -SOC	K -SOC	0.41	LCEBR	Yes	Comp.Exfo

TABLE S45: Computationally stable materials with valley type: hexagonal- K -SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
---------	----	----	-----	----------	---------	------------	------------	-------------	----------	------	-----------

HfCl ₂	78	3.3.493	0.89	C2DB	hexagonal	<i>K</i> -SOC	nHSP-SOC	0.67	OAI	/	Stable
CrS ₂	78	3.3.497	0.90	C2DB	hexagonal	<i>K</i> -SOC	<i>K</i>	0.66	OAI	/	Stable
ZrBr ₂	78	3.3.483	0.83	C2DB	hexagonal	<i>K</i> -SOC	nHSP	0.65	OAI	/	Stable
WSSe	69	3.3.292	1.42	C2DB	hexagonal	<i>K</i> -SOC	<i>K</i> -SOC	0.65	OAI	/	Stable
TiBr ₂	78	3.3.482	0.76	C2DB	hexagonal	<i>K</i> -SOC	/	0.63	OAI	/	Stable
WSeTe	69	3.3.294	1.06	C2DB	hexagonal	<i>K</i> -SOC	<i>K</i> -SOC	0.63	OAI	/	Stable
HfBr ₂	78	3.3.481	0.72	C2DB	hexagonal	<i>K</i> -SOC	nHSP-SOC	0.62	OAI	/	Stable
ZrBrCl	69	3.3.267	0.91	C2DB	hexagonal	<i>K</i> -SOC	nHSP	0.62	OAI	/	Stable
ZrI ₂	78	3.3.507	0.70	C2DB	hexagonal	<i>K</i> -SOC	nHSP	0.61	OAI	/	Stable
ZrClI	69	3.3.275	0.88	C2DB	hexagonal	<i>K</i> -SOC	nHSP	0.61	OAI	/	Stable
WSTe	69	3.3.293	1.17	C2DB	hexagonal	Γ -SOC	<i>K</i> -SOC	0.60	OAI	/	Stable
HfBrCl	69	3.3.265	0.82	C2DB	hexagonal	<i>K</i> -SOC	nHSP-SOC	0.59	OAI	/	Stable
GeI ₂	78	6.3.2642	1.84	C2DB	hexagonal	nHSP-SOC	<i>K</i> -SOC	0.59	LCEBR	/	Stable
HfI ₂	78	3.3.505	0.62	C2DB	hexagonal	<i>K</i> -SOC	nHSP-SOC	0.59	OAI	/	Stable
GaSe	78	3.1.33	0.68	C2DB	hexagonal	/	<i>K</i> -SOC	0.59	OAI	Yes	Stable
HfClI	69	3.3.273	0.81	C2DB	hexagonal	<i>K</i> -SOC	nHSP-SOC	0.59	OAI	/	Stable
SnBrHO	69	6.3.2076	1.74	C2DB	hexagonal	<i>K</i> -SOC	Γ -SOC	0.58	LCEBR	/	Stable
TiI ₂	78	3.3.506	0.60	C2DB	hexagonal	<i>K</i> -SOC	/	0.58	OAI	/	Stable
ZrBrI	69	3.3.270	0.78	C2DB	hexagonal	<i>K</i> -SOC	nHSP	0.58	OAI	/	Stable
AsBrTe	69	6.3.1931	1.10	C2DB	hexagonal	Γ -SOC	<i>K</i> -SOC	0.57	LCEBR	/	Stable
TiClI	69	3.3.274	0.75	C2DB	hexagonal	<i>K</i> -SOC	/	0.57	OAI	/	Stable
AsClTe	69	6.3.1936	1.32	C2DB	hexagonal	Γ -SOC	<i>K</i> -SOC	0.57	LCEBR	/	Stable
MoSeTe	69	3.3.287	1.16	C2DB	hexagonal	<i>K</i> -SOC	<i>K</i>	0.56	OAI	/	Stable
HfBrI	69	3.3.268	0.70	C2DB	hexagonal	<i>K</i> -SOC	nHSP-SOC	0.55	OAI	/	Stable
TiBrI	69	3.3.269	0.68	C2DB	hexagonal	<i>K</i> -SOC	/	0.55	OAI	/	Stable
HgF ₂	78	6.3.2639	1.26	C2DB	hexagonal	<i>K</i> -SOC	Γ	0.54	LCEBR	/	Stable
CrSe ₂	78	3.3.498	0.70	C2DB	hexagonal	<i>K</i> -SOC	<i>K</i>	0.53	OAI	/	Stable
BiO	78	3.3.479	0.45	C2DB	hexagonal	Γ	<i>K</i> -SOC	0.52	OAI	/	Stable
CrSSe	69	3.3.276	0.80	C2DB	hexagonal	<i>K</i> -SOC	<i>K</i>	0.51	OAI	/	Stable
Sn ₂ BrIS	69	6.3.2001	0.93	C2DB	hexagonal	<i>K</i> -SOC	Γ -SOC	0.49	LCEBR	/	Stable
PbTe	72	6.3.2560	0.73	C2DB	hexagonal	<i>K</i> -SOC	Γ	0.46	LCEBR	/	Stable
IrBrSe	69	6.3.2006	1.24	C2DB	hexagonal	nHSP-SOC	<i>K</i> -SOC	0.46	LCEBR	/	Stable
Hf ₃ N ₂ O ₂	78	3.3.503	0.32	C2DB	hexagonal	<i>K</i> -SOC	<i>M</i>	0.45	OAI	/	Stable
CrTe ₂	78	3.3.499	0.47	C2DB	hexagonal	<i>K</i> -SOC	<i>K</i>	0.42	OAI	/	Stable
InSbSeTe	69	6.3.2128	0.34	C2DB	hexagonal	<i>K</i> -SOC	/	0.42	LCEBR	/	Stable
InPbBrSe	69	6.3.2005	0.34	C2DB	hexagonal	nHSP-SOC	<i>K</i> -SOC	0.42	LCEBR	/	Stable
AsITe	69	6.3.1945	0.42	C2DB	hexagonal	Γ -SOC	<i>K</i> -SOC	0.40	LCEBR	/	Stable
RhISe	69	6.3.2109	0.55	C2DB	hexagonal	nHSP-SOC	<i>K</i> -SOC	0.39	LCEBR	/	Stable
AgAlP ₂ Te ₆	67	3.3.215	0.52	C2DB	hexagonal	Γ -SOC	<i>K</i> -SOC	0.22	OAI	/	Stable
BiCuP ₂ S ₆	65	6.3.1835	1.60	C2DB	hexagonal	/	<i>KA</i> -SOC	0.44	LCEBR	/	Stable
AgP ₂ S ₆ Sb	65	6.3.1824	1.69	C2DB	hexagonal	/	<i>KA</i> -SOC	0.43	LCEBR	/	Stable
CuP ₂ S ₆ Sb	65	6.3.1839	1.69	C2DB	hexagonal	/	<i>KA</i> -SOC	0.42	LCEBR	/	Stable
AuP ₂ S ₆ Sb	65	6.3.1832	1.71	C2DB	hexagonal	/	<i>KA</i> -SOC	0.40	LCEBR	/	Stable

TABLE S46: Computationally unstable materials with valley type: hexagonal-*K*-SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
I ₂ Si	78	6.4.719	1.38	C2DB	hexagonal	nHSP-SOC	<i>K</i> -SOC	0.65	LCEBR	/	Unstable
HfBrF	69	3.4.88	1.09	C2DB	hexagonal	<i>K</i> -SOC	nHSP-SOC	0.65	OAI	/	Unstable
HfClF	69	3.4.99	1.18	C2DB	hexagonal	<i>K</i> -SOC	nHSP-SOC	0.65	OAI	/	Unstable

ZrFI	69	3.4.109	1.07	C2DB	hexagonal	K -SOC	/	0.65	OAI	/	Unstable
HfFI	69	3.4.107	0.96	C2DB	hexagonal	K -SOC	nHSP-SOC	0.63	OAI	/	Unstable
SrO	78	6.4.725	1.75	C2DB	hexagonal	K -SOC	Γ	0.63	LCEBR	/	Unstable
Br ₂ Si	78	6.4.697	1.98	C2DB	hexagonal	nHSP-SOC	K -SOC	0.59	LCEBR	/	Unstable
ClPTe	69	6.4.544	0.94	C2DB	hexagonal	nHSP-SOC	K -SOC	0.57	LCEBR	/	Unstable
ClPSe	69	6.4.543	1.22	C2DB	hexagonal	nHSP-SOC	K -SOC	0.55	LCEBR	/	Unstable
BiTl	69	3.4.84	0.55	C2DB	hexagonal	nHSP-SOC	K -SOC	0.55	OAI	/	Unstable
BrPSe	69	6.4.513	1.01	C2DB	hexagonal	nHSP-SOC	K -SOC	0.53	LCEBR	/	Unstable
BrPTe	69	6.4.514	0.75	C2DB	hexagonal	nHSP-SOC	K -SOC	0.52	LCEBR	/	Unstable

e. M

TABLE S47: Experimental materials with valley type: hexagonal- M .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
SnS ₂	72	6.1.75	1.58	C2DB	hexagonal	/	M	0.70	LCEBR	Yes	Exp.M.Exfo
HfS ₂	72	6.1.43	1.24	C2DB	hexagonal	/	M	0.64	LCEBR	Yes	Exp.M.Exfo
SnSe ₂	72	6.1.71	0.76	C2DB	hexagonal	Γ -SOC	M	0.63	LCEBR	Yes	Exp.M.Exfo
CdI ₂	72	6.1.38	2.18	C2DB	hexagonal	Γ -SOC	M	0.60	LCEBR	Yes	Exp.Substr
C ₃ N	80	3.1.48	0.39	C2DB	hexagonal	M	/	0.59	OAI	Yes	Exp.
HSi	72	3.1.19	2.18	C2DB	hexagonal	/	M	0.57	OAI	Yes	Exp.
ZrS ₂	72	6.1.61	1.16	C2DB	hexagonal	/	M	0.55	LCEBR	Yes	Exp.M.Exfo
HfSe ₂	72	6.1.44	0.45	C2DB	hexagonal	Γ -SOC	M	0.49	LCEBR	Yes	Exp.M.Exfo
ZrSe ₂	72	6.1.73	0.34	C2DB	hexagonal	Γ -SOC	M	0.39	LCEBR	Yes	Exp.M.Exfo
Ti ₂ CO ₂	72	6.1.34	0.31	C2DB	hexagonal	/	M	0.24	LCEBR	Yes	Exp.

TABLE S48: Computationally exfoliable materials with valley type: hexagonal- M .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
Tl ₂ S	72	6.2.1302	1.27	MC2D	hexagonal	Γ	M	0.71	LCEBR	Yes	Comp.Exfo
Lu ₂ CCl ₂	72	6.2.1199	1.04	MC2D	hexagonal	/	M	0.68	LCEBR	Yes	Comp.Exfo
BC ₃	80	3.2.206	0.63	MC2D	hexagonal	/	M	0.67	OAI	Yes	Comp.Exfo
Y ₂ Br ₂ C	72	6.2.1198	0.81	MC2D	hexagonal	/	M	0.62	LCEBR	Yes	Comp.Exfo
Tl ₂ O	72	6.2.1288	0.93	MC2D	hexagonal	M	M	0.59	LCEBR	Yes	Comp.Exfo
HgNa ₄ P ₂	72	6.2.1261	1.15	MC2D	hexagonal	/	M	0.57	LCEBR	Yes	Comp.Exfo
Ga ₂ S ₃	72	6.2.1237	0.52	MC2D	hexagonal	/	M	0.52	LCEBR	Yes	Comp.Exfo
La ₂ GeI ₂	72	6.2.1240	0.30	MC2D	hexagonal	/	M	0.45	LCEBR	Yes	Comp.Exfo
Y ₂ Cl ₂	72	6.2.1201	0.24	MC2D	hexagonal	Γ -SOC	M	0.44	LCEBR	Yes	Comp.Exfo
KPt ₂ Se ₃	72	6.2.1276	1.11	MC2D	hexagonal	/	M	0.42	LCEBR	Yes	Comp.Exfo

TABLE S49: Computationally stable materials with valley type: hexagonal- M .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
HgI ₂	72	6.3.2498	1.15	C2DB	hexagonal	Γ -SOC	M	0.71	LCEBR	/	Stable
S ₂ Si	72	6.3.2577	1.39	C2DB	hexagonal	nHSP	M	0.71	LCEBR	/	Stable
CdI ₂	78	6.3.2630	1.52	C2DB	hexagonal	Γ -SOC	M	0.70	LCEBR	/	Stable
AlO	78	3.3.475	1.32	C2DB	hexagonal	K	M	0.69	OAI	/	Stable
Sc ₂ CF ₂	72	6.3.2360	1.01	C2DB	hexagonal	/	M	0.68	LCEBR	/	Stable
In ₂ S ₃	72	6.1.47	1.12	C2DB	hexagonal	/	M	0.68	LCEBR	/	Stable
Y ₂ CF ₂	72	6.3.2362	1.11	C2DB	hexagonal	/	M	0.68	LCEBR	/	Stable

Sc ₂ CH ₂	72	6.3.2371	1.00	C2DB	hexagonal	/	<i>M</i>	0.67	LCEBR	/	Stable
Al ₂ S ₃	72	6.3.2280	1.53	C2DB	hexagonal	/	<i>M</i>	0.67	LCEBR	/	Stable
Hf ₂ CO ₂	72	6.3.2377	0.97	C2DB	hexagonal	/	<i>M</i>	0.67	LCEBR	/	Stable
ZnI ₂	72	6.3.2510	1.78	C2DB	hexagonal	/	<i>M</i>	0.66	LCEBR	Yes	Stable
Y ₂ CCl ₂	72	6.3.2357	0.96	C2DB	hexagonal	/	<i>M</i>	0.66	LCEBR	/	Stable
SnO	69	6.3.2139	1.68	C2DB	hexagonal	<i>K</i>	<i>M</i>	0.66	LCEBR	/	Stable
AlISe	69	6.3.1921	1.47	C2DB	hexagonal	Γ-SOC	<i>M</i>	0.65	LCEBR	/	Stable
BrSSb	69	6.3.2008	1.44	C2DB	hexagonal	nHSP-SOC	<i>M</i>	0.65	LCEBR	/	Stable
GaClSe	69	6.3.2032	1.27	C2DB	hexagonal	Γ-SOC	<i>M</i>	0.65	LCEBR	/	Stable
Y ₂ CH ₂	72	6.3.2375	0.91	C2DB	hexagonal	/	<i>M</i>	0.65	LCEBR	/	Stable
Sc ₂ CCl ₂	72	6.3.2355	0.87	C2DB	hexagonal	/	<i>M</i>	0.64	LCEBR	Yes	Stable
PbS ₂	72	6.3.2561	0.74	C2DB	hexagonal	/	<i>M</i>	0.63	LCEBR	/	Stable
GeS ₂	72	6.3.2455	0.73	C2DB	hexagonal	nHSP	<i>M</i>	0.62	LCEBR	/	Stable
GaTe	72	3.3.436	1.27	C2DB	hexagonal	/	<i>M</i>	0.62	OAI	/	Stable
Zr ₂ CO ₂	72	6.3.2383	0.95	C2DB	hexagonal	/	<i>M</i>	0.62	LCEBR	/	Stable
ClSSb	69	6.3.2039	1.68	C2DB	hexagonal	nHSP	<i>M</i>	0.62	LCEBR	/	Stable
ISbSe	69	6.3.2114	1.08	C2DB	hexagonal	Γ-SOC	<i>M</i>	0.60	LCEBR	/	Stable
AlSe	78	3.3.477	2.00	C2DB	hexagonal	/	<i>M</i>	0.60	OAI	/	Stable
Cd ₂ BrIS	69	6.3.1985	0.97	C2DB	hexagonal	Γ-SOC	<i>M</i>	0.60	LCEBR	/	Stable
ISSb	69	6.3.2111	0.87	C2DB	hexagonal	Γ-SOC	<i>M</i>	0.60	LCEBR	/	Stable
SnSSe	69	6.3.2148	0.84	C2DB	hexagonal	Γ-SOC	<i>M</i>	0.59	LCEBR	/	Stable
GeO	69	6.3.2066	2.09	C2DB	hexagonal	<i>K</i>	<i>M</i>	0.59	LCEBR	/	Stable
AlS	78	3.3.476	2.10	C2DB	hexagonal	/	<i>M</i>	0.59	OAI	/	Stable
BrSbSe	69	6.3.2010	1.47	C2DB	hexagonal	nHSP-SOC	<i>M</i>	0.58	LCEBR	/	Stable
Al ₂ Se ₃	72	6.3.2281	0.69	C2DB	hexagonal	/	<i>M</i>	0.58	LCEBR	/	Stable
AsBrS	69	6.3.1927	1.43	C2DB	hexagonal	nHSP-SOC	<i>M</i>	0.58	LCEBR	/	Stable
Sc ₂ Br ₂ C	72	6.3.2353	0.65	C2DB	hexagonal	/	<i>M</i>	0.57	LCEBR	/	Stable
Se ₂ Si	72	6.3.2584	0.46	C2DB	hexagonal	nHSP	<i>M</i>	0.54	LCEBR	/	Stable
AlS	72	3.3.375	2.15	C2DB	hexagonal	/	<i>M</i>	0.53	OAI	/	Stable
AlSe	72	3.3.377	2.14	C2DB	hexagonal	/	<i>M</i>	0.50	OAI	/	Stable
In ₂ Se ₃	72	6.3.2527	0.44	C2DB	hexagonal	/	<i>M</i>	0.50	LCEBR	Yes	Stable
HfSSe	69	6.3.2094	0.71	C2DB	hexagonal	Γ-SOC	<i>M</i>	0.49	LCEBR	/	Stable
Zr ₃ C ₂ O ₂	78	6.3.2626	0.38	C2DB	hexagonal	/	<i>M</i>	0.47	LCEBR	/	Stable
MgI ₂	78	6.3.2650	2.59	C2DB	hexagonal	Γ-SOC	<i>M</i>	0.46	LCEBR	/	Stable
CaI ₂	78	6.3.2628	2.99	C2DB	hexagonal	Γ-SOC	<i>M</i>	0.46	LCEBR	/	Stable
ScClTe	69	6.3.2044	0.82	C2DB	hexagonal	Γ-SOC	<i>M</i>	0.44	LCEBR	/	Stable
AlTe	78	3.3.478	1.76	C2DB	hexagonal	nHSP	<i>M</i>	0.43	OAI	/	Stable
CaH ₂ Te ₂	72	6.3.2465	2.34	C2DB	hexagonal	Γ-SOC	<i>M</i>	0.40	LCEBR	/	Stable
AsISe	69	6.3.1943	0.52	C2DB	hexagonal	Γ-SOC	<i>M</i>	0.40	LCEBR	/	Stable
AlGaSe ₂	69	6.3.1919	2.05	C2DB	hexagonal	/	<i>M</i>	0.38	LCEBR	/	Stable
ZrSSe	69	6.3.2151	0.62	C2DB	hexagonal	Γ-SOC	<i>M</i>	0.38	LCEBR	/	Stable
Hf ₃ N ₂ O ₂	78	3.3.503	0.32	C2DB	hexagonal	<i>K</i> -SOC	<i>M</i>	0.35	OAI	/	Stable
RhPS ₃	70	6.3.2181	0.78	C2DB	hexagonal	/	<i>M</i>	0.35	LCEBR	/	Stable
SrH ₂ Te ₂	72	6.3.2489	2.56	C2DB	hexagonal	Γ-SOC	<i>M</i>	0.33	LCEBR	/	Stable
Zr ₃ N ₂ O ₂	78	3.3.514	0.40	C2DB	hexagonal	Γ	<i>M</i>	0.29	OAI	/	Stable
Al ₂ FeTe ₄	72	6.3.2264	0.39	C2DB	hexagonal	/	<i>M</i>	0.27	LCEBR	/	Stable
FeGa ₂ Se ₄	72	6.3.2437	0.47	C2DB	hexagonal	/	<i>M</i>	0.26	LCEBR	/	Stable

TABLE S50: Computationally unstable materials with valley type: hexagonal- M .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
AlO	72	3.4.124	1.18	C2DB	hexagonal	K	M	0.69	OAI	/	Unstable
ZnI ₂	78	6.4.720	0.93	C2DB	hexagonal	Γ -SOC	M	0.69	LCEBR	/	Unstable
O ₂ Sb ₂ Se	72	6.4.675	0.92	C2DB	hexagonal	nHSP	M	0.65	LCEBR	/	Unstable
CIOsB	69	6.4.541	1.53	C2DB	hexagonal	K	M	0.64	LCEBR	/	Unstable
SnS ₂	78	6.1.80	0.75	C2DB	hexagonal	/	M	0.63	LCEBR	/	Unstable
CIPS	69	6.4.542	1.12	C2DB	hexagonal	nHSP	M	0.58	LCEBR	/	Unstable
SnF ₂	78	6.4.709	2.31	C2DB	hexagonal	K	M	0.57	LCEBR	/	Unstable
F ₂ GeO ₂	72	6.4.634	1.09	C2DB	hexagonal	K	M	0.57	LCEBR	/	Unstable
AsClS	69	6.4.483	1.73	C2DB	hexagonal	nHSP	M	0.54	LCEBR	/	Unstable
BrPS	69	6.4.512	0.85	C2DB	hexagonal	nHSP-SOC	M	0.52	LCEBR	/	Unstable
ZnF ₂ S ₂	72	6.4.645	1.07	C2DB	hexagonal	M	Γ	0.51	LCEBR	/	Unstable
OSi	69	6.4.587	0.39	C2DB	hexagonal	K	M	0.50	LCEBR	/	Unstable
CdF ₂ S ₂	72	6.4.624	1.08	C2DB	hexagonal	M	Γ	0.49	LCEBR	/	Unstable
F ₂ Ge	78	6.4.706	2.80	C2DB	hexagonal	K	M	0.49	LCEBR	/	Unstable
FeF ₂ S ₂	72	6.4.633	1.01	C2DB	hexagonal	nHSP	M	0.47	LCEBR	/	Unstable
AsIS	69	6.4.487	0.29	C2DB	hexagonal	Γ -SOC	M	0.39	LCEBR	/	Unstable
ScO	78	3.4.198	0.69	C2DB	hexagonal	/	M	0.37	OAI	/	Unstable
VS	78	3.4.211	0.21	C2DB	hexagonal	M	/	0.31	OAI	/	Unstable
VSe	78	3.4.215	0.25	C2DB	hexagonal	M	/	0.30	OAI	/	Unstable
VTe	78	3.4.216	0.22	C2DB	hexagonal	M	/	0.28	OAI	/	Unstable

f. M-SOC

TABLE S51: Experimental materials with valley type: hexagonal- M -SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
GaTe	78	3.1.35	1.29	C2DB	hexagonal	/	M -SOC	0.58	OAI	Yes	Exp.M.Exfo

TABLE S52: Computationally stable materials with valley type: hexagonal- M -SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
HgI ₂	78	6.3.2649	0.66	C2DB	hexagonal	Γ -SOC	M -SOC	0.60	LCEBR	/	Stable
SnCl ₂	78	6.3.2635	2.76	C2DB	hexagonal	/	M -SOC	0.50	LCEBR	/	Stable
Hf ₃ C ₂ O ₂	78	6.3.2622	0.42	C2DB	hexagonal	/	M -SOC	0.48	LCEBR	/	Stable

TABLE S53: Computationally unstable materials with valley type: hexagonal- M -SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
BrOSb	69	6.4.511	1.21	C2DB	hexagonal	Γ -SOC	M -SOC	0.65	LCEBR	/	Unstable
IrSe	78	3.4.189	0.29	C2DB	hexagonal	M -SOC	nHSP-SOC	0.28	OAI	/	Unstable

g. nHSP

TABLE S54: Experimental materials with valley type: hexagonal-nHSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
---------	----	----	-----	----------	---------	------------	------------	-------------	----------	------	-----------

Sb	72	3.1.25	1.01	C2DB	hexagonal	Γ -SOC	nHSP	0.75	OAI	Yes	Exp.W.Exfo
As	72	3.1.11	1.48	C2DB	hexagonal	Γ -SOC	nHSP	0.75	OAI	Yes	Exp.W.Exfo
P	72	3.1.23	1.95	C2DB	hexagonal	/	nHSP	0.68	OAI	Yes	Exp.Substr
PtSe ₂	72	6.1.58	1.18	C2DB	hexagonal	Γ -SOC	nHSP	0.53	LCEBR	Yes	Exp.M.Exfo
InSe	78	3.1.37	1.40	C2DB	hexagonal	nHSP	Γ	0.50	OAI	Yes	Exp.M.Exfo
GaS	78	3.1.30	2.30	C2DB	hexagonal	nHSP	Γ	0.48	OAI	Yes	Exp.M.Exfo
GaSe	78	3.1.32	1.74	C2DB	hexagonal	nHSP	Γ	0.46	OAI	Yes	Exp.M.Exfo
ZrBrN	72	6.3.2323	1.62	C2DB	hexagonal	nHSP	K	0.44	LCEBR	Yes	Exp.W.Exfo
TiO ₂	72	6.1.49	2.66	C2DB	hexagonal	nHSP	/	0.27	LCEBR	Yes	Exp.
Sb ₂ SeTe ₂	72	6.1.67	0.44	C2DB	hexagonal	nHSP	Γ	0.27	LCEBR	Yes	Exp.M.Exfo

TABLE S55: Computationally exfoliable materials with valley type: hexagonal-nHSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
GeTe	69	6.2.1108	1.25	MC2D	hexagonal	Γ -SOC	nHSP	0.69	LCEBR	Yes	Comp.Exfo
SnTl ₂ As ₂ S ₆	66	6.2.1065	1.59	MC2D	hexagonal	/	nHSP	0.51	LCEBR	Yes	Comp.Exfo
KSnAs	69	6.2.1089	0.62	MC2D	hexagonal	nHSP	/	0.33	LCEBR	Yes	Comp.Exfo
SSb ₂ Te ₂	72	6.2.1301	0.50	MC2D	hexagonal	nHSP	Γ	0.31	LCEBR	Yes	Comp.Exfo
NdIS	72	6.2.1266	2.47	MC2D	hexagonal	nHSP	K	0.26	LCEBR	Yes	Comp.Exfo
PrIS	72	6.2.1268	2.47	MC2D	hexagonal	nHSP	K	0.26	LCEBR	Yes	Comp.Exfo
GdIS	72	6.2.1238	2.57	MC2D	hexagonal	nHSP	K	0.25	LCEBR	Yes	Comp.Exfo
DyIS	72	6.2.1220	2.65	MC2D	hexagonal	nHSP	/	0.23	LCEBR	Yes	Comp.Exfo

TABLE S56: Computationally stable materials with valley type: hexagonal-nHSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
InI	72	6.3.2500	1.01	C2DB	hexagonal	nHSP	K	0.69	LCEBR	/	Stable
GeTe	69	6.3.2069	1.49	C2DB	hexagonal	Γ -SOC	nHSP	0.69	LCEBR	/	Stable
InBr	72	6.3.2321	1.34	C2DB	hexagonal	nHSP	K	0.68	LCEBR	/	Stable
SnTe	69	6.3.2164	1.59	C2DB	hexagonal	Γ -SOC	nHSP	0.67	LCEBR	/	Stable
PtO ₂	72	6.3.2546	1.65	C2DB	hexagonal	nHSP	/	0.67	LCEBR	Yes	Stable
HfSe ₂	78	6.3.2647	0.83	C2DB	hexagonal	nHSP-SOC	nHSP	0.65	LCEBR	/	Stable
ClSSb	69	6.3.2038	1.33	C2DB	hexagonal	nHSP	Γ -SOC	0.65	LCEBR	/	Stable
AsClS	69	6.3.1932	1.53	C2DB	hexagonal	nHSP	Γ -SOC	0.64	LCEBR	/	Stable
HfSSe	69	6.3.2095	0.91	C2DB	hexagonal	/	nHSP	0.62	LCEBR	/	Stable
ClSSb	69	6.3.2039	1.68	C2DB	hexagonal	nHSP	M	0.60	LCEBR	/	Stable
PdO ₂	72	6.3.2545	1.36	C2DB	hexagonal	nHSP	/	0.60	LCEBR	/	Stable
AlPS ₃	70	6.3.2166	1.30	C2DB	hexagonal	nHSP	/	0.59	LCEBR	/	Stable
GeSe	69	6.3.2068	2.22	C2DB	hexagonal	/	nHSP	0.57	LCEBR	/	Stable
ScAsS ₃	70	6.3.2170	1.41	C2DB	hexagonal	nHSP	/	0.54	LCEBR	/	Stable
AlAsS ₃	70	6.3.2165	1.14	C2DB	hexagonal	nHSP	/	0.54	LCEBR	/	Stable
ScPS ₃	70	6.3.2183	0.83	C2DB	hexagonal	nHSP	/	0.53	LCEBR	/	Stable
GaS	72	3.3.432	2.16	C2DB	hexagonal	nHSP	Γ	0.53	OAI	Yes	Stable
GeS	69	6.3.2067	2.47	C2DB	hexagonal	/	nHSP	0.53	LCEBR	/	Stable
InSe	72	3.3.456	1.31	C2DB	hexagonal	nHSP	Γ	0.51	OAI	/	Stable
GaSe	72	3.3.434	1.61	C2DB	hexagonal	nHSP	Γ	0.50	OAI	/	Stable
InF	72	6.3.2424	1.34	C2DB	hexagonal	nHSP	nHSP	0.50	LCEBR	/	Stable
NiO ₂	72	6.3.2540	1.17	C2DB	hexagonal	nHSP	nHSP	0.49	LCEBR	Yes	Stable
OsBr ₂	72	6.3.2325	1.14	C2DB	hexagonal	/	nHSP	0.49	LCEBR	/	Stable

OsCl ₂	72	6.3.2410	1.32	C2DB	hexagonal	/	nHSP	0.49	LCEBR	/	Stable
GeI ₂	72	6.3.2453	1.98	C2DB	hexagonal	nHSP	Γ	0.48	LCEBR	Yes	Stable
ZrTe ₂	78	6.1.81	0.28	C2DB	hexagonal	Γ-SOC	nHSP	0.48	LCEBR	/	Stable
S ₂ Si	72	6.3.2577	1.39	C2DB	hexagonal	nHSP	<i>M</i>	0.48	LCEBR	/	Stable
PbSe	72	6.3.2559	1.21	C2DB	hexagonal	nHSP	Γ	0.47	LCEBR	/	Stable
SnSe	72	6.3.2585	1.23	C2DB	hexagonal	nHSP	/	0.47	LCEBR	/	Stable
InSeSi	72	3.3.455	1.51	C2DB	hexagonal	nHSP	Γ	0.46	OAI	/	Stable
ZrCl ₂	78	3.3.495	0.99	C2DB	hexagonal	<i>K</i>	nHSP	0.46	OAI	Yes	Stable
TlS	78	3.3.525	0.67	C2DB	hexagonal	nHSP	Γ	0.45	OAI	/	Stable
TlS	72	3.3.470	0.62	C2DB	hexagonal	nHSP	Γ	0.45	OAI	/	Stable
AlSiTe	72	3.3.378	1.52	C2DB	hexagonal	nHSP	/	0.45	OAI	/	Stable
InTe	72	3.3.458	1.16	C2DB	hexagonal	nHSP	Γ	0.44	OAI	/	Stable
SnTe	72	6.3.2588	0.72	C2DB	hexagonal	nHSP	Γ	0.44	LCEBR	/	Stable
ZrI ₂	78	3.3.507	0.70	C2DB	hexagonal	<i>K</i> -SOC	nHSP	0.43	OAI	/	Stable
BiClS	69	6.3.1960	1.84	C2DB	hexagonal	nHSP	Γ-SOC	0.43	LCEBR	/	Stable
ZrBr ₂	78	3.3.483	0.83	C2DB	hexagonal	<i>K</i> -SOC	nHSP	0.43	OAI	/	Stable
Ta ₃ Br ₇ Te	69	6.3.1984	0.74	C2DB	hexagonal	/	nHSP	0.42	LCEBR	/	Stable
ZrSeTe	69	6.3.2163	0.28	C2DB	hexagonal	Γ-SOC	nHSP	0.42	LCEBR	/	Stable
CoBrTe	69	6.3.1993	0.83	C2DB	hexagonal	/	nHSP	0.42	LCEBR	/	Stable
ZrClI	69	3.3.275	0.88	C2DB	hexagonal	<i>K</i> -SOC	nHSP	0.41	OAI	/	Stable
As ₂ S ₃	72	6.3.2291	0.92	C2DB	hexagonal	nHSP	Γ	0.41	LCEBR	/	Stable
PtSeTe	69	6.3.2146	0.75	C2DB	hexagonal	Γ-SOC	nHSP	0.41	LCEBR	/	Stable
ZrClF	69	3.3.272	1.25	C2DB	hexagonal	<i>K</i>	nHSP	0.40	OAI	/	Stable
AlTe	72	3.3.379	1.97	C2DB	hexagonal	nHSP	/	0.40	OAI	/	Stable
AlTe	78	3.3.478	1.76	C2DB	hexagonal	nHSP	<i>M</i>	0.40	OAI	/	Stable
GaInS ₂	69	6.3.2063	1.77	C2DB	hexagonal	nHSP	Γ	0.39	LCEBR	/	Stable
TiS ₂	78	6.3.2657	0.73	C2DB	hexagonal	nHSP	/	0.39	LCEBR	/	Stable
ZrBrCl	69	3.3.267	0.91	C2DB	hexagonal	<i>K</i> -SOC	nHSP	0.39	OAI	/	Stable
PdSe ₂	72	6.3.2570	0.53	C2DB	hexagonal	Γ-SOC	nHSP	0.39	LCEBR	/	Stable
HfBrN	72	6.3.2318	1.97	C2DB	hexagonal	nHSP	<i>K</i>	0.38	LCEBR	Yes	Stable
ZrBrI	69	3.3.270	0.78	C2DB	hexagonal	<i>K</i> -SOC	nHSP	0.38	OAI	/	Stable
GeS ₂	72	6.3.2455	0.73	C2DB	hexagonal	nHSP	<i>M</i>	0.38	LCEBR	/	Stable
As ₂ S ₂ Se	72	6.3.2290	0.82	C2DB	hexagonal	nHSP	Γ	0.37	LCEBR	/	Stable
P ₂ STe ₂	72	6.3.2554	0.66	C2DB	hexagonal	nHSP	Γ	0.36	LCEBR	/	Stable
As ₂ SSe ₂	72	6.3.2292	0.72	C2DB	hexagonal	nHSP	Γ	0.36	LCEBR	/	Stable
As ₂ STe ₂	72	6.3.2293	0.74	C2DB	hexagonal	nHSP	Γ	0.36	LCEBR	/	Stable
P ₂ SSe ₂	72	6.3.2553	0.50	C2DB	hexagonal	nHSP	nHSP	0.34	LCEBR	/	Stable
SnF	72	1.3.271	0.28	C2DB	hexagonal	nHSP	Γ	0.34	SEBR	/	Stable
NiS ₂	72	6.3.2541	0.49	C2DB	hexagonal	/	nHSP	0.33	LCEBR	/	Stable
TlSe	78	3.3.526	0.49	C2DB	hexagonal	nHSP	Γ	0.33	OAI	/	Stable
As ₂ Se ₂ Te	72	6.3.2294	0.64	C2DB	hexagonal	nHSP	nHSP	0.32	LCEBR	/	Stable
GePTe ₃	66	3.3.210	0.84	C2DB	hexagonal	nHSP	/	0.32	OAI	/	Stable
Se ₂ Si	72	6.3.2584	0.46	C2DB	hexagonal	nHSP	<i>M</i>	0.32	LCEBR	/	Stable
TlSe	72	3.3.471	0.44	C2DB	hexagonal	nHSP	Γ	0.32	OAI	/	Stable
As ₂ Se ₃	72	6.3.2295	0.62	C2DB	hexagonal	nHSP	Γ	0.31	LCEBR	/	Stable
PtI	72	3.3.450	0.39	C2DB	hexagonal	nHSP	/	0.30	OAI	/	Stable
P ₂ SeTe ₂	72	6.3.2556	0.51	C2DB	hexagonal	nHSP	Γ	0.30	LCEBR	/	Stable
SnAs ₂ Te ₄	72	6.3.2298	0.39	C2DB	hexagonal	nHSP	Γ	0.29	LCEBR	/	Stable
P ₂ Se ₃	72	6.3.2555	0.42	C2DB	hexagonal	nHSP	Γ	0.28	LCEBR	/	Stable
Sb ₂ Se ₃	72	6.1.65	0.44	C2DB	hexagonal	nHSP	Γ	0.25	LCEBR	/	Stable
YIS	72	6.3.2506	2.56	C2DB	hexagonal	nHSP	<i>K</i>	0.24	LCEBR	/	Stable

Sb ₂ Te ₃	72	6.3.2583	0.40	C2DB	hexagonal	nHSP	Γ	0.24	LCEBR	/	Stable
CoITe	69	6.3.2048	0.43	C2DB	hexagonal	Γ -SOC	nHSP	0.22	LCEBR	/	Stable
P ₂ Te ₃	72	6.3.2557	0.29	C2DB	hexagonal	nHSP	nHSP	0.22	LCEBR	/	Stable
InNi ₂ Te ₃	72	6.3.2520	0.29	C2DB	hexagonal	/	nHSP	0.21	LCEBR	/	Stable
SnAsTe ₃	66	3.3.209	0.49	C2DB	hexagonal	nHSP	/	0.21	OAI	/	Stable

TABLE S57: Computationally unstable materials with valley type: hexagonal-nHSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
TiO ₂	78	6.4.723	1.16	C2DB	hexagonal	/	nHSP	0.71	LCEBR	/	Unstable
HfS ₂	78	6.4.718	1.08	C2DB	hexagonal	/	nHSP	0.71	LCEBR	/	Unstable
I ₂ Si	72	6.4.669	1.60	C2DB	hexagonal	nHSP	Γ	0.69	LCEBR	/	Unstable
PbH	72	1.4.179	0.96	C2DB	hexagonal	nHSP	Γ	0.66	SEBR	/	Unstable
SeSi	69	6.4.594	2.07	C2DB	hexagonal	nHSP-SOC	nHSP	0.59	LCEBR	/	Unstable
ClOP	69	6.4.540	1.95	C2DB	hexagonal	<i>K</i>	nHSP	0.57	LCEBR	/	Unstable
ClPS	69	6.4.542	1.12	C2DB	hexagonal	nHSP	<i>M</i>	0.56	LCEBR	/	Unstable
SSb	72	3.4.165	0.36	C2DB	hexagonal	nHSP	/	0.49	OAI	/	Unstable
O ₂ SSb ₂	72	6.4.674	0.96	C2DB	hexagonal	nHSP	nHSP	0.48	LCEBR	/	Unstable
AsClS	69	6.4.483	1.73	C2DB	hexagonal	nHSP	<i>M</i>	0.48	LCEBR	/	Unstable
FeF ₂ S ₂	72	6.4.633	1.01	C2DB	hexagonal	nHSP	<i>M</i>	0.47	LCEBR	/	Unstable
SbSe	72	3.4.170	0.22	C2DB	hexagonal	nHSP	/	0.44	OAI	/	Unstable
ZnZrCl ₂	69	3.4.98	0.70	C2DB	hexagonal	/	nHSP	0.44	OAI	/	Unstable
O ₂ Sb ₂ Se	72	6.4.675	0.92	C2DB	hexagonal	nHSP	<i>M</i>	0.44	LCEBR	/	Unstable
ZrBrF	69	3.4.90	1.16	C2DB	hexagonal	<i>K</i>	nHSP	0.43	OAI	/	Unstable
FeF ₂ O ₂	72	6.4.632	0.75	C2DB	hexagonal	/	nHSP	0.39	LCEBR	/	Unstable
P ₂ S ₃	72	6.4.684	0.57	C2DB	hexagonal	nHSP	/	0.36	LCEBR	/	Unstable
P ₂ S ₂ Se	72	6.4.683	0.58	C2DB	hexagonal	nHSP	/	0.33	LCEBR	/	Unstable

h. nHSP-SOC

TABLE S58: Experimental materials with valley type: hexagonal-nHSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
BiTe	69	6.1.13	0.70	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.34	LCEBR	Yes	Exp.M.Exfo

TABLE S59: Computationally exfoliable materials with valley type: hexagonal-nHSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
AsSb	69	6.2.1090	1.18	MC2D	hexagonal	Γ -SOC	nHSP-SOC	0.69	LCEBR	Yes	Comp.Exfo
NaSnP	69	6.2.1128	1.07	MC2D	hexagonal	nHSP-SOC	Γ	0.41	LCEBR	Yes	Comp.Exfo
Bi ₂ STe ₂	69	6.2.1092	0.36	MC2D	hexagonal	nHSP-SOC	Γ -SOC	0.17	LCEBR	Yes	Comp.Exfo

TABLE S60: Computationally stable materials with valley type: hexagonal-nHSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
BrSSb	69	6.3.2007	1.23	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.65	LCEBR	/	Stable
BrSbSe	69	6.3.2009	1.07	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.65	LCEBR	/	Stable
FSbTe	69	6.3.2059	1.57	C2DB	hexagonal	Γ -SOC	nHSP-SOC	0.63	LCEBR	/	Stable

ClSbSe	69	6.3.2040	1.18	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.63	LCEBR	/	Stable
AsFTe	69	6.3.1939	1.65	C2DB	hexagonal	Γ -SOC	nHSP-SOC	0.62	LCEBR	/	Stable
AsClSe	69	6.3.1933	1.36	C2DB	hexagonal	nHSP-SOC	Γ	0.61	LCEBR	/	Stable
AsBrS	69	6.3.1926	1.38	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.60	LCEBR	/	Stable
AsBrSe	69	6.3.1928	1.21	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.59	LCEBR	/	Stable
BiBrS	69	6.3.1954	1.23	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.58	LCEBR	/	Stable
SnSe	69	6.3.2159	2.16	C2DB	hexagonal	/	nHSP-SOC	0.58	LCEBR	/	Stable
IrClS	69	6.3.2037	1.43	C2DB	hexagonal	nHSP-SOC	/	0.57	LCEBR	/	Stable
SnS	69	6.3.2153	2.30	C2DB	hexagonal	/	nHSP-SOC	0.55	LCEBR	/	Stable
HfCl ₂	78	3.3.493	0.89	C2DB	hexagonal	K -SOC	nHSP-SOC	0.54	OAI	/	Stable
BiBrISb	69	6.3.1953	0.69	C2DB	hexagonal	Γ -SOC	nHSP-SOC	0.53	LCEBR	/	Stable
BrSSb	69	6.3.2008	1.44	C2DB	hexagonal	nHSP-SOC	M	0.52	LCEBR	/	Stable
IrBrSe	69	6.3.2006	1.24	C2DB	hexagonal	nHSP-SOC	K -SOC	0.52	LCEBR	/	Stable
BiBrSe	69	6.3.1956	1.03	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.51	LCEBR	/	Stable
WO _{Te}	69	3.3.291	0.56	C2DB	hexagonal	Γ	nHSP-SOC	0.51	OAI	/	Stable
BrSbSe	69	6.3.2010	1.47	C2DB	hexagonal	nHSP-SOC	M	0.50	LCEBR	/	Stable
ISbSe	69	6.3.2113	1.06	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.50	LCEBR	/	Stable
IrITe	69	6.3.2108	1.04	C2DB	hexagonal	nHSP-SOC	nHSP-SOC	0.50	LCEBR	/	Stable
HfBr ₂	78	3.3.481	0.72	C2DB	hexagonal	K -SOC	nHSP-SOC	0.50	OAI	/	Stable
ISSb	69	6.3.2110	1.28	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.50	LCEBR	/	Stable
AsBrTe	69	6.3.1930	1.25	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.49	LCEBR	/	Stable
BrSbTe	69	6.3.2011	1.09	C2DB	hexagonal	nHSP-SOC	Γ	0.48	LCEBR	/	Stable
ISbTe	69	6.3.2115	0.89	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.47	LCEBR	/	Stable
AsITe	69	6.3.1944	1.01	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.47	LCEBR	/	Stable
BiClSe	69	6.3.1961	1.14	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.47	LCEBR	/	Stable
ClSbSe	69	6.3.2041	1.68	C2DB	hexagonal	nHSP-SOC	nHSP-SOC	0.47	LCEBR	/	Stable
AlPSe ₃	70	6.3.2167	0.61	C2DB	hexagonal	nHSP-SOC	Γ	0.46	LCEBR	/	Stable
BiS	78	3.3.480	0.28	C2DB	hexagonal	nHSP-SOC	/	0.46	OAI	/	Stable
HfBrCl	69	3.3.265	0.82	C2DB	hexagonal	K -SOC	nHSP-SOC	0.46	OAI	/	Stable
HfClI	69	3.3.273	0.81	C2DB	hexagonal	K -SOC	nHSP-SOC	0.46	OAI	/	Stable
HfI ₂	78	3.3.505	0.62	C2DB	hexagonal	K -SOC	nHSP-SOC	0.46	OAI	/	Stable
AsClTe	69	6.3.1935	1.50	C2DB	hexagonal	nHSP-SOC	Γ	0.45	LCEBR	/	Stable
AsISe	69	6.3.1942	1.16	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.45	LCEBR	/	Stable
HfOS	69	6.3.2092	1.92	C2DB	hexagonal	/	nHSP-SOC	0.45	LCEBR	/	Stable
SnI ₂	78	6.3.2652	1.96	C2DB	hexagonal	nHSP-SOC	/	0.44	LCEBR	/	Stable
ScAsSe ₃	70	6.3.2172	0.82	C2DB	hexagonal	nHSP-SOC	/	0.44	LCEBR	/	Stable
BiBrS	69	6.3.1955	1.59	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.43	LCEBR	/	Stable
AsClSe	69	6.3.1934	1.71	C2DB	hexagonal	nHSP-SOC	/	0.43	LCEBR	/	Stable
ZrSe ₂	78	6.3.2660	0.73	C2DB	hexagonal	nHSP-SOC	/	0.43	LCEBR	/	Stable
HfSe ₂	78	6.3.2647	0.83	C2DB	hexagonal	nHSP-SOC	nHSP	0.43	LCEBR	/	Stable
AsBrSe	69	6.3.1929	1.49	C2DB	hexagonal	nHSP-SOC	/	0.43	LCEBR	/	Stable
BiBrSe	69	6.3.1957	1.38	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.43	LCEBR	/	Stable
GeI ₂	78	6.3.2642	1.84	C2DB	hexagonal	nHSP-SOC	K -SOC	0.43	LCEBR	/	Stable
ISbTe	69	6.3.2116	1.03	C2DB	hexagonal	nHSP-SOC	K	0.43	LCEBR	/	Stable
ClSbTe	69	6.3.2042	1.29	C2DB	hexagonal	nHSP-SOC	Γ	0.43	LCEBR	/	Stable
HfBrI	69	3.3.268	0.70	C2DB	hexagonal	K -SOC	nHSP-SOC	0.42	OAI	/	Stable
BrSbTe	69	6.3.2012	1.33	C2DB	hexagonal	nHSP-SOC	/	0.42	LCEBR	/	Stable
AsBrS	69	6.3.1927	1.43	C2DB	hexagonal	nHSP-SOC	M	0.42	LCEBR	/	Stable
InPbBrSe	69	6.3.2005	0.34	C2DB	hexagonal	nHSP-SOC	K -SOC	0.42	LCEBR	/	Stable
ScSbSe ₃	70	6.3.2186	1.11	C2DB	hexagonal	nHSP-SOC	/	0.42	LCEBR	/	Stable
PtSSe	69	6.3.2145	1.33	C2DB	hexagonal	nHSP-SOC	nHSP-SOC	0.41	LCEBR	/	Stable

BiISe	69	6.3.1971	0.93	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.41	LCEBR	/	Stable
BiClSe	69	6.3.1962	1.60	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.40	LCEBR	/	Stable
Br ₂ Ge	78	6.3.2613	2.54	C2DB	hexagonal	nHSP-SOC	/	0.39	LCEBR	/	Stable
BiBrTe	69	6.3.1958	0.88	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.36	LCEBR	/	Stable
ZrSSe	69	6.3.2152	0.83	C2DB	hexagonal	nHSP-SOC	/	0.36	LCEBR	/	Stable
BiPTe ₃	70	6.3.2175	0.51	C2DB	hexagonal	nHSP-SOC	/	0.34	LCEBR	/	Stable
RhISe	69	6.3.2109	0.55	C2DB	hexagonal	nHSP-SOC	<i>K</i> -SOC	0.30	LCEBR	/	Stable
ZrTe	78	3.3.530	0.46	C2DB	hexagonal	/	nHSP-SOC	0.30	OAI	/	Stable
PSbTe ₃	70	6.3.2185	0.53	C2DB	hexagonal	nHSP-SOC	/	0.29	LCEBR	/	Stable
AgPbITe	69	6.3.1907	0.62	C2DB	hexagonal	nHSP-SOC	Γ -SOC	0.28	LCEBR	/	Stable
ScSbTe ₃	70	6.3.2187	0.57	C2DB	hexagonal	nHSP-SOC	/	0.23	LCEBR	/	Stable

TABLE S61: Computationally unstable materials with valley type: hexagonal-nHSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
SiTe	69	6.4.596	1.53	C2DB	hexagonal	Γ -SOC	nHSP-SOC	0.68	LCEBR	/	Unstable
ZrO ₂	78	6.4.724	1.68	C2DB	hexagonal	/	nHSP-SOC	0.68	LCEBR	/	Unstable
HfO ₂	78	6.4.716	1.90	C2DB	hexagonal	/	nHSP-SOC	0.64	LCEBR	/	Unstable
BiBrO	69	6.4.490	1.54	C2DB	hexagonal	Γ -SOC	nHSP-SOC	0.64	LCEBR	/	Unstable
InClSeSi	69	6.4.537	1.07	C2DB	hexagonal	nHSP-SOC	/	0.62	LCEBR	/	Unstable
Br ₂ Si	78	6.4.697	1.98	C2DB	hexagonal	nHSP-SOC	<i>K</i> -SOC	0.62	LCEBR	/	Unstable
IrFO	69	6.4.555	0.91	C2DB	hexagonal	nHSP-SOC	nHSP-SOC	0.59	LCEBR	/	Unstable
AsBrO	69	6.4.481	2.04	C2DB	hexagonal	Γ -SOC	nHSP-SOC	0.56	LCEBR	/	Unstable
BiClO	69	6.4.491	2.13	C2DB	hexagonal	/	nHSP-SOC	0.54	LCEBR	/	Unstable
I ₂ Si	78	6.4.719	1.38	C2DB	hexagonal	nHSP-SOC	<i>K</i> -SOC	0.54	LCEBR	/	Unstable
IOP	69	6.4.574	0.65	C2DB	hexagonal	Γ -SOC	nHSP-SOC	0.53	LCEBR	/	Unstable
AsIO	69	6.4.486	0.63	C2DB	hexagonal	Γ -SOC	nHSP-SOC	0.53	LCEBR	/	Unstable
ClPSe	69	6.4.543	1.22	C2DB	hexagonal	nHSP-SOC	<i>K</i> -SOC	0.53	LCEBR	/	Unstable
AsClO	69	6.4.482	2.25	C2DB	hexagonal	<i>K</i>	nHSP-SOC	0.52	LCEBR	/	Unstable
HfOSe	69	6.4.569	0.97	C2DB	hexagonal	Γ -SOC	nHSP-SOC	0.52	LCEBR	/	Unstable
BiTl	69	3.4.84	0.55	C2DB	hexagonal	nHSP-SOC	<i>K</i> -SOC	0.51	OAI	/	Unstable
BrPSe	69	6.4.513	1.01	C2DB	hexagonal	nHSP-SOC	<i>K</i> -SOC	0.45	LCEBR	/	Unstable
BrOP	69	6.4.510	1.79	C2DB	hexagonal	nHSP-SOC	nHSP-SOC	0.45	LCEBR	/	Unstable
ClPTe	69	6.4.544	0.94	C2DB	hexagonal	nHSP-SOC	<i>K</i> -SOC	0.43	LCEBR	/	Unstable
HfFI	69	3.4.107	0.96	C2DB	hexagonal	<i>K</i> -SOC	nHSP-SOC	0.43	OAI	/	Unstable
HgO	78	1.4.265	0.30	C2DB	hexagonal	nHSP-SOC	Γ	0.42	NLC	/	Unstable
HfBrF	69	3.4.88	1.09	C2DB	hexagonal	<i>K</i> -SOC	nHSP-SOC	0.41	OAI	/	Unstable
HfClF	69	3.4.99	1.18	C2DB	hexagonal	<i>K</i> -SOC	nHSP-SOC	0.40	OAI	/	Unstable
BrPS	69	6.4.512	0.85	C2DB	hexagonal	nHSP-SOC	<i>M</i>	0.40	LCEBR	/	Unstable
SeSi	69	6.4.594	2.07	C2DB	hexagonal	nHSP-SOC	nHSP	0.37	LCEBR	/	Unstable
BrPTe	69	6.4.514	0.75	C2DB	hexagonal	nHSP-SOC	<i>K</i> -SOC	0.37	LCEBR	/	Unstable
AuCl	78	1.4.247	0.29	C2DB	hexagonal	nHSP-SOC	Γ	0.32	NLC	/	Unstable
IrSe	78	3.4.189	0.29	C2DB	hexagonal	<i>M</i> -SOC	nHSP-SOC	0.28	OAI	/	Unstable

3. Square lattice

a. Γ

TABLE S62: Computationally exfoliable materials with valley type: square- Γ .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
---------	----	----	-----	----------	---------	------------	------------	-------------	----------	------	-----------

AgCsO	61	6.2.944	1.12	MC2D	square	/	Γ	0.69	LCEBR	Yes	Comp.Exfo
Ba ₃ In ₂ Br ₂ O ₅	61	6.2.946	1.51	MC2D	square	/	Γ	0.69	LCEBR	Yes	Comp.Exfo
NiC ₂ N ₂	61	6.2.949	1.56	MC2D	square	/	Γ	0.68	LCEBR	Yes	Comp.Exfo
TlO ₄ P	57	6.2.931	1.30	MC2D	square	<i>M</i>	Γ	0.62	LCEBR	Yes	Comp.Exfo
AuCsO	61	6.2.945	0.77	MC2D	square	/	Γ	0.62	LCEBR	Yes	Comp.Exfo
MgNaAs	64	6.2.972	0.95	MC2D	square	/	Γ	0.59	LCEBR	Yes	Comp.Exfo
PbFI	64	6.2.1017	1.99	MC2D	square	/	Γ	0.57	LCEBR	Yes	Comp.Exfo
CuNaTe	64	6.2.1008	0.73	MC2D	square	Γ -SOC	Γ	0.56	LCEBR	Yes	Comp.Exfo
ZnF ₂	61	6.2.956	2.71	MC2D	square	<i>M</i>	Γ	0.55	LCEBR	Yes	Comp.Exfo
AgKTe	64	6.2.970	1.37	MC2D	square	Γ -SOC	Γ	0.53	LCEBR	Yes	Comp.Exfo
AgKSe	64	6.2.969	0.48	MC2D	square	/	Γ	0.51	LCEBR	Yes	Comp.Exfo
BiIO	64	6.2.982	1.23	MC2D	square	/	Γ	0.50	LCEBR	Yes	Comp.Exfo
CuNaSe	64	6.2.1007	0.26	MC2D	square	/	Γ	0.48	LCEBR	Yes	Comp.Exfo
CaO	64	6.2.1000	2.46	MC2D	square	/	Γ	0.45	LCEBR	Yes	Comp.Exfo
Ba ₂ OTe	64	6.2.976	1.74	MC2D	square	/	Γ	0.44	LCEBR	Yes	Comp.Exfo
PbBrF	64	6.2.991	2.71	MC2D	square	/	Γ	0.44	LCEBR	Yes	Comp.Exfo
PtO ₄ S	52	6.2.923	1.32	MC2D	square	/	Γ	0.43	LCEBR	Yes	Comp.Exfo
HgI ₂	59	6.2.942	1.59	MC2D	square	/	Γ	0.41	LCEBR	Yes	Comp.Exfo
AgClO ₄	57	6.2.926	2.82	MC2D	square	<i>X</i>	Γ	0.40	LCEBR	Yes	Comp.Exfo
PdO ₄ S	52	6.2.922	0.76	MC2D	square	/	Γ	0.38	LCEBR	Yes	Comp.Exfo
BiBrO	64	6.2.977	2.16	MC2D	square	/	Γ	0.37	LCEBR	Yes	Comp.Exfo
CuKTe	64	6.2.1006	0.32	MC2D	square	Γ -SOC	Γ	0.33	LCEBR	Yes	Comp.Exfo
Na ₃ PS ₄	50	6.2.918	2.78	MC2D	square	/	Γ	0.20	LCEBR	Yes	Comp.Exfo

TABLE S63: Computationally stable materials with valley type: square- Γ .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
CuCl	64	6.3.1751	1.45	C2DB	square	/	Γ	0.73	LCEBR	/	Stable
CuBr	64	6.3.1738	1.50	C2DB	square	/	Γ	0.73	LCEBR	Yes	Stable
AgBr	64	6.3.1721	1.85	C2DB	square	/	Γ	0.67	LCEBR	/	Stable
GeI ₂	59	6.3.1658	1.06	C2DB	square	nHSP-SOC	Γ	0.67	LCEBR	/	Stable
Br ₂ Ge	59	6.3.1631	1.31	C2DB	square	nHSP-SOC	Γ	0.67	LCEBR	/	Stable
Cl ₂ Ge	59	6.3.1642	1.38	C2DB	square	<i>M</i>	Γ	0.67	LCEBR	/	Stable
SnI ₂	59	6.3.1672	1.14	C2DB	square	nHSP-SOC	Γ	0.67	LCEBR	/	Stable
SnS ₂	59	6.3.1685	1.45	C2DB	square	<i>X</i>	Γ	0.67	LCEBR	Yes	Stable
AgI	64	6.3.1724	1.92	C2DB	square	Γ -SOC	Γ	0.66	LCEBR	Yes	Stable
AgCl	64	6.3.1722	2.02	C2DB	square	/	Γ	0.64	LCEBR	/	Stable
SnF ₂	59	6.3.1653	1.66	C2DB	square	<i>M</i>	Γ	0.64	LCEBR	/	Stable
SnSe ₂	59	6.1.9	0.85	C2DB	square	<i>X</i>	Γ	0.62	LCEBR	/	Stable
GeO	64	6.3.1769	2.12	C2DB	square	/	Γ	0.61	LCEBR	/	Stable
CuI	64	6.3.1761	1.90	C2DB	square	Γ -SOC	Γ	0.60	LCEBR	Yes	Stable
AgF	64	6.3.1723	0.58	C2DB	square	/	Γ	0.60	LCEBR	/	Stable
HgBr ₂	59	6.3.1632	1.94	C2DB	square	/	Γ	0.59	LCEBR	/	Stable
HgF ₂	59	6.3.1651	1.99	C2DB	square	/	Γ	0.58	LCEBR	/	Stable
ZnTe	64	6.3.1814	0.51	C2DB	square	Γ -SOC	Γ	0.58	LCEBR	/	Stable
SnO ₂	59	6.3.1677	2.06	C2DB	square	/	Γ	0.57	LCEBR	/	Stable
AuI	64	6.3.1728	0.79	C2DB	square	Γ -SOC	Γ	0.57	LCEBR	/	Stable
PbS ₂	59	6.3.1680	0.67	C2DB	square	/	Γ	0.56	LCEBR	/	Stable
GeS ₂	59	6.3.1660	1.36	C2DB	square	<i>X</i>	Γ	0.56	LCEBR	Yes	Stable
PbF ₄	61	6.3.1699	2.62	C2DB	square	/	Γ	0.53	LCEBR	Yes	Stable

HgCl ₂	59	6.3.1643	2.40	C2DB	square	/	Γ	0.52	LCEBR	/	Stable
ZnSe	64	6.3.1812	2.02	C2DB	square	/	Γ	0.49	LCEBR	Yes	Stable
GeSe ₂	59	6.3.1661	0.56	C2DB	square	<i>X</i>	Γ	0.49	LCEBR	/	Stable
Zn ₂ Cl ₂ O	59	6.3.1646	2.45	C2DB	square	/	Γ	0.48	LCEBR	/	Stable
S ₂ Si	59	6.3.1684	1.71	C2DB	square	<i>X</i>	Γ	0.47	LCEBR	/	Stable
KHSe	64	6.3.1784	2.95	C2DB	square	/	Γ	0.47	LCEBR	/	Stable
PbSnBr ₂ O ₂	55	6.3.1601	0.46	C2DB	square	nHSP-SOC	Γ	0.46	LCEBR	/	Stable
SnTe ₂	59	6.3.1692	0.39	C2DB	square	<i>X</i>	Γ	0.44	LCEBR	/	Stable
LiHTe	64	6.3.1791	2.42	C2DB	square	Γ -SOC	Γ	0.44	LCEBR	/	Stable
CdBr ₂	59	6.3.1630	2.94	C2DB	square	/	Γ	0.43	LCEBR	/	Stable
GeO ₂	59	6.3.1659	2.94	C2DB	square	/	Γ	0.43	LCEBR	/	Stable
HgI ₂	59	6.3.1668	1.64	C2DB	square	/	Γ	0.39	LCEBR	Yes	Stable
PbO	64	6.3.1804	2.48	C2DB	square	Γ	/	0.39	LCEBR	Yes	Stable
KHTe	64	6.3.1785	2.67	C2DB	square	/	Γ	0.39	LCEBR	/	Stable
CaS	64	6.3.1749	2.63	C2DB	square	/	Γ	0.38	LCEBR	/	Stable
NaHS	64	6.3.1795	2.92	C2DB	square	/	Γ	0.34	LCEBR	/	Stable
ScCl	64	3.3.199	0.20	C2DB	square	/	Γ	0.31	OAI	/	Stable
NaHO	64	6.3.1792	2.76	C2DB	square	/	Γ	0.29	LCEBR	Yes	Stable
KH	64	6.3.1786	2.90	C2DB	square	/	Γ	0.29	LCEBR	/	Stable
KHO	64	6.3.1780	2.83	C2DB	square	/	Γ	0.27	LCEBR	/	Stable
NaHTe	64	6.3.1797	2.73	C2DB	square	/	Γ	0.26	LCEBR	/	Stable
SiTe ₂	59	6.3.1691	0.27	C2DB	square	<i>X</i>	Γ	0.22	LCEBR	/	Stable

TABLE S64: Computationally unstable materials with valley type: square- Γ .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
PbO ₂	59	6.4.394	1.08	C2DB	square	/	Γ	0.67	LCEBR	/	Unstable
F ₂ Ge	59	6.4.377	1.62	C2DB	square	<i>M</i>	Γ	0.65	LCEBR	/	Unstable
LiFS	64	6.4.441	1.63	C2DB	square	/	Γ	0.63	LCEBR	/	Unstable
NaFSe	64	6.4.445	1.47	C2DB	square	/	Γ	0.56	LCEBR	/	Unstable
NaFTe	64	6.4.446	1.11	C2DB	square	/	Γ	0.54	LCEBR	/	Unstable
NaFO	64	6.4.443	2.01	C2DB	square	/	Γ	0.53	LCEBR	/	Unstable
NaFS	64	6.4.444	1.93	C2DB	square	/	Γ	0.52	LCEBR	/	Unstable
I ₂ Si	59	6.4.392	0.33	C2DB	square	nHSP-SOC	Γ	0.46	LCEBR	/	Unstable
PbSe ₂	59	6.4.398	0.29	C2DB	square	<i>X</i>	Γ	0.44	LCEBR	/	Unstable
InF	64	6.4.438	1.94	C2DB	square	/	Γ	0.43	LCEBR	/	Unstable
LiFO	64	6.4.440	2.57	C2DB	square	/	Γ	0.39	LCEBR	/	Unstable
ZnS	64	6.4.469	2.73	C2DB	square	/	Γ	0.34	LCEBR	/	Unstable
AuBr	64	6.4.429	0.39	C2DB	square	Γ	Γ	0.32	LCEBR	/	Unstable

b. Γ -SOC

TABLE S65: Computationally exfoliable materials with valley type: square- Γ -SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
AgKTe	64	6.2.970	1.37	MC2D	square	Γ -SOC	Γ	0.48	LCEBR	Yes	Comp.Exfo
CuNaTe	64	6.2.1008	0.73	MC2D	square	Γ -SOC	Γ	0.40	LCEBR	Yes	Comp.Exfo
CuKTe	64	6.2.1006	0.32	MC2D	square	Γ -SOC	Γ	0.27	LCEBR	Yes	Comp.Exfo

TABLE S66: Computationally stable materials with valley type: square- Γ -SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
SnBr ₂	59	6.3.1635	1.28	C2DB	square	M -SOC	Γ -SOC	0.67	LCEBR	/	Stable
SnCl ₂	59	6.3.1648	1.46	C2DB	square	M	Γ -SOC	0.67	LCEBR	/	Stable
PbI ₂	59	6.3.1671	1.53	C2DB	square	nHSP-SOC	Γ -SOC	0.66	LCEBR	/	Stable
PbBr ₂	59	6.3.1634	1.88	C2DB	square	nHSP-SOC	Γ -SOC	0.60	LCEBR	/	Stable
CdI ₂	59	6.3.1641	2.38	C2DB	square	/	Γ -SOC	0.52	LCEBR	/	Stable
AgI	64	6.3.1724	1.92	C2DB	square	Γ -SOC	Γ	0.44	LCEBR	Yes	Stable
CuI	64	6.3.1761	1.90	C2DB	square	Γ -SOC	Γ	0.44	LCEBR	Yes	Stable
HgI ₂	59	6.3.1669	1.51	C2DB	square	Γ -SOC	Γ -SOC	0.44	LCEBR	Yes	Stable
AuI	64	6.3.1728	0.79	C2DB	square	Γ -SOC	Γ	0.43	LCEBR	/	Stable
LiHTe	64	6.3.1791	2.42	C2DB	square	Γ -SOC	Γ	0.40	LCEBR	/	Stable
ZnTe	64	6.3.1814	0.51	C2DB	square	Γ -SOC	Γ	0.39	LCEBR	/	Stable
ZrTe ₂	59	6.3.1695	0.81	C2DB	square	Γ -SOC	/	0.38	LCEBR	/	Stable
ZnI ₂	59	6.3.1674	2.47	C2DB	square	Γ -SOC	Γ -SOC	0.29	LCEBR	/	Stable
TiTe ₂	59	6.3.1693	0.40	C2DB	square	Γ -SOC	/	0.25	LCEBR	/	Stable

c. M

TABLE S67: Computationally exfoliable materials with valley type: square- M .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
ZnF ₂	61	6.2.956	2.71	MC2D	square	M	Γ	0.55	LCEBR	Yes	Comp.Exfo
TiO ₄ P	57	6.2.931	1.30	MC2D	square	M	Γ	0.41	LCEBR	Yes	Comp.Exfo

TABLE S68: Computationally stable materials with valley type: square- M .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
Cl ₂ Ge	59	6.3.1642	1.38	C2DB	square	M	Γ	0.67	LCEBR	/	Stable
SnCl ₂	59	6.3.1648	1.46	C2DB	square	M	Γ -SOC	0.67	LCEBR	/	Stable
SnF ₂	59	6.3.1653	1.66	C2DB	square	M	Γ	0.64	LCEBR	/	Stable
PbCl ₂	59	6.3.1647	2.16	C2DB	square	M	nHSP-SOC	0.56	LCEBR	/	Stable
Au ₂ WSe ₄	57	6.3.1615	0.78	C2DB	square	M	/	0.48	LCEBR	/	Stable
Ag ₂ MoS ₄	57	6.3.1605	0.99	C2DB	square	M	/	0.48	LCEBR	/	Stable
Ag ₂ WS ₄	57	6.3.1608	1.41	C2DB	square	M	/	0.47	LCEBR	/	Stable
Ag ₂ WSe ₄	57	6.3.1609	1.09	C2DB	square	M	/	0.47	LCEBR	/	Stable
Au ₂ MoSe ₄	57	6.3.1612	0.63	C2DB	square	M	/	0.44	LCEBR	/	Stable
Cu ₂ WSe ₄	57	6.3.1621	1.24	C2DB	square	M	/	0.42	LCEBR	/	Stable
Cu ₂ MoS ₄	57	6.3.1617	1.20	C2DB	square	M	/	0.40	LCEBR	/	Stable
Cu ₂ MoSe ₄	57	6.3.1618	0.92	C2DB	square	M	/	0.40	LCEBR	/	Stable
Ag ₂ MoSe ₄	57	6.3.1606	0.73	C2DB	square	M	/	0.39	LCEBR	/	Stable
Cu ₂ WS ₄	57	6.3.1620	1.55	C2DB	square	M	/	0.39	LCEBR	Yes	Stable
Au ₂ WTe ₄	57	6.3.1616	0.35	C2DB	square	M	/	0.36	LCEBR	/	Stable
Ag ₂ WTe ₄	57	6.3.1610	0.62	C2DB	square	M	/	0.35	LCEBR	/	Stable
Cu ₂ WTe ₄	57	6.3.1622	0.67	C2DB	square	M	/	0.35	LCEBR	/	Stable
Au ₂ MoTe ₄	57	6.3.1613	0.25	C2DB	square	M	/	0.32	LCEBR	/	Stable
Ag ₂ MoTe ₄	57	6.3.1607	0.35	C2DB	square	M	/	0.28	LCEBR	/	Stable
Cu ₂ MoTe ₄	57	6.3.1619	0.40	C2DB	square	M	/	0.26	LCEBR	/	Stable

TABLE S69: Computationally unstable materials with valley type: square- M .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
F ₂ Ge	59	6.4.377	1.62	C2DB	square	M	Γ	0.65	LCEBR	/	Unstable
F ₂ Si	59	6.4.381	0.66	C2DB	square	M	/	0.56	LCEBR	/	Unstable
PbF ₂	59	6.4.379	2.77	C2DB	square	M	nHSP-SOC	0.46	LCEBR	/	Unstable

d. M -SOC

TABLE S70: Computationally stable materials with valley type: square- M -SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
SnBr ₂	59	6.3.1635	1.28	C2DB	square	M -SOC	Γ -SOC	0.67	LCEBR	/	Stable
Au ₂ WS ₄	57	6.3.1614	1.10	C2DB	square	M -SOC	/	0.54	LCEBR	/	Stable
Au ₂ MoS ₄	57	6.3.1611	0.84	C2DB	square	M -SOC	/	0.49	LCEBR	/	Stable

TABLE S71: Computationally unstable materials with valley type: square- M -SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
HgH ₂	59	6.4.385	0.79	C2DB	square	nHSP-SOC	M -SOC	0.60	LCEBR	/	Unstable

e. X

TABLE S72: Computationally exfoliable materials with valley type: square- X .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
AgClO ₄	57	6.2.926	2.82	MC2D	square	X	Γ	0.34	LCEBR	Yes	Comp.Exfo
K ₂ MgH ₄	61	6.2.960	2.82	MC2D	square	X	/	0.30	LCEBR	Yes	Comp.Exfo

TABLE S73: Computationally stable materials with valley type: square- X .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
Se ₂ Si	59	6.3.1688	1.12	C2DB	square	X	/	0.55	LCEBR	/	Stable
S ₂ Si	59	6.3.1684	1.71	C2DB	square	X	Γ	0.49	LCEBR	/	Stable
GeS ₂	59	6.3.1660	1.36	C2DB	square	X	Γ	0.49	LCEBR	Yes	Stable
SnS ₂	59	6.3.1685	1.45	C2DB	square	X	Γ	0.45	LCEBR	Yes	Stable
SnSe ₂	59	6.1.9	0.85	C2DB	square	X	Γ	0.43	LCEBR	/	Stable
GeSe ₂	59	6.3.1661	0.56	C2DB	square	X	Γ	0.38	LCEBR	/	Stable
SiTe ₂	59	6.3.1691	0.27	C2DB	square	X	Γ	0.34	LCEBR	/	Stable
SnTe ₂	59	6.3.1692	0.39	C2DB	square	X	Γ	0.31	LCEBR	/	Stable

TABLE S74: Computationally unstable materials with valley type: square- X .

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
PbTe	61	1.4.57	0.26	C2DB	square	nHSP	X	0.56	SEBR	/	Unstable
PbSe	61	1.4.56	0.21	C2DB	square	X	X	0.53	SEBR	/	Unstable
PbH ₄	61	6.4.414	1.48	C2DB	square	X	nHSP	0.48	LCEBR	/	Unstable
SnH ₄	61	6.4.415	2.28	C2DB	square	X	nHSP	0.39	LCEBR	/	Unstable
PbSe ₂	59	6.4.398	0.29	C2DB	square	X	Γ	0.23	LCEBR	/	Unstable

f. X-SOC

TABLE S75: Computationally unstable materials with valley type: square-*X*-SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
OsCl ₂	59	6.4.370	0.32	C2DB	square	<i>X</i> -SOC	nHSP-SOC	0.34	LCEBR	/	Unstable

g. nHSP

TABLE S76: Computationally exfoliable materials with valley type: square-nHSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
CuTlSe	64	6.2.1010	0.69	MC2D	square	nHSP	/	0.41	LCEBR	Yes	Comp.Exfo

TABLE S77: Computationally stable materials with valley type: square-nHSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
PbS	64	6.3.1807	1.35	C2DB	square	nHSP	nHSP	0.49	LCEBR	Yes	Stable
PbSe	64	6.3.1808	0.95	C2DB	square	nHSP	nHSP	0.48	LCEBR	/	Stable
PbTe	64	6.3.1809	0.70	C2DB	square	nHSP	nHSP	0.41	LCEBR	Yes	Stable

TABLE S78: Computationally unstable materials with valley type: square-nHSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
PbH ₄	61	6.4.414	1.48	C2DB	square	<i>X</i>	nHSP	0.72	LCEBR	/	Unstable
CuH	64	6.4.452	1.48	C2DB	square	nHSP	nHSP	0.72	LCEBR	/	Unstable
AgH	64	6.4.450	1.73	C2DB	square	nHSP	nHSP	0.69	LCEBR	/	Unstable
AuH	64	6.4.451	0.70	C2DB	square	nHSP	nHSP	0.64	LCEBR	/	Unstable
SnH ₄	61	6.4.415	2.28	C2DB	square	<i>X</i>	nHSP	0.54	LCEBR	/	Unstable
GeS	64	6.4.449	1.12	C2DB	square	/	nHSP	0.52	LCEBR	/	Unstable
PbSe	64	6.4.465	0.26	C2DB	square	/	nHSP	0.47	LCEBR	/	Unstable
PbTe	64	6.4.466	0.21	C2DB	square	/	nHSP	0.40	LCEBR	/	Unstable
PbTe	61	1.4.57	0.26	C2DB	square	nHSP	<i>X</i>	0.40	SEBR	/	Unstable

h. nHSP-SOC

TABLE S79: Computationally stable materials with valley type: square-nHSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
Br ₂ Ge	59	6.3.1631	1.31	C2DB	square	nHSP-SOC	Γ	0.67	LCEBR	/	Stable
SnI ₂	59	6.3.1672	1.14	C2DB	square	nHSP-SOC	Γ	0.67	LCEBR	/	Stable
GeI ₂	59	6.3.1658	1.06	C2DB	square	nHSP-SOC	Γ	0.65	LCEBR	/	Stable
PbBr ₂	59	6.3.1634	1.88	C2DB	square	nHSP-SOC	Γ-SOC	0.56	LCEBR	/	Stable
PbCl ₂	59	6.3.1647	2.16	C2DB	square	<i>M</i>	nHSP-SOC	0.56	LCEBR	/	Stable
PbI ₂	59	6.3.1671	1.53	C2DB	square	nHSP-SOC	Γ-SOC	0.54	LCEBR	/	Stable
PbSnBr ₂ O ₂	55	6.3.1601	0.46	C2DB	square	nHSP-SOC	Γ	0.34	LCEBR	/	Stable

TABLE S80: Computationally unstable materials with valley type: square-nHSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
HgH ₂	59	6.4.385	0.79	C2DB	square	nHSP-SOC	<i>M</i> -SOC	0.60	LCEBR	/	Unstable
I ₂ Si	59	6.4.392	0.33	C2DB	square	nHSP-SOC	Γ	0.46	LCEBR	/	Unstable
PbF ₂	59	6.4.379	2.77	C2DB	square	<i>M</i>	nHSP-SOC	0.46	LCEBR	/	Unstable
OsCl ₂	59	6.4.370	0.32	C2DB	square	<i>X</i> -SOC	nHSP-SOC	0.23	LCEBR	/	Unstable

4. Rectangular lattice

a. HSP

TABLE S81: Experimental materials with valley type: rectangular-HSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
P	42	3.1.7	0.91	C2DB	rectangular	Γ	Γ	0.62	OAI	Yes	Exp.M.Exfo
ZrS ₃	46	6.1.6	1.18	C2DB	rectangular	/	Γ	0.41	LCEBR	Yes	Exp.W.Exfo
ZrSe ₃	46	6.1.7	0.41	C2DB	rectangular	Γ	/	0.18	LCEBR	Yes	Exp.M.Exfo
TiS ₃	46	6.1.8	0.29	C2DB	rectangular	/	Γ	0.18	LCEBR	Yes	Exp.M.Exfo

TABLE S82: Computationally exfoliable materials with valley type: rectangular-HSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
KTIO	15	6.2.416	1.53	MC2D	rectangular	/	<i>X</i>	0.56	LCEBR	Yes	Comp.Exfo
PbCN ₂	15	6.2.365	1.82	MC2D	rectangular	/	<i>X</i>	0.50	LCEBR	Yes	Comp.Exfo
Tl ₂ ZrS ₃	15	6.2.438	1.07	MC2D	rectangular	<i>X</i>	/	0.42	LCEBR	Yes	Comp.Exfo
HfTl ₂ S ₃	15	6.2.408	1.18	MC2D	rectangular	<i>X</i>	/	0.41	LCEBR	Yes	Comp.Exfo
NbTlBr ₄ O	8	6.2.227	1.24	MC2D	rectangular	<i>X</i>	<i>Y</i>	0.52	LCEBR	Yes	Comp.Exfo
S ₃ Sb ₂	15	6.2.437	1.17	MC2D	rectangular	/	<i>X</i>	0.38	LCEBR	Yes	Comp.Exfo
HfTl ₂ Se ₃	15	6.2.409	0.82	MC2D	rectangular	<i>X</i>	/	0.32	LCEBR	Yes	Comp.Exfo
Sb ₂ Se ₃	15	6.2.440	0.70	MC2D	rectangular	/	<i>X</i>	0.31	LCEBR	Yes	Comp.Exfo
CuFO ₂	9	6.2.253	0.77	MC2D	rectangular	<i>X</i>	/	0.30	LCEBR	Yes	Comp.Exfo
AgFO ₂	9	6.2.230	0.80	MC2D	rectangular	<i>X</i>	/	0.28	LCEBR	Yes	Comp.Exfo
CuHfNaSe ₃	15	6.2.377	0.44	MC2D	rectangular	Γ	<i>X</i>	0.18	LCEBR	Yes	Comp.Exfo
AuK ₃ Sn ₄	27	6.2.649	0.30	MC2D	rectangular	<i>X</i>	<i>X</i>	0.14	LCEBR	Yes	Comp.Exfo
CuNaZrSe ₃	15	6.2.380	0.32	MC2D	rectangular	Γ	<i>X</i>	0.13	LCEBR	Yes	Comp.Exfo
AgBr	15	6.2.345	1.24	MC2D	rectangular	/	Γ	0.60	LCEBR	Yes	Comp.Exfo
GaKH ₂	41	3.2.124	0.94	MC2D	rectangular	Γ	Γ	0.60	OAI	Yes	Comp.Exfo
N	46	3.2.132	0.82	MC2D	rectangular	Γ	nHSP	0.59	OAI	Yes	Comp.Exfo
AgClO ₂	48	6.2.908	1.29	MC2D	rectangular	/	Γ	0.55	LCEBR	Yes	Comp.Exfo
PtO ₄ S	38	6.2.775	1.09	MC2D	rectangular	/	Γ	0.54	LCEBR	Yes	Comp.Exfo
AgN ₃	38	6.2.765	1.09	MC2D	rectangular	Γ	Γ	0.51	LCEBR	Yes	Comp.Exfo
Hg ₃ O ₆ S	13	6.2.322	0.86	MC2D	rectangular	/	Γ	0.50	LCEBR	Yes	Comp.Exfo
Tl ₂ S	47	6.2.907	0.50	MC2D	rectangular	/	Γ	0.47	LCEBR	Yes	Comp.Exfo
Ag ₂ K ₂ GeSe ₄	22	6.2.631	1.72	MC2D	rectangular	/	Γ	0.46	LCEBR	Yes	Comp.Exfo
Cu ₂ O ₄ S	22	6.2.635	2.07	MC2D	rectangular	<i>Y</i>	Γ	0.36	LCEBR	Yes	Comp.Exfo
SnPS ₃	18	3.2.113	1.11	MC2D	rectangular	Γ	nHSP	0.45	OAI	Yes	Comp.Exfo
AuI	26	6.2.648	1.84	MC2D	rectangular	Γ	/	0.43	LCEBR	Yes	Comp.Exfo

K ₂ As ₂ Si	38	6.2.769	1.04	MC2D	rectangular	Γ	/	0.42	LCEBR	Yes	Comp.Exfo
PtO ₄ S	19	6.2.619	1.29	MC2D	rectangular	/	Γ	0.42	LCEBR	Yes	Comp.Exfo
TlF ₃	29	6.2.679	2.40	MC2D	rectangular	/	Γ	0.42	LCEBR	Yes	Comp.Exfo
Li ₅ Br ₂ N	37	6.2.756	2.38	MC2D	rectangular	/	Γ	0.42	LCEBR	Yes	Comp.Exfo
InK ₃ P ₂	38	6.2.773	0.71	MC2D	rectangular	/	Γ	0.41	LCEBR	Yes	Comp.Exfo
Cu ₂ RbI ₃	41	6.2.810	2.20	MC2D	rectangular	/	Γ	0.40	LCEBR	Yes	Comp.Exfo
AlMgF ₅	37	6.2.755	2.86	MC2D	rectangular	/	Γ	0.39	LCEBR	Yes	Comp.Exfo
PdO ₄ S	19	6.2.618	0.87	MC2D	rectangular	/	Γ	0.38	LCEBR	Yes	Comp.Exfo
HgK ₂ S ₂	24	6.2.645	2.06	MC2D	rectangular	/	Γ	0.38	LCEBR	Yes	Comp.Exfo
InK ₂ NaAs ₂	38	6.2.768	0.53	MC2D	rectangular	/	Γ	0.38	LCEBR	Yes	Comp.Exfo
GaK ₂ NaAs ₂	38	6.2.766	0.62	MC2D	rectangular	/	Γ	0.37	LCEBR	Yes	Comp.Exfo
AgBrH ₃ N	15	6.2.405	2.51	MC2D	rectangular	/	Γ	0.36	LCEBR	Yes	Comp.Exfo
CuK ₂ NbSe ₄	22	6.2.637	1.57	MC2D	rectangular	/	Γ	0.36	LCEBR	Yes	Comp.Exfo
LaI ₃	46	6.2.891	1.98	MC2D	rectangular	Γ	/	0.36	LCEBR	Yes	Comp.Exfo
KNO ₃	32	6.2.733	2.14	MC2D	rectangular	/	Γ	0.35	LCEBR	Yes	Comp.Exfo
GaClO	33	6.2.744	2.80	MC2D	rectangular	/	Γ	0.35	LCEBR	Yes	Comp.Exfo
PrI ₃	46	6.2.893	1.89	MC2D	rectangular	Γ	/	0.35	LCEBR	Yes	Comp.Exfo
NdI ₃	46	6.2.892	1.88	MC2D	rectangular	Γ	/	0.34	LCEBR	Yes	Comp.Exfo
SmI ₃	46	6.2.894	1.88	MC2D	rectangular	Γ	/	0.34	LCEBR	Yes	Comp.Exfo
GdI ₃	46	6.2.879	1.86	MC2D	rectangular	Γ	/	0.33	LCEBR	Yes	Comp.Exfo
TbI ₃	46	6.2.895	1.84	MC2D	rectangular	Γ	/	0.33	LCEBR	Yes	Comp.Exfo
Ag ₂ K ₂ GeS ₄	22	6.2.630	2.43	MC2D	rectangular	/	Γ	0.31	LCEBR	Yes	Comp.Exfo
CuK ₂ NbS ₄	22	6.2.636	1.95	MC2D	rectangular	/	Γ	0.29	LCEBR	Yes	Comp.Exfo
KH ₂ N	15	6.2.402	2.25	MC2D	rectangular	/	Γ	0.29	LCEBR	Yes	Comp.Exfo
O ₃ Sb ₂	46	6.2.900	2.50	MC2D	rectangular	Γ	/	0.28	LCEBR	Yes	Comp.Exfo
SnCl ₂	15	6.2.376	2.82	MC2D	rectangular	/	Γ	0.28	LCEBR	Yes	Comp.Exfo
TmISe	46	6.2.890	2.19	MC2D	rectangular	Γ	Γ	0.28	LCEBR	Yes	Comp.Exfo
CuBrSe ₂	20	6.2.621	0.79	MC2D	rectangular	Y	Γ	0.29	LCEBR	Yes	Comp.Exfo
ErBrSe	46	6.2.844	2.26	MC2D	rectangular	Γ	Γ	0.27	LCEBR	Yes	Comp.Exfo
HoISe	46	6.2.883	2.21	MC2D	rectangular	Γ	/	0.27	LCEBR	Yes	Comp.Exfo
HgClH ₂ N	41	6.2.813	2.32	MC2D	rectangular	Γ	Γ	0.27	LCEBR	Yes	Comp.Exfo
TbISe	46	6.2.889	2.23	MC2D	rectangular	Γ	/	0.26	LCEBR	Yes	Comp.Exfo
Ag ₃ KSe ₂	18	6.2.560	0.22	MC2D	rectangular	/	Γ	0.26	LCEBR	Yes	Comp.Exfo
GdISe	46	6.2.878	2.25	MC2D	rectangular	Γ	/	0.26	LCEBR	Yes	Comp.Exfo
HgINO ₃	28	6.2.669	2.10	MC2D	rectangular	/	Γ	0.24	LCEBR	Yes	Comp.Exfo
LuIS	46	6.2.884	2.48	MC2D	rectangular	Γ	/	0.23	LCEBR	Yes	Comp.Exfo
Pb ₂ HIO ₂	18	6.2.599	2.31	MC2D	rectangular	/	Γ	0.21	LCEBR	Yes	Comp.Exfo
NaHO	46	6.2.880	2.75	MC2D	rectangular	/	Γ	0.21	LCEBR	Yes	Comp.Exfo
CuHoPbSe ₃	41	6.2.806	0.46	MC2D	rectangular	Γ	Γ	0.21	LCEBR	Yes	Comp.Exfo
TmIS	46	6.2.888	2.60	MC2D	rectangular	Γ	/	0.20	LCEBR	Yes	Comp.Exfo
ErIS	46	6.2.876	2.64	MC2D	rectangular	Γ	/	0.19	LCEBR	Yes	Comp.Exfo
Sb ₂ Te ₃	18	6.2.615	0.53	MC2D	rectangular	/	Γ	0.19	LCEBR	Yes	Comp.Exfo
DyIS	46	6.2.875	2.70	MC2D	rectangular	Γ	/	0.18	LCEBR	Yes	Comp.Exfo
Ca ₃ In ₂ As ₄	14	6.2.324	0.32	MC2D	rectangular	Γ	Γ	0.16	LCEBR	Yes	Comp.Exfo
PdO ₃ Se	18	6.2.611	0.26	MC2D	rectangular	Γ	Γ	0.15	LCEBR	Yes	Comp.Exfo
ZrGeTe ₄	32	6.2.724	0.49	MC2D	rectangular	Γ	/	0.15	LCEBR	Yes	Comp.Exfo
DyBrS	46	6.2.842	2.89	MC2D	rectangular	Γ	/	0.15	LCEBR	Yes	Comp.Exfo
PrBr ₃	46	6.2.857	2.97	MC2D	rectangular	Γ	/	0.15	LCEBR	Yes	Comp.Exfo
NdBr ₃	46	6.2.856	2.96	MC2D	rectangular	Γ	/	0.15	LCEBR	Yes	Comp.Exfo
TiS ₃	46	6.2.902	0.28	MC2D	rectangular	Γ	Γ	0.14	LCEBR	Yes	Comp.Exfo
LuBrS	46	6.2.848	2.93	MC2D	rectangular	/	Γ	0.14	LCEBR	Yes	Comp.Exfo

Ag ₃ KTe ₂	18	6.2.561	0.30	MC2D	rectangular	Γ	Γ	0.14	LCEBR	Yes	Comp.Exfo
GdBr ₃	46	6.2.854	2.97	MC2D	rectangular	Γ	/	0.13	LCEBR	Yes	Comp.Exfo
TbBr ₃	46	6.2.858	2.97	MC2D	rectangular	Γ	/	0.13	LCEBR	Yes	Comp.Exfo
DyBr ₃	46	6.2.853	2.98	MC2D	rectangular	Γ	/	0.12	LCEBR	Yes	Comp.Exfo
HoBr ₃	46	6.2.855	2.97	MC2D	rectangular	Γ	/	0.12	LCEBR	Yes	Comp.Exfo
SnTl ₂ S ₃	41	6.2.823	1.27	MC2D	rectangular	/	Y	0.37	LCEBR	Yes	Comp.Exfo
PdPS	16	3.2.80	1.12	MC2D	rectangular	Y	/	0.32	OAI	Yes	Comp.Exfo
PdPSe	16	3.2.81	1.00	MC2D	rectangular	Y	/	0.32	OAI	Yes	Comp.Exfo
K ₂ PdAs ₂	41	6.2.790	0.43	MC2D	rectangular	Y	/	0.27	LCEBR	Yes	Comp.Exfo
K ₂ PdP ₂	41	6.2.818	0.38	MC2D	rectangular	Y	/	0.24	LCEBR	Yes	Comp.Exfo
PbClHO	18	6.2.598	1.30	MC2D	rectangular	/	S	0.48	LCEBR	Yes	Comp.Exfo
SnO	18	6.2.610	2.10	MC2D	rectangular	/	S	0.31	LCEBR	Yes	Comp.Exfo
PbCClO ₂	18	3.2.100	2.89	MC2D	rectangular	S	/	0.09	OAI	Yes	Comp.Exfo
In ₂ Se ₃	10	6.2.309	0.96	MC2D	rectangular	/	Y	0.56	LCEBR	Yes	Comp.Exfo
GaTe	18	3.2.106	1.29	MC2D	rectangular	Y	/	0.36	OAI	Yes	Comp.Exfo
AsGe	18	3.2.94	1.36	MC2D	rectangular	Y	/	0.32	OAI	Yes	Comp.Exfo
C ₂ F	48	3.2.135	2.27	MC2D	rectangular	Y	Y	0.25	OAI	Yes	Comp.Exfo
Cu ₃ TlS ₂	18	6.2.592	0.53	MC2D	rectangular	Y	Y	0.21	LCEBR	Yes	Comp.Exfo
CdPb ₂ Cl ₂ O ₂	18	6.2.576	2.97	MC2D	rectangular	Y	/	0.15	LCEBR	Yes	Comp.Exfo
Cu ₃ TlSe ₂	18	6.2.593	0.31	MC2D	rectangular	Y	Y	0.10	LCEBR	Yes	Comp.Exfo

TABLE S83: Computationally stable materials with valley type: rectangular-HSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
Ga ₂ ClI	11	6.3.472	1.87	C2DB	rectangular	X	X	0.52	LCEBR	/	Stable
Bi ₂ OSe ₂	15	6.3.637	1.22	C2DB	rectangular	/	X	0.50	LCEBR	/	Stable
Bi ₂ OS ₂	15	6.3.636	1.57	C2DB	rectangular	/	X	0.47	LCEBR	/	Stable
InI ₂	14	6.3.605	0.81	C2DB	rectangular	X	/	0.46	LCEBR	/	Stable
AuSe	14	6.3.580	0.98	C2DB	rectangular	X	nHSP	0.44	LCEBR	Yes	Stable
Bi ₂ OTe ₂	15	6.3.638	0.76	C2DB	rectangular	/	X	0.44	LCEBR	/	Stable
AuTe	14	6.3.581	0.67	C2DB	rectangular	X	nHSP	0.42	LCEBR	/	Stable
CdFO ₂ Sb	15	6.3.665	2.45	C2DB	rectangular	/	X	0.41	LCEBR	/	Stable
OSb ₂ Te ₂	15	6.3.777	0.81	C2DB	rectangular	/	X	0.41	LCEBR	/	Stable
IrClTe	15	6.3.677	1.08	C2DB	rectangular	/	X	0.39	LCEBR	/	Stable
IrBrTe	15	6.3.644	0.96	C2DB	rectangular	/	X	0.39	LCEBR	/	Stable
IrClSe	15	6.3.676	1.16	C2DB	rectangular	/	X	0.39	LCEBR	/	Stable
RhClTe	15	6.3.684	1.03	C2DB	rectangular	/	X	0.38	LCEBR	Yes	Stable
IrBrSe	15	6.3.643	1.06	C2DB	rectangular	/	X	0.38	LCEBR	/	Stable
IrFSe	15	6.3.702	1.03	C2DB	rectangular	/	X	0.38	LCEBR	/	Stable
BiAsS ₄	15	6.3.612	1.50	C2DB	rectangular	/	X	0.38	LCEBR	/	Stable
RhFSe	15	6.3.705	0.94	C2DB	rectangular	/	X	0.38	LCEBR	/	Stable
OSb ₂ Se ₂	15	6.3.776	1.45	C2DB	rectangular	/	X	0.38	LCEBR	/	Stable
IrClS	15	6.3.675	1.12	C2DB	rectangular	/	X	0.37	LCEBR	/	Stable
BiHgFO ₂	15	6.3.627	2.16	C2DB	rectangular	/	X	0.37	LCEBR	/	Stable
RhClSe	15	6.3.683	1.08	C2DB	rectangular	/	X	0.37	LCEBR	/	Stable
RhBrTe	15	6.3.648	0.95	C2DB	rectangular	/	X	0.37	LCEBR	/	Stable
RhBrSe	15	6.3.647	1.01	C2DB	rectangular	/	X	0.36	LCEBR	/	Stable
IrBrS	15	6.3.642	1.04	C2DB	rectangular	/	X	0.36	LCEBR	/	Stable
RhClS	15	6.3.682	1.05	C2DB	rectangular	/	X	0.36	LCEBR	/	Stable
IrFS	15	6.3.701	0.95	C2DB	rectangular	/	X	0.36	LCEBR	/	Stable

RhBrS	15	6.3.646	0.99	C2DB	rectangular	/	X	0.35	LCEBR	/	Stable
BiBr	15	1.3.6	0.64	C2DB	rectangular	nHSP	X	0.35	NLC	/	Stable
RhFS	15	6.3.704	0.88	C2DB	rectangular	/	X	0.35	LCEBR	/	Stable
AgTe	14	6.3.575	0.49	C2DB	rectangular	X	nHSP	0.33	LCEBR	/	Stable
BrSb	15	1.3.7	0.28	C2DB	rectangular	X	X	0.33	NLC	/	Stable
PS ₄ Sb	15	6.3.790	0.85	C2DB	rectangular	/	X	0.31	LCEBR	/	Stable
AgSe	14	6.3.574	0.74	C2DB	rectangular	X	nHSP	0.31	LCEBR	/	Stable
InCl ₂	14	6.3.586	2.47	C2DB	rectangular	/	X	0.29	LCEBR	/	Stable
TlI ₂	14	6.3.606	0.52	C2DB	rectangular	X	/	0.26	LCEBR	/	Stable
WF ₂ O ₂	29	6.3.1225	2.38	C2DB	rectangular	X	nHSP-SOC	0.26	LCEBR	/	Stable
TiBrISe	11	6.3.465	0.57	C2DB	rectangular	X	nHSP	0.25	LCEBR	/	Stable
CuSe	14	6.3.592	0.44	C2DB	rectangular	X	nHSP	0.20	LCEBR	/	Stable
MoF ₂ O ₂	29	6.3.1224	2.83	C2DB	rectangular	X	nHSP-SOC	0.15	LCEBR	/	Stable
NaNO ₃	15	6.3.760	2.93	C2DB	rectangular	/	X	0.14	LCEBR	/	Stable
AlClSe	46	6.3.1405	1.41	C2DB	rectangular	Γ	/	0.62	LCEBR	/	Stable
SnClN	46	6.3.1487	1.40	C2DB	rectangular	/	Γ	0.62	LCEBR	/	Stable
TlClO	46	6.3.1497	1.01	C2DB	rectangular	/	Γ	0.62	LCEBR	/	Stable
YBrS	23	6.3.1097	1.30	C2DB	rectangular	nHSP-SOC	Γ	0.62	LCEBR	/	Stable
AlBrSe	46	6.3.1401	1.52	C2DB	rectangular	Γ	/	0.62	LCEBR	/	Stable
TlBrO	46	6.3.1457	0.98	C2DB	rectangular	/	Γ	0.62	LCEBR	/	Stable
InIO	46	6.3.1545	1.23	C2DB	rectangular	/	Γ	0.62	LCEBR	/	Stable
HfIN	46	6.3.1541	1.63	C2DB	rectangular	/	Γ	0.60	LCEBR	/	Stable
CdH ₂ Se ₂	18	6.3.972	1.39	C2DB	rectangular	S	Γ	0.39	LCEBR	/	Stable
AuInF ₄	14	6.3.583	1.09	C2DB	rectangular	Y	Γ	0.58	LCEBR	/	Stable
MoWO ₄	27	6.3.1141	1.08	C2DB	rectangular	Γ	nHSP	0.58	LCEBR	/	Stable
HgTe ₂	18	3.3.122	0.97	C2DB	rectangular	Γ	nHSP	0.58	OAI	/	Stable
CdCuIS	28	6.3.1197	1.20	C2DB	rectangular	/	Γ	0.57	LCEBR	/	Stable
AgCdClS	28	6.3.1156	1.33	C2DB	rectangular	/	Γ	0.57	LCEBR	/	Stable
AgCdISe	28	6.3.1160	1.28	C2DB	rectangular	/	Γ	0.57	LCEBR	/	Stable
CdCuISe	28	6.3.1198	1.04	C2DB	rectangular	/	Γ	0.57	LCEBR	/	Stable
AgCdBrS	28	6.3.1150	1.37	C2DB	rectangular	/	Γ	0.57	LCEBR	/	Stable
AgCdBrSe	28	6.3.1151	1.10	C2DB	rectangular	/	Γ	0.57	LCEBR	/	Stable
AuHgClS	28	6.3.1182	1.00	C2DB	rectangular	/	Γ	0.57	LCEBR	/	Stable
AgCdClSe	28	6.3.1157	1.06	C2DB	rectangular	/	Γ	0.57	LCEBR	/	Stable
AgCdIS	28	6.3.1159	1.54	C2DB	rectangular	/	Γ	0.57	LCEBR	/	Stable
In ₂ O ₃	32	6.3.1313	1.50	C2DB	rectangular	/	Γ	0.57	LCEBR	/	Stable
GaTlO ₃	32	6.3.1280	1.03	C2DB	rectangular	/	Γ	0.57	LCEBR	/	Stable
ScFS	46	6.3.1529	1.61	C2DB	rectangular	Γ	/	0.56	LCEBR	/	Stable
Ag ₂ O ₄ Se	22	6.3.1054	1.59	C2DB	rectangular	Y	Γ	0.47	LCEBR	/	Stable
CdCuBrS	28	6.3.1187	0.96	C2DB	rectangular	/	Γ	0.56	LCEBR	/	Stable
AgHgBrS	28	6.3.1153	1.31	C2DB	rectangular	/	Γ	0.56	LCEBR	/	Stable
AgHgIS	28	6.3.1167	1.10	C2DB	rectangular	/	Γ	0.56	LCEBR	/	Stable
SnBrN	46	6.3.1447	1.42	C2DB	rectangular	/	Γ	0.55	LCEBR	/	Stable
GaClS	46	6.3.1474	1.40	C2DB	rectangular	Γ	/	0.55	LCEBR	/	Stable
AlFS	46	6.3.1408	1.87	C2DB	rectangular	Γ	/	0.55	LCEBR	/	Stable
AlSe	18	3.3.101	1.64	C2DB	rectangular	nHSP	Γ	0.55	OAI	/	Stable
ZrFN	46	6.3.1534	1.93	C2DB	rectangular	Γ	Γ	0.55	LCEBR	/	Stable
CdCuBrSe	28	6.3.1188	0.89	C2DB	rectangular	/	Γ	0.54	LCEBR	/	Stable
CdCuClS	28	6.3.1193	0.89	C2DB	rectangular	/	Γ	0.54	LCEBR	/	Stable
AgHgClS	28	6.3.1162	1.38	C2DB	rectangular	/	Γ	0.54	LCEBR	/	Stable
ScFSe	46	6.3.1533	0.85	C2DB	rectangular	Γ	/	0.54	LCEBR	/	Stable

TiFN	46	6.3.1522	0.70	C2DB	rectangular	Γ	Γ	0.53	LCEBR	/	Stable
Au ₂ O ₄ S	22	6.3.1055	1.49	C2DB	rectangular	Y	Γ	0.53	LCEBR	/	Stable
In ₂ Se ₃	32	6.3.1315	1.13	C2DB	rectangular	/	Γ	0.53	LCEBR	/	Stable
AuCdClS	28	6.3.1180	1.51	C2DB	rectangular	/	Γ	0.52	LCEBR	/	Stable
Au ₂ O ₄ Se	22	6.3.1056	0.83	C2DB	rectangular	/	Γ	0.52	LCEBR	/	Stable
AgHgISe	28	6.3.1168	1.01	C2DB	rectangular	/	Γ	0.52	LCEBR	/	Stable
AuCdBrS	28	6.3.1178	1.48	C2DB	rectangular	/	Γ	0.52	LCEBR	/	Stable
AgBr ₂ H	13	6.3.553	1.94	C2DB	rectangular	/	Γ	0.51	LCEBR	/	Stable
CdCuClSe	28	6.3.1194	0.84	C2DB	rectangular	/	Γ	0.51	LCEBR	/	Stable
BiHgIO ₂	15	6.3.628	1.70	C2DB	rectangular	/	Γ	0.51	LCEBR	/	Stable
In ₂ I ₂ STe	11	6.3.494	0.84	C2DB	rectangular	Γ	Γ	0.51	LCEBR	/	Stable
SSi	32	6.3.1327	1.43	C2DB	rectangular	Γ	/	0.50	LCEBR	/	Stable
Hf ₂ Br ₃ IO ₂	26	6.3.1125	1.93	C2DB	rectangular	/	Γ	0.50	LCEBR	/	Stable
InFO	46	6.3.1516	2.25	C2DB	rectangular	/	Γ	0.50	LCEBR	/	Stable
AlIS	46	6.3.1410	1.66	C2DB	rectangular	/	Γ	0.50	LCEBR	/	Stable
AlS	18	3.3.100	1.93	C2DB	rectangular	nHSP	Γ	0.50	OAI	/	Stable
In ₂ S ₃	32	6.3.1314	1.75	C2DB	rectangular	/	Γ	0.49	LCEBR	/	Stable
InBrO	46	6.3.1439	2.29	C2DB	rectangular	/	Γ	0.49	LCEBR	Yes	Stable
PbS ₂	18	3.3.137	1.22	C2DB	rectangular	Γ	Y	0.62	OAI	/	Stable
TlFO	46	6.3.1527	0.56	C2DB	rectangular	/	Γ	0.49	LCEBR	/	Stable
AlClS	46	6.3.1404	2.34	C2DB	rectangular	Γ	Γ	0.48	LCEBR	/	Stable
AgClGeTe	23	6.3.1062	1.19	C2DB	rectangular	nHSP-SOC	Γ	0.48	LCEBR	/	Stable
HfFN	46	6.3.1515	2.35	C2DB	rectangular	Γ	/	0.48	LCEBR	/	Stable
TlF ₃	37	6.3.1363	2.49	C2DB	rectangular	S	Γ	0.25	LCEBR	/	Stable
ScClSe	46	6.3.1504	1.40	C2DB	rectangular	Γ	/	0.48	LCEBR	/	Stable
Al ₂ Se ₅	18	6.3.935	1.46	C2DB	rectangular	Y	Γ	0.38	LCEBR	/	Stable
AgHgBrSe	28	6.3.1154	1.27	C2DB	rectangular	/	Γ	0.47	LCEBR	/	Stable
InClSe	46	6.3.1480	1.07	C2DB	rectangular	Γ	/	0.47	LCEBR	/	Stable
HfClN	46	6.3.1477	2.14	C2DB	rectangular	Γ	Γ	0.47	LCEBR	/	Stable
Cu ₂ O ₄ S	22	6.3.1057	2.03	C2DB	rectangular	/	Γ	0.47	LCEBR	Yes	Stable
Ag ₂ O ₄ S	22	6.3.1053	2.16	C2DB	rectangular	Y	Γ	0.38	LCEBR	/	Stable
GaBrS	46	6.3.1435	1.47	C2DB	rectangular	Γ	/	0.47	LCEBR	/	Stable
GaIO	46	6.3.1536	1.04	C2DB	rectangular	/	Γ	0.46	LCEBR	/	Stable
TiClN	46	6.3.1488	0.60	C2DB	rectangular	Γ	Γ	0.46	LCEBR	Yes	Stable
PbSe ₂	18	3.3.138	0.85	C2DB	rectangular	Γ	Y	0.58	OAI	/	Stable
CuHgBrS	28	6.3.1190	0.75	C2DB	rectangular	/	Γ	0.46	LCEBR	/	Stable
GaInO ₃	32	6.3.1278	2.15	C2DB	rectangular	/	Γ	0.46	LCEBR	/	Stable
ZrClN	46	6.3.1490	1.85	C2DB	rectangular	Γ	Γ	0.46	LCEBR	/	Stable
InFS	46	6.3.1517	1.01	C2DB	rectangular	Γ	Γ	0.46	LCEBR	/	Stable
InBrSe	46	6.3.1441	1.22	C2DB	rectangular	Γ	/	0.45	LCEBR	/	Stable
AgCdITe	28	6.3.1161	1.23	C2DB	rectangular	/	Γ	0.45	LCEBR	/	Stable
ZrBrClO	11	6.3.460	2.31	C2DB	rectangular	/	Γ	0.45	LCEBR	/	Stable
AgHgClSe	28	6.3.1163	1.34	C2DB	rectangular	/	Γ	0.45	LCEBR	/	Stable
AlISe	46	6.3.1411	1.49	C2DB	rectangular	Γ	Γ	0.45	LCEBR	/	Stable
AgHgFS	28	6.3.1165	1.26	C2DB	rectangular	/	Γ	0.44	LCEBR	/	Stable
InClO	46	6.3.1478	2.59	C2DB	rectangular	/	Γ	0.44	LCEBR	Yes	Stable
Sc ₂ Se ₃	47	6.3.1585	1.03	C2DB	rectangular	Γ	/	0.44	LCEBR	/	Stable
CuHgClS	28	6.3.1200	0.77	C2DB	rectangular	/	Γ	0.44	LCEBR	/	Stable
GaBrO	46	6.3.1434	2.52	C2DB	rectangular	/	Γ	0.43	LCEBR	/	Stable
HgH ₂ S ₂	10	6.3.389	2.32	C2DB	rectangular	/	Γ	0.43	LCEBR	/	Stable
ScBrSe	46	6.3.1464	1.50	C2DB	rectangular	Γ	/	0.43	LCEBR	/	Stable

CdCuITe	28	6.3.1199	1.18	C2DB	rectangular	/	Γ	0.43	LCEBR	/	Stable
InClS	46	6.3.1479	1.80	C2DB	rectangular	Γ	Γ	0.43	LCEBR	/	Stable
CuMgBrS	23	6.3.1088	2.53	C2DB	rectangular	/	Γ	0.42	LCEBR	/	Stable
ScBrTe	46	6.3.1465	0.57	C2DB	rectangular	Γ	/	0.42	LCEBR	/	Stable
ScISe	46	6.3.1566	1.41	C2DB	rectangular	Γ	/	0.42	LCEBR	/	Stable
ScClTe	46	6.3.1505	0.41	C2DB	rectangular	Γ	/	0.42	LCEBR	/	Stable
GaBrSe	46	6.3.1436	0.72	C2DB	rectangular	Γ	/	0.42	LCEBR	/	Stable
BrGeN	46	6.3.1437	1.51	C2DB	rectangular	/	Γ	0.42	LCEBR	/	Stable
SnIN	46	6.3.1553	1.11	C2DB	rectangular	/	Γ	0.42	LCEBR	/	Stable
GaClSe	46	6.3.1475	0.60	C2DB	rectangular	Γ	/	0.42	LCEBR	/	Stable
HfS ₃	46	6.3.1543	1.16	C2DB	rectangular	/	Γ	0.42	LCEBR	Yes	Stable
CdIO ₂ Sb	15	6.3.666	1.58	C2DB	rectangular	/	Γ	0.42	LCEBR	/	Stable
TiIO	46	6.3.1558	0.34	C2DB	rectangular	/	Γ	0.41	LCEBR	/	Stable
NaH ₂ N	48	6.3.1587	2.43	C2DB	rectangular	/	Γ	0.41	LCEBR	/	Stable
AlBrS	46	6.3.1400	2.27	C2DB	rectangular	Γ	Γ	0.41	LCEBR	/	Stable
InSe	18	3.3.130	1.63	C2DB	rectangular	Y	Γ	0.52	OAI	Yes	Stable
HfBrN	46	6.3.1438	2.10	C2DB	rectangular	Γ	Γ	0.41	LCEBR	Yes	Stable
PSb	32	6.3.1325	0.80	C2DB	rectangular	Γ	Γ	0.41	LCEBR	/	Stable
Hg ₂ GeO ₄	22	6.3.1058	2.52	C2DB	rectangular	/	Γ	0.41	LCEBR	Yes	Stable
ZrBrN	46	6.3.1450	1.82	C2DB	rectangular	Γ	Γ	0.40	LCEBR	Yes	Stable
PtSnS ₄	14	6.3.610	1.39	C2DB	rectangular	Γ	nHSP	0.40	LCEBR	/	Stable
ScIO	46	6.3.1557	1.86	C2DB	rectangular	/	Γ	0.40	LCEBR	/	Stable
CdCuFS	28	6.3.1196	0.70	C2DB	rectangular	/	Γ	0.40	LCEBR	/	Stable
ScIS	46	6.3.1562	1.70	C2DB	rectangular	Γ	/	0.39	LCEBR	/	Stable
AlTe	18	3.3.102	1.48	C2DB	rectangular	nHSP	Γ	0.39	OAI	/	Stable
BiFO	46	6.3.1424	2.12	C2DB	rectangular	/	Γ	0.39	LCEBR	/	Stable
ClGeN	46	6.3.1476	1.87	C2DB	rectangular	Γ	/	0.39	LCEBR	/	Stable
InClSe	32	6.3.1272	2.12	C2DB	rectangular	/	Γ	0.39	LCEBR	/	Stable
Sc ₂ S ₃	47	6.3.1584	1.50	C2DB	rectangular	Γ	/	0.39	LCEBR	Yes	Stable
Ga ₂ O ₃	32	6.3.1281	2.59	C2DB	rectangular	/	Γ	0.38	LCEBR	/	Stable
AgCdBrTe	28	6.3.1152	1.27	C2DB	rectangular	/	Γ	0.38	LCEBR	/	Stable
Sc ₂ Cl ₂ SSe	23	6.3.1100	1.60	C2DB	rectangular	Γ	/	0.38	LCEBR	/	Stable
As	42	3.3.152	0.80	C2DB	rectangular	nHSP	Γ	0.38	OAI	Yes	Stable
CuHgIS	28	6.3.1205	0.77	C2DB	rectangular	/	Γ	0.38	LCEBR	/	Stable
ZrIN	46	6.3.1554	1.16	C2DB	rectangular	Γ	Γ	0.38	LCEBR	Yes	Stable
CaAs	17	3.3.85	1.00	C2DB	rectangular	Γ	/	0.38	OAI	Yes	Stable
ScITe	46	6.3.1567	0.66	C2DB	rectangular	Γ	/	0.38	LCEBR	/	Stable
CuHgBrSe	28	6.3.1191	0.79	C2DB	rectangular	/	Γ	0.38	LCEBR	/	Stable
BiHgBrO ₂	15	6.3.622	2.35	C2DB	rectangular	/	Γ	0.37	LCEBR	/	Stable
Hf ₄ Br ₃ ClN ₄	26	6.3.1123	2.11	C2DB	rectangular	Γ	Γ	0.37	LCEBR	/	Stable
Ga ₂ S ₃	32	6.3.1282	1.78	C2DB	rectangular	/	Γ	0.37	LCEBR	/	Stable
TaBrO ₂	41	6.3.1369	1.66	C2DB	rectangular	/	Γ	0.37	LCEBR	/	Stable
AgHgITe	28	6.3.1169	1.12	C2DB	rectangular	/	Γ	0.37	LCEBR	/	Stable
Ga ₂ Se ₅	18	6.3.970	1.43	C2DB	rectangular	Y	Γ	0.38	LCEBR	/	Stable
SnBr ₂ S ₂	14	3.3.58	0.81	C2DB	rectangular	Γ	Y	0.53	OAI	/	Stable
CaHIO	11	6.3.488	2.78	C2DB	rectangular	Γ	Γ	0.37	LCEBR	/	Stable
AlITe	46	6.3.1412	0.36	C2DB	rectangular	Γ	/	0.37	LCEBR	/	Stable
AgHgFSe	28	6.3.1166	1.11	C2DB	rectangular	/	Γ	0.37	LCEBR	/	Stable
CdCuBrTe	28	6.3.1189	1.12	C2DB	rectangular	/	Γ	0.37	LCEBR	/	Stable
GaIS	46	6.3.1537	0.88	C2DB	rectangular	/	Γ	0.36	LCEBR	/	Stable
InBrS	46	6.3.1440	1.90	C2DB	rectangular	Γ	/	0.36	LCEBR	/	Stable

InS	18	3.3.129	1.98	C2DB	rectangular	Y	Γ	0.50	OAI	/	Stable
AllnO ₃	32	6.3.1236	2.82	C2DB	rectangular	/	Γ	0.35	LCEBR	/	Stable
AgCdClTe	28	6.3.1158	1.31	C2DB	rectangular	/	Γ	0.35	LCEBR	/	Stable
AsSb	32	6.3.1242	0.75	C2DB	rectangular	Γ	Γ	0.35	LCEBR	/	Stable
CuHgISe	28	6.3.1206	0.75	C2DB	rectangular	/	Γ	0.34	LCEBR	/	Stable
Hf ₂ Br ₄ OSe	47	6.3.1581	0.38	C2DB	rectangular	Y	Γ	0.29	LCEBR	/	Stable
ZnS ₂	17	3.3.99	1.72	C2DB	rectangular	Γ	/	0.34	OAI	/	Stable
GaInS ₃	32	6.3.1279	1.98	C2DB	rectangular	/	Γ	0.34	LCEBR	Yes	Stable
CuHgClSe	28	6.3.1201	0.81	C2DB	rectangular	/	Γ	0.34	LCEBR	Yes	Stable
LiH ₂ N	48	6.3.1586	2.79	C2DB	rectangular	Γ	Γ	0.34	LCEBR	Yes	Stable
AgAuBr ₂	18	6.3.934	2.39	C2DB	rectangular	Γ	Γ	0.34	LCEBR	/	Stable
CuHgITe	28	6.3.1207	0.91	C2DB	rectangular	/	Γ	0.34	LCEBR	/	Stable
CdCuClTe	28	6.3.1195	1.13	C2DB	rectangular	/	Γ	0.33	LCEBR	/	Stable
In ₂ S ₅	10	6.3.392	1.68	C2DB	rectangular	/	Γ	0.33	LCEBR	/	Stable
In ₂ Se ₅	10	6.3.393	1.48	C2DB	rectangular	Y	Γ	0.37	LCEBR	/	Stable
AuCuBr ₂	18	6.3.937	2.08	C2DB	rectangular	Γ	/	0.32	LCEBR	/	Stable
GaS	18	3.3.119	2.01	C2DB	rectangular	nHSP	Γ	0.31	OAI	/	Stable
Tl ₂ Se ₅	10	6.3.401	0.85	C2DB	rectangular	/	Γ	0.31	LCEBR	/	Stable
IrClS	46	6.3.1482	0.34	C2DB	rectangular	Γ	/	0.31	LCEBR	/	Stable
TaIO ₂	41	6.3.1376	0.69	C2DB	rectangular	/	Γ	0.31	LCEBR	/	Stable
PbTe ₂	18	3.3.139	0.21	C2DB	rectangular	Γ	Y	0.38	OAI	/	Stable
CdBrO ₂ Sb	15	6.3.639	2.38	C2DB	rectangular	/	Γ	0.31	LCEBR	/	Stable
AllnSe ₃	32	6.3.1238	1.68	C2DB	rectangular	/	Γ	0.30	LCEBR	/	Stable
Hg ₂ I ₂ S	35	6.3.1353	2.27	C2DB	rectangular	/	Γ	0.30	LCEBR	/	Stable
PdAsS	16	3.3.73	0.88	C2DB	rectangular	/	Γ	0.30	OAI	/	Stable
As ₂ Se ₃	32	6.3.1248	1.73	C2DB	rectangular	/	Γ	0.29	LCEBR	Yes	Stable
PdPTe	16	3.3.81	0.73	C2DB	rectangular	/	Γ	0.29	OAI	/	Stable
PdAsSe	16	3.3.74	0.73	C2DB	rectangular	/	Γ	0.29	OAI	/	Stable
IrFS	46	6.3.1519	0.42	C2DB	rectangular	Γ	/	0.29	LCEBR	/	Stable
CuISe ₂	20	6.3.1020	0.82	C2DB	rectangular	/	Γ	0.29	LCEBR	/	Stable
InISe	17	6.3.913	1.82	C2DB	rectangular	/	Γ	0.28	LCEBR	/	Stable
IrBrS	46	6.3.1443	0.33	C2DB	rectangular	Γ	/	0.28	LCEBR	/	Stable
OsSe ₂	15	3.3.67	0.61	C2DB	rectangular	nHSP	Γ	0.28	OAI	/	Stable
ScClS	46	6.3.1500	2.10	C2DB	rectangular	Γ	/	0.28	LCEBR	/	Stable
InF ₂	14	6.3.596	2.00	C2DB	rectangular	/	Γ	0.27	LCEBR	/	Stable
IrClO	46	6.3.1481	0.42	C2DB	rectangular	Γ	/	0.27	LCEBR	/	Stable
CuHgFS	28	6.3.1203	0.48	C2DB	rectangular	/	Γ	0.27	LCEBR	/	Stable
InIS	17	6.3.912	1.94	C2DB	rectangular	/	Γ	0.27	LCEBR	/	Stable
TiBrN	46	6.3.1448	0.60	C2DB	rectangular	Γ	Γ	0.26	LCEBR	Yes	Stable
AuHgISe	28	6.3.1184	0.28	C2DB	rectangular	/	Γ	0.26	LCEBR	/	Stable
AgGeIS	13	6.3.521	0.61	C2DB	rectangular	Γ	Γ -SOC	0.26	LCEBR	/	Stable
P ₂ Se ₃	32	6.3.1326	1.99	C2DB	rectangular	/	Γ	0.25	LCEBR	/	Stable
TaClO ₂	41	6.3.1373	2.38	C2DB	rectangular	/	Γ	0.24	LCEBR	/	Stable
OsS ₂	15	3.3.66	0.55	C2DB	rectangular	nHSP	Γ	0.24	OAI	/	Stable
PdSSb	16	3.3.84	0.64	C2DB	rectangular	/	Γ	0.24	OAI	/	Stable
CdClO ₂ Sb	15	6.3.663	2.88	C2DB	rectangular	/	Γ	0.24	LCEBR	/	Stable
AgS ₂ Sb	28	6.3.1170	0.68	C2DB	rectangular	Γ	/	0.24	LCEBR	/	Stable
InBrSe	17	6.3.876	2.26	C2DB	rectangular	/	Γ	0.23	LCEBR	/	Stable
P ₂ Se ₂ Te	10	6.3.400	0.36	C2DB	rectangular	nHSP-SOC	Γ	0.23	LCEBR	/	Stable
OsO ₂	15	3.3.64	0.21	C2DB	rectangular	/	Γ	0.23	OAI	/	Stable
O ₂ Te	17	6.3.930	2.68	C2DB	rectangular	/	Γ	0.22	LCEBR	Yes	Stable

GaClSe	32	6.3.1271	2.58	C2DB	rectangular	/	Γ	0.22	LCEBR	/	Stable
InFSe	46	6.3.1518	0.27	C2DB	rectangular	Γ	Γ	0.21	LCEBR	/	Stable
InITe	46	6.3.1548	0.38	C2DB	rectangular	Γ	/	0.21	LCEBR	/	Stable
InClSe	17	6.3.892	2.49	C2DB	rectangular	/	Γ	0.21	LCEBR	/	Stable
GaClTe	17	6.3.890	2.17	C2DB	rectangular	Γ	Γ	0.21	LCEBR	/	Stable
NiPSe	16	3.3.78	0.58	C2DB	rectangular	/	Γ	0.21	OAI	/	Stable
IrBrO	46	6.3.1442	0.26	C2DB	rectangular	Γ	nHSP	0.21	LCEBR	/	Stable
As ₂ S ₃	32	6.3.1247	2.27	C2DB	rectangular	/	Γ	0.21	LCEBR	Yes	Stable
AgAsS ₂	28	6.3.1146	0.59	C2DB	rectangular	Γ	/	0.20	LCEBR	/	Stable
HfSiTe ₄	32	6.3.1307	0.64	C2DB	rectangular	Γ	/	0.20	LCEBR	/	Stable
MgI ₂	41	6.3.1377	2.67	C2DB	rectangular	Γ	/	0.20	LCEBR	/	Stable
NiAsS	16	3.3.72	0.46	C2DB	rectangular	/	Γ	0.19	OAI	/	Stable
IrS	46	6.3.1550	0.21	C2DB	rectangular	Γ	/	0.19	LCEBR	/	Stable
HfGeTe ₄	32	6.3.1285	0.59	C2DB	rectangular	Γ	/	0.19	LCEBR	Yes	Stable
BiClTe	46	6.3.1423	0.32	C2DB	rectangular	Γ	/	0.18	LCEBR	/	Stable
HfSnTe ₄	32	6.3.1308	0.53	C2DB	rectangular	Γ	/	0.17	LCEBR	/	Stable
CuHgFSe	28	6.3.1204	0.51	C2DB	rectangular	/	Γ	0.17	LCEBR	/	Stable
AgBiS ₂	28	6.3.1149	0.42	C2DB	rectangular	Γ	/	0.17	LCEBR	/	Stable
SnZrTe ₄	32	6.3.1337	0.52	C2DB	rectangular	Γ	/	0.16	LCEBR	/	Stable
AuHgITe	28	6.3.1185	0.45	C2DB	rectangular	/	Γ	0.16	LCEBR	/	Stable
CuS ₂ Sb	28	6.3.1208	0.38	C2DB	rectangular	/	Γ	0.16	LCEBR	Yes	Stable
HfSe ₃	46	6.3.1544	0.28	C2DB	rectangular	Γ	/	0.15	LCEBR	Yes	Stable
NbO ₂	18	6.3.987	0.46	C2DB	rectangular	/	Γ	0.15	LCEBR	/	Stable
InClS	17	6.3.891	2.59	C2DB	rectangular	/	Γ	0.14	LCEBR	/	Stable
AgSbSe ₂	28	6.3.1171	0.32	C2DB	rectangular	Γ	/	0.13	LCEBR	/	Stable
AgBrS ₂	20	6.3.997	1.19	C2DB	rectangular	Y	/	0.40	LCEBR	/	Stable
AgGaI ₂	11	6.3.425	1.77	C2DB	rectangular	Y	Y	0.38	LCEBR	/	Stable
AgClS ₂	20	6.3.998	1.20	C2DB	rectangular	Y	/	0.37	LCEBR	/	Stable
TaBr ₂ O	37	3.3.145	0.84	C2DB	rectangular	/	Y	0.36	OAI	/	Stable
TaI ₂ O	37	3.3.147	0.87	C2DB	rectangular	/	Y	0.36	OAI	Yes	Stable
TaCl ₂ O	37	3.3.146	0.80	C2DB	rectangular	/	Y	0.35	OAI	/	Stable
CuFO ₂	20	6.3.1018	0.37	C2DB	rectangular	/	Y	0.23	LCEBR	/	Stable
VFO ₂	11	6.3.477	2.68	C2DB	rectangular	nHSP	Y	0.16	LCEBR	/	Stable
RhF ₃	23	6.3.1108	0.30	C2DB	rectangular	Y	nHSP	0.15	LCEBR	/	Stable
Hf ₂ Br ₂ S ₃	10	6.3.378	1.39	C2DB	rectangular	nHSP	S	0.46	LCEBR	/	Stable
Zr ₂ Br ₂ S ₃	10	6.3.380	1.21	C2DB	rectangular	/	S	0.45	LCEBR	/	Stable
AuS	14	6.3.579	1.24	C2DB	rectangular	S	nHSP	0.45	LCEBR	/	Stable
Tl ₂ BrI	13	6.3.540	2.14	C2DB	rectangular	S	S	0.37	LCEBR	/	Stable
AgS	14	6.3.573	0.95	C2DB	rectangular	S	nHSP	0.36	LCEBR	/	Stable
AuPdClSe	11	6.3.441	0.76	C2DB	rectangular	S	nHSP	0.33	LCEBR	/	Stable
AsTe	18	3.3.103	0.96	C2DB	rectangular	/	Y	0.50	OAI	/	Stable
InTe	18	3.3.131	1.09	C2DB	rectangular	Y	nHSP	0.47	OAI	/	Stable
SbTe	18	3.3.143	0.55	C2DB	rectangular	/	Y	0.45	OAI	/	Stable
Zr ₂ Cl ₂ SSe ₂	18	6.3.966	0.59	C2DB	rectangular	/	Y	0.45	LCEBR	/	Stable
CdSn ₂ Cl ₂ S ₂	18	6.3.954	2.09	C2DB	rectangular	Y	/	0.42	LCEBR	/	Stable
NbI ₂ S ₂	18	3.3.123	1.42	C2DB	rectangular	/	Y	0.40	OAI	/	Stable
Ga ₂ Te ₅	18	6.3.971	0.85	C2DB	rectangular	/	Y	0.39	LCEBR	/	Stable
NbBr ₂ S ₂	18	3.3.104	1.55	C2DB	rectangular	/	Y	0.38	OAI	Yes	Stable
BrClGe ₂ Se ₂	13	6.3.534	1.71	C2DB	rectangular	Y	nHSP	0.35	LCEBR	/	Stable
AgGaBr ₂	13	6.3.519	2.32	C2DB	rectangular	nHSP-SOC	Y	0.35	LCEBR	/	Stable
CdPb ₂ Cl ₂ S ₂	18	6.3.953	2.12	C2DB	rectangular	Y	/	0.33	LCEBR	/	Stable

CdSn ₂ F ₂ O ₂	18	6.3.956	2.69	C2DB	rectangular	/	Y	0.31	LCEBR	/	Stable
Ga ₂ S ₅	10	6.3.384	1.79	C2DB	rectangular	/	Y	0.30	LCEBR	/	Stable
Al ₂ S ₅	10	6.3.359	2.21	C2DB	rectangular	Y	Y	0.29	LCEBR	/	Stable
CdSn ₂ I ₂ O ₂	18	6.3.959	2.01	C2DB	rectangular	Y	Y	0.27	LCEBR	/	Stable
CdPb ₂ F ₂ O ₂	18	6.3.955	2.95	C2DB	rectangular	/	Y	0.23	LCEBR	/	Stable
HgPb ₂ Br ₂ O ₂	18	6.3.946	2.39	C2DB	rectangular	Y	nHSP	0.21	LCEBR	/	Stable
HgPb ₂ Cl ₂ O ₂	18	6.3.962	2.67	C2DB	rectangular	Y	nHSP	0.17	LCEBR	/	Stable
CdPb ₂ Br ₂ O ₂	18	6.3.942	2.77	C2DB	rectangular	Y	/	0.15	LCEBR	/	Stable
CdSn ₂ Cl ₂ O ₂	18	6.3.952	2.72	C2DB	rectangular	/	Y	0.13	LCEBR	/	Stable

TABLE S84: Computationally unstable materials with valley type: rectangular-HSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
Mg ₂ OSe	11	6.4.76	1.21	C2DB	rectangular	X	Γ	0.58	LCEBR	/	Unstable
AlBr ₂	14	6.4.140	1.96	C2DB	rectangular	X	/	0.51	LCEBR	/	Unstable
SnBrClO	11	6.4.57	1.51	C2DB	rectangular	X	Γ	0.58	LCEBR	/	Unstable
LiFO	15	6.4.152	1.69	C2DB	rectangular	X	Γ	0.55	LCEBR	/	Unstable
SnBrIO	11	6.4.62	0.24	C2DB	rectangular	nHSP-SOC	X	0.35	LCEBR	/	Unstable
ScFS	23	6.4.234	1.12	C2DB	rectangular	Γ	Γ	0.62	LCEBR	/	Unstable
MgF ₂ Se ₂	18	6.4.179	1.24	C2DB	rectangular	nHSP	Γ	0.59	LCEBR	/	Unstable
CaF ₂ Te ₂	18	6.4.173	1.26	C2DB	rectangular	/	Γ	0.59	LCEBR	/	Unstable
SrF ₂ Te ₂	18	6.4.184	1.29	C2DB	rectangular	/	Γ	0.59	LCEBR	/	Unstable
AuI	48	6.4.334	1.81	C2DB	rectangular	Γ	/	0.59	LCEBR	/	Unstable
CaF ₂ Se ₂	18	6.4.172	1.57	C2DB	rectangular	nHSP	Γ	0.58	LCEBR	/	Unstable
CaF ₂ S ₂	18	6.4.171	1.39	C2DB	rectangular	Γ	Γ	0.54	LCEBR	/	Unstable
CaF ₂ S ₂	18	6.4.170	1.92	C2DB	rectangular	nHSP	Γ	0.52	LCEBR	/	Unstable
MgF ₂ Te ₂	18	6.4.180	0.73	C2DB	rectangular	nHSP	Γ	0.51	LCEBR	/	Unstable
CdH ₂ Te ₂	18	6.4.186	1.68	C2DB	rectangular	S	Γ	0.45	LCEBR	/	Unstable
Ag ₂ WO ₄	26	6.4.244	1.99	C2DB	rectangular	/	Γ	0.50	LCEBR	/	Unstable
FOSb	46	6.4.324	1.54	C2DB	rectangular	/	Γ	0.49	LCEBR	/	Unstable
SrF ₂ S ₂	18	6.4.182	1.58	C2DB	rectangular	Γ	Γ	0.48	LCEBR	/	Unstable
Ag ₂ MoO ₄	26	6.4.243	2.12	C2DB	rectangular	/	Γ	0.47	LCEBR	/	Unstable
OSSi	13	6.4.135	1.08	C2DB	rectangular	Γ	Γ	0.47	LCEBR	/	Unstable
As ₂ OS ₂	10	6.4.37	0.68	C2DB	rectangular	nHSP	Γ	0.47	LCEBR	/	Unstable
CdH ₂ S ₂	18	6.4.185	2.27	C2DB	rectangular	/	Γ	0.46	LCEBR	/	Unstable
CdSe ₂	18	3.4.12	1.36	C2DB	rectangular	Γ	nHSP	0.46	OAI	/	Unstable
BrNSi	46	6.4.315	2.17	C2DB	rectangular	/	Γ	0.46	LCEBR	/	Unstable
CdF ₂ Se ₂	18	6.4.174	0.57	C2DB	rectangular	S	Γ	0.27	LCEBR	/	Unstable
PtO ₃ Se	18	6.4.198	0.86	C2DB	rectangular	/	Γ	0.45	LCEBR	/	Unstable
InBrS	32	6.4.262	1.77	C2DB	rectangular	/	Γ	0.44	LCEBR	/	Unstable
AgCl	48	6.4.330	2.54	C2DB	rectangular	Γ	Γ	0.44	LCEBR	/	Unstable
InIS	32	6.4.282	1.05	C2DB	rectangular	/	Γ	0.44	LCEBR	/	Unstable
InBrSe	32	6.4.263	1.74	C2DB	rectangular	/	Γ	0.44	LCEBR	/	Unstable
Ga ₂ Se ₃	32	6.4.280	0.98	C2DB	rectangular	/	Γ	0.43	LCEBR	/	Unstable
As ₂ O ₂ S	10	6.4.35	1.87	C2DB	rectangular	nHSP	Γ	0.43	LCEBR	/	Unstable
AlFSe	46	6.4.311	0.47	C2DB	rectangular	Γ	Γ	0.43	LCEBR	/	Unstable
GaBrS ₂	13	6.4.106	1.22	C2DB	rectangular	nHSP	Γ	0.42	LCEBR	/	Unstable
LiCNTe	32	6.4.269	1.61	C2DB	rectangular	Γ	/	0.42	LCEBR	/	Unstable
CdS ₂	18	3.4.11	1.74	C2DB	rectangular	Γ	nHSP	0.42	OAI	/	Unstable
InISe	32	6.4.283	1.11	C2DB	rectangular	/	Γ	0.42	LCEBR	/	Unstable

HgBr ₂	18	6.4.166	2.73	C2DB	rectangular	/	Γ	0.42	LCEBR	/	Unstable
AlIS	32	6.4.253	1.56	C2DB	rectangular	/	Γ	0.40	LCEBR	/	Unstable
As ₂ O ₂ Se	10	6.4.36	1.85	C2DB	rectangular	nHSP-SOC	Γ	0.40	LCEBR	/	Unstable
HfClISe	11	6.4.65	0.56	C2DB	rectangular	Γ	Γ	0.40	LCEBR	/	Unstable
AgBr	48	6.4.329	2.45	C2DB	rectangular	Γ	Γ	0.40	LCEBR	/	Unstable
CINSi	46	6.4.320	2.80	C2DB	rectangular	Γ	Γ	0.40	LCEBR	/	Unstable
PdO ₃ Se	18	6.4.195	0.64	C2DB	rectangular	/	Γ	0.39	LCEBR	/	Unstable
AuBr	48	6.4.332	1.99	C2DB	rectangular	Γ	/	0.39	LCEBR	/	Unstable
HfBrNSe	13	6.4.110	1.47	C2DB	rectangular	Γ	Y	0.44	LCEBR	/	Unstable
PdO ₃ S	18	6.4.194	0.67	C2DB	rectangular	/	Γ	0.38	LCEBR	/	Unstable
WBr ₂ O ₂	35	6.4.292	1.01	C2DB	rectangular	Γ	/	0.37	LCEBR	/	Unstable
InITe	32	6.4.284	1.33	C2DB	rectangular	/	Γ	0.37	LCEBR	/	Unstable
P ₂ S ₂ Te	10	6.4.50	0.35	C2DB	rectangular	nHSP-SOC	Γ	0.37	LCEBR	/	Unstable
InClS	32	6.4.272	2.34	C2DB	rectangular	/	Γ	0.36	LCEBR	/	Unstable
GaIS	32	6.4.277	1.11	C2DB	rectangular	/	Γ	0.34	LCEBR	/	Unstable
AgI	48	6.4.331	2.52	C2DB	rectangular	Γ	Γ	0.34	LCEBR	/	Unstable
GaSe	32	6.4.278	1.20	C2DB	rectangular	/	Γ	0.34	LCEBR	/	Unstable
PtO ₃ S	18	6.4.197	0.87	C2DB	rectangular	Γ	Γ	0.33	LCEBR	/	Unstable
ScBr ₂ N	13	6.4.103	1.77	C2DB	rectangular	Γ	Y	0.54	LCEBR	/	Unstable
InFTe	32	6.4.276	1.88	C2DB	rectangular	nHSP-SOC	Γ	0.32	LCEBR	/	Unstable
PdO ₃ Te	18	6.4.196	0.38	C2DB	rectangular	/	Γ	0.31	LCEBR	/	Unstable
CuBr	48	6.4.336	2.39	C2DB	rectangular	Γ	Γ	0.29	LCEBR	/	Unstable
In ₂ Te ₃	32	6.4.285	0.62	C2DB	rectangular	/	Γ	0.29	LCEBR	/	Unstable
GaBrSe	32	6.4.260	2.06	C2DB	rectangular	/	Γ	0.29	LCEBR	/	Unstable
GaBrS	32	6.4.259	2.13	C2DB	rectangular	/	Γ	0.28	LCEBR	/	Unstable
CuCl	48	6.4.337	2.61	C2DB	rectangular	Γ	Γ	0.25	LCEBR	/	Unstable
TaClIN	11	6.4.66	0.51	C2DB	rectangular	Γ	nHSP-SOC	0.21	LCEBR	/	Unstable
GaFSe	32	6.4.275	2.81	C2DB	rectangular	Γ -SOC	Γ	0.19	LCEBR	/	Unstable
NiO ₃ Se	18	6.4.192	0.25	C2DB	rectangular	/	Γ	0.19	LCEBR	/	Unstable
LiCNSe	32	6.4.268	2.78	C2DB	rectangular	Γ	/	0.16	LCEBR	/	Unstable
AlBrS	32	6.4.245	2.89	C2DB	rectangular	/	Γ	0.16	LCEBR	/	Unstable
GaClS	32	6.4.270	2.92	C2DB	rectangular	/	Γ	0.16	LCEBR	/	Unstable
SnS ₂ Si	11	6.4.91	1.01	C2DB	rectangular	/	Y	0.58	LCEBR	/	Unstable
ZnBrGeI	13	6.4.107	0.95	C2DB	rectangular	Y	/	0.57	LCEBR	/	Unstable
AlInH ₄	14	3.4.4	0.74	C2DB	rectangular	S	Y	0.50	OAI	/	Unstable
Li ₄ CS ₄	35	6.4.294	2.38	C2DB	rectangular	/	Y	0.42	LCEBR	/	Unstable
AgBrSe ₂	20	6.4.199	1.11	C2DB	rectangular	Y	/	0.40	LCEBR	/	Unstable
AgClSe ₂	20	6.4.201	1.13	C2DB	rectangular	Y	/	0.39	LCEBR	/	Unstable
AuClS ₂	20	6.4.205	1.02	C2DB	rectangular	/	Y	0.35	LCEBR	/	Unstable
AuBrTe ₂	20	6.4.204	0.71	C2DB	rectangular	Y	Γ -SOC	0.27	LCEBR	/	Unstable
AlIH ₄	14	6.4.142	0.58	C2DB	rectangular	Y	Y	0.27	LCEBR	/	Unstable
NiZnCl ₂	13	6.4.120	1.05	C2DB	rectangular	/	S	0.58	LCEBR	/	Unstable
SnS ₂	18	3.4.20	0.89	C2DB	rectangular	nHSP	Y	0.59	OAI	/	Unstable
AuCl	18	3.4.9	1.11	C2DB	rectangular	Y	/	0.47	OAI	/	Unstable
SnSe ₂	18	3.4.21	0.48	C2DB	rectangular	nHSP	Y	0.46	OAI	/	Unstable
AuCl	48	6.4.333	2.14	C2DB	rectangular	Y	/	0.41	LCEBR	/	Unstable
CdTe ₂	18	3.4.13	1.08	C2DB	rectangular	nHSP	Y	0.41	OAI	/	Unstable
GeS ₂	18	3.4.15	0.27	C2DB	rectangular	nHSP	Y	0.40	OAI	/	Unstable

b. HSP-SOC

TABLE S85: Computationally stable materials with valley type: rectangular-HSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
AuCuClI	13	6.3.522	1.93	C2DB	rectangular	Y-SOC	/	0.34	LCEBR	/	Stable
BaSnS ₂	11	6.3.442	1.18	C2DB	rectangular	nHSP	X-SOC	0.51	LCEBR	/	Stable
PbSe ₃	9	6.3.354	0.63	C2DB	rectangular	/	X-SOC	0.23	LCEBR	/	Stable
AgGeIS	13	6.3.521	0.61	C2DB	rectangular	Γ	Γ -SOC	0.46	LCEBR	/	Stable
Bi ₂ OSe ₂	10	6.3.376	0.60	C2DB	rectangular	/	Γ -SOC	0.45	LCEBR	/	Stable
As ₂ OSe ₂	10	6.3.370	0.49	C2DB	rectangular	nHSP-SOC	Γ -SOC	0.41	LCEBR	/	Stable
OSb ₂ Te ₂	10	6.3.398	0.47	C2DB	rectangular	/	Γ -SOC	0.41	LCEBR	/	Stable
As ₂ OTe ₂	10	6.3.371	0.41	C2DB	rectangular	/	Γ -SOC	0.38	LCEBR	/	Stable
GaFTe	32	6.3.1276	2.07	C2DB	rectangular	Γ -SOC	nHSP	0.36	LCEBR	/	Stable
PdZnI ₂	13	6.3.564	1.28	C2DB	rectangular	Γ -SOC	nHSP-SOC	0.35	LCEBR	/	Stable
CuHgClTe	28	6.3.1202	0.85	C2DB	rectangular	/	Γ -SOC	0.31	LCEBR	/	Stable
CuHgBrTe	28	6.3.1192	0.94	C2DB	rectangular	/	Γ -SOC	0.31	LCEBR	/	Stable
CuClSe ₂	20	6.3.1016	0.83	C2DB	rectangular	/	Γ -SOC	0.28	LCEBR	Yes	Stable
AuHgClTe	28	6.3.1183	0.41	C2DB	rectangular	/	Γ -SOC	0.22	LCEBR	/	Stable
AuHgBrTe	28	6.3.1179	0.46	C2DB	rectangular	/	Γ -SOC	0.20	LCEBR	/	Stable
NiPd ₃ Se ₈	14	6.3.607	0.35	C2DB	rectangular	Γ -SOC	/	0.13	LCEBR	/	Stable
BiCuS ₂	28	6.3.1186	0.26	C2DB	rectangular	/	Γ -SOC	0.12	LCEBR	Yes	Stable

TABLE S86: Computationally unstable materials with valley type: rectangular-HSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
OTe	11	6.4.83	0.60	C2DB	rectangular	Y-SOC	nHSP	0.52	LCEBR	/	Unstable
AuYBrI	11	6.4.54	0.51	C2DB	rectangular	Y-SOC	X-SOC	0.43	LCEBR	/	Unstable
TiCl ₂	13	6.4.117	0.62	C2DB	rectangular	Γ -SOC	Y-SOC	0.34	LCEBR	/	Unstable
TlClSe	13	6.4.121	1.13	C2DB	rectangular	Γ -SOC	Γ -SOC	0.40	LCEBR	/	Unstable
InBrTe	32	6.4.264	1.69	C2DB	rectangular	nHSP-SOC	Γ -SOC	0.37	LCEBR	/	Unstable
Bi ₂ OTe ₂	10	6.4.38	0.32	C2DB	rectangular	/	Γ -SOC	0.36	LCEBR	/	Unstable
InClTe	32	6.4.273	1.87	C2DB	rectangular	nHSP-SOC	Γ -SOC	0.35	LCEBR	/	Unstable
BiISe ₂	13	6.4.99	0.41	C2DB	rectangular	/	Γ -SOC	0.34	LCEBR	/	Unstable
OP ₂ Te ₂	10	6.4.49	0.36	C2DB	rectangular	nHSP-SOC	Γ -SOC	0.33	LCEBR	/	Unstable
GaBrTe	32	6.4.261	1.91	C2DB	rectangular	Γ -SOC	/	0.31	LCEBR	/	Unstable
GaClTe	32	6.4.271	2.13	C2DB	rectangular	Γ -SOC	/	0.29	LCEBR	/	Unstable
AuBrTe ₂	20	6.4.204	0.71	C2DB	rectangular	Y	Γ -SOC	0.27	LCEBR	/	Unstable
NbBSTe ₂	13	6.4.97	0.27	C2DB	rectangular	Γ -SOC	nHSP-SOC	0.20	LCEBR	/	Unstable
GaFSe	32	6.4.275	2.81	C2DB	rectangular	Γ -SOC	Γ	0.19	LCEBR	/	Unstable
AlFTe	32	6.4.252	2.90	C2DB	rectangular	Γ -SOC	nHSP	0.17	LCEBR	/	Unstable
AlBrTe	32	6.4.247	2.74	C2DB	rectangular	Γ -SOC	/	0.17	LCEBR	/	Unstable
AlClTe	32	6.4.249	2.89	C2DB	rectangular	Γ -SOC	/	0.15	LCEBR	/	Unstable

c. nHSP

TABLE S87: Experimental materials with valley type: rectangular-nHSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
GeSe	32	6.1.1	1.12	C2DB	rectangular	nHSP	/	0.41	LCEBR	Yes	Exp.M.Exfo
SnS	32	6.1.2	1.43	C2DB	rectangular	nHSP	nHSP-SOC	0.38	LCEBR	Yes	Exp.M.Exfo
SnSe	32	6.1.4	0.89	C2DB	rectangular	nHSP	nHSP-SOC	0.37	LCEBR	Yes	Exp.M.Exfo

TABLE S88: Computationally exfoliable materials with valley type: rectangular-nHSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
Hg ₂ IO	47	3.2.134	1.24	MC2D	rectangular	/	nHSP	0.61	OAI	Yes	Comp.Exfo
N	46	3.2.132	0.82	MC2D	rectangular	Γ	nHSP	0.59	OAI	Yes	Comp.Exfo
HgO	40	6.2.785	1.93	MC2D	rectangular	/	nHSP	0.57	LCEBR	Yes	Comp.Exfo
SnPS ₃	18	3.2.113	1.11	MC2D	rectangular	Γ	nHSP	0.52	OAI	Yes	Comp.Exfo
Tl ₂ CS ₃	10	6.2.293	1.21	MC2D	rectangular	nHSP	/	0.51	LCEBR	Yes	Comp.Exfo
PbSnS ₂	11	6.2.313	1.05	MC2D	rectangular	nHSP	nHSP-SOC	0.47	LCEBR	Yes	Comp.Exfo
K ₂ P ₂ Si	38	6.2.774	1.22	MC2D	rectangular	nHSP	/	0.46	LCEBR	Yes	Comp.Exfo
K ₂ ZrTe ₃	36	6.2.752	0.51	MC2D	rectangular	/	nHSP	0.38	LCEBR	Yes	Comp.Exfo
GeS	32	6.2.721	1.61	MC2D	rectangular	nHSP	nHSP-SOC	0.37	LCEBR	Yes	Comp.Exfo
AuKS	40	6.2.777	1.65	MC2D	rectangular	/	nHSP	0.36	LCEBR	Yes	Comp.Exfo
O ₂ Te	17	6.2.554	2.21	MC2D	rectangular	/	nHSP	0.28	LCEBR	Yes	Comp.Exfo
PtSiTe	17	6.2.558	0.46	MC2D	rectangular	nHSP	/	0.23	LCEBR	Yes	Comp.Exfo
BaBiO ₂	41	6.2.792	2.86	MC2D	rectangular	/	nHSP	0.16	LCEBR	Yes	Comp.Exfo

TABLE S89: Computationally stable materials with valley type: rectangular-nHSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
AuS	14	6.3.579	1.24	C2DB	rectangular	S	nHSP	0.60	LCEBR	/	Stable
AuSe	14	6.3.580	0.98	C2DB	rectangular	X	nHSP	0.60	LCEBR	Yes	Stable
AgS	14	6.3.573	0.95	C2DB	rectangular	S	nHSP	0.59	LCEBR	/	Stable
BaSnS ₂	11	6.3.442	1.18	C2DB	rectangular	nHSP	X-SOC	0.58	LCEBR	/	Stable
SrGeS ₂	11	6.3.482	1.21	C2DB	rectangular	nHSP	nHSP-SOC	0.58	LCEBR	/	Stable
AlSe	18	3.3.101	1.64	C2DB	rectangular	nHSP	Γ	0.58	OAI	/	Stable
GaSe	18	3.3.120	1.58	C2DB	rectangular	nHSP	nHSP	0.54	OAI	/	Stable
AlTe	18	3.3.102	1.48	C2DB	rectangular	nHSP	Γ	0.54	OAI	/	Stable
AlS	18	3.3.100	1.93	C2DB	rectangular	nHSP	Γ	0.53	OAI	/	Stable
AgSe	14	6.3.574	0.74	C2DB	rectangular	X	nHSP	0.52	LCEBR	/	Stable
GaS	18	3.3.119	2.01	C2DB	rectangular	nHSP	Γ	0.52	OAI	/	Stable
Ge ₂ STe	11	6.3.479	0.92	C2DB	rectangular	nHSP	nHSP-SOC	0.52	LCEBR	/	Stable
MoWO ₄	27	6.3.1141	1.08	C2DB	rectangular	Γ	nHSP	0.51	LCEBR	/	Stable
AuPdClSe	11	6.3.441	0.76	C2DB	rectangular	S	nHSP	0.51	LCEBR	/	Stable
AuTe	14	6.3.581	0.67	C2DB	rectangular	X	nHSP	0.50	LCEBR	/	Stable
InTe	18	3.3.131	1.09	C2DB	rectangular	Y	nHSP	0.50	OAI	/	Stable
CuS	14	6.3.591	0.61	C2DB	rectangular	/	nHSP	0.48	LCEBR	/	Stable
HfBr ₂	15	6.3.649	0.84	C2DB	rectangular	/	nHSP	0.47	LCEBR	/	Stable
GeS	32	6.3.1289	1.76	C2DB	rectangular	nHSP	nHSP	0.47	LCEBR	/	Stable
HfCl ₂	15	6.3.685	0.85	C2DB	rectangular	/	nHSP	0.45	LCEBR	/	Stable
Ge ₂ SSe	11	6.3.478	1.27	C2DB	rectangular	nHSP	nHSP	0.45	LCEBR	/	Stable
AgTe	14	6.3.575	0.49	C2DB	rectangular	X	nHSP	0.44	LCEBR	/	Stable
BrClGe ₂ Se ₂	13	6.3.534	1.71	C2DB	rectangular	Y	nHSP	0.44	LCEBR	/	Stable
CrMoS ₄	27	6.3.1133	1.04	C2DB	rectangular	nHSP-SOC	nHSP	0.43	LCEBR	/	Stable
CuSe	14	6.3.592	0.44	C2DB	rectangular	X	nHSP	0.43	LCEBR	/	Stable
GaTe	18	3.3.121	0.93	C2DB	rectangular	nHSP	nHSP	0.43	OAI	/	Stable
CrWS ₄	27	6.3.1136	0.97	C2DB	rectangular	nHSP-SOC	nHSP	0.43	LCEBR	/	Stable
ISb	18	1.3.39	0.41	C2DB	rectangular	nHSP	nHSP	0.42	SEBR	/	Stable

As	42	3.3.152	0.80	C2DB	rectangular	nHSP	Γ	0.42	OAI	Yes	Stable
HgTe ₂	18	3.3.122	0.97	C2DB	rectangular	Γ	nHSP	0.42	OAI	/	Stable
HgClS ₂ Sb	15	6.3.674	1.32	C2DB	rectangular	/	nHSP	0.41	LCEBR	/	Stable
HgBrS ₂ Sb	15	6.3.641	1.36	C2DB	rectangular	/	nHSP	0.41	LCEBR	/	Stable
AuFS ₂	20	6.3.1009	1.26	C2DB	rectangular	/	nHSP	0.41	LCEBR	/	Stable
BiClS	46	6.3.1421	1.21	C2DB	rectangular	/	nHSP	0.41	LCEBR	/	Stable
HfSnS ₄	32	6.3.1305	1.18	C2DB	rectangular	nHSP	/	0.41	LCEBR	/	Stable
SnZrS ₄	32	6.3.1328	1.07	C2DB	rectangular	nHSP	/	0.41	LCEBR	/	Stable
HgIS ₂ Sb	15	6.3.736	1.38	C2DB	rectangular	/	nHSP	0.41	LCEBR	/	Stable
HfI ₂	15	6.3.735	0.62	C2DB	rectangular	/	nHSP	0.41	LCEBR	/	Stable
BiFS	46	6.3.1425	1.30	C2DB	rectangular	/	nHSP	0.40	LCEBR	/	Stable
BiBrS	46	6.3.1417	1.21	C2DB	rectangular	/	nHSP	0.40	LCEBR	/	Stable
HfGeS ₄	32	6.3.1283	1.21	C2DB	rectangular	nHSP	/	0.40	LCEBR	/	Stable
SeSi	32	6.3.1331	1.20	C2DB	rectangular	nHSP	/	0.40	LCEBR	/	Stable
CdS ₂	17	3.3.86	1.53	C2DB	rectangular	/	nHSP	0.40	OAI	/	Stable
BiBrO	46	6.3.1416	1.77	C2DB	rectangular	/	nHSP	0.40	LCEBR	/	Stable
ZrGeS ₄	32	6.3.1290	1.09	C2DB	rectangular	nHSP	/	0.39	LCEBR	/	Stable
GeTe	32	6.3.1293	0.81	C2DB	rectangular	nHSP	/	0.39	LCEBR	Yes	Stable
Hf ₂ Br ₂ S ₃	10	6.3.378	1.39	C2DB	rectangular	nHSP	S	0.39	LCEBR	/	Stable
BiBr	15	1.3.6	0.64	C2DB	rectangular	nHSP	X	0.39	NLC	/	Stable
BiS	46	6.3.1427	1.08	C2DB	rectangular	/	nHSP	0.39	LCEBR	/	Stable
SnS	32	6.1.3	1.84	C2DB	rectangular	nHSP	nHSP	0.38	LCEBR	/	Stable
PtSnS ₄	14	6.3.610	1.39	C2DB	rectangular	Γ	nHSP	0.38	LCEBR	/	Stable
HfSnSe ₄	32	6.3.1306	0.94	C2DB	rectangular	nHSP	/	0.38	LCEBR	/	Stable
TiBrISe	11	6.3.465	0.57	C2DB	rectangular	X	nHSP	0.38	LCEBR	/	Stable
BiClO	46	6.3.1420	2.08	C2DB	rectangular	/	nHSP	0.37	LCEBR	/	Stable
HgPb ₂ I ₂ O ₂	18	6.3.978	1.91	C2DB	rectangular	/	nHSP	0.37	LCEBR	/	Stable
HgSn ₂ I ₂ S ₂	18	6.3.980	1.79	C2DB	rectangular	/	nHSP	0.36	LCEBR	/	Stable
HfGeSe ₄	32	6.3.1284	1.07	C2DB	rectangular	nHSP	/	0.36	LCEBR	/	Stable
SnZrSe ₄	32	6.3.1334	0.89	C2DB	rectangular	nHSP	/	0.36	LCEBR	/	Stable
Al ₂ Te ₃	32	6.3.1241	1.00	C2DB	rectangular	/	nHSP	0.36	LCEBR	/	Stable
IrLiO ₄	8	6.3.277	0.34	C2DB	rectangular	nHSP	/	0.35	LCEBR	/	Stable
AsBr	18	1.3.32	0.20	C2DB	rectangular	nHSP	nHSP	0.35	SEBR	/	Stable
SnSe	32	6.3.1332	1.57	C2DB	rectangular	/	nHSP	0.35	LCEBR	/	Stable
ZrGeSe ₄	32	6.3.1292	1.00	C2DB	rectangular	nHSP	/	0.35	LCEBR	/	Stable
CdClS ₂ Sb	15	6.3.664	1.17	C2DB	rectangular	/	nHSP	0.35	LCEBR	/	Stable
SnI ₂	18	6.3.982	1.57	C2DB	rectangular	/	nHSP	0.35	LCEBR	/	Stable
CdBrS ₂ Sb	15	6.3.640	1.18	C2DB	rectangular	/	nHSP	0.35	LCEBR	/	Stable
ZrSe ₄ Si	32	6.3.1333	1.01	C2DB	rectangular	nHSP	/	0.35	LCEBR	/	Stable
GeSiTe ₂	11	6.3.483	0.58	C2DB	rectangular	nHSP	/	0.34	LCEBR	/	Stable
GeS	32	6.3.1288	1.71	C2DB	rectangular	nHSP	nHSP-SOC	0.34	LCEBR	Yes	Stable
CdIS ₂ Sb	15	6.3.667	1.04	C2DB	rectangular	/	nHSP	0.34	LCEBR	/	Stable
VFO ₂	11	6.3.477	2.68	C2DB	rectangular	nHSP	Y	0.34	LCEBR	/	Stable
PdF ₂	42	6.3.1379	0.77	C2DB	rectangular	/	nHSP	0.33	LCEBR	/	Stable
MoWS ₄	27	6.3.1142	1.55	C2DB	rectangular	nHSP-SOC	nHSP	0.33	LCEBR	/	Stable
ZrBr ₂	15	6.3.652	0.57	C2DB	rectangular	/	nHSP	0.33	LCEBR	/	Stable
BiHgIS ₂	15	6.3.629	1.03	C2DB	rectangular	/	nHSP	0.32	LCEBR	/	Stable
CdSn ₂ I ₂ S ₂	18	6.3.961	1.91	C2DB	rectangular	/	nHSP	0.32	LCEBR	/	Stable
RhF ₃	23	6.3.1108	0.30	C2DB	rectangular	Y	nHSP	0.32	LCEBR	/	Stable
HgSn ₂ Br ₂ S ₂	18	6.3.948	1.93	C2DB	rectangular	/	nHSP	0.31	LCEBR	/	Stable
ZrI ₂	15	6.3.751	0.41	C2DB	rectangular	/	nHSP	0.31	LCEBR	/	Stable

IrS	15	6.3.740	0.85	C2DB	rectangular	/	nHSP	0.31	LCEBR	/	Stable
SnTe	32	6.3.1336	0.59	C2DB	rectangular	nHSP	/	0.30	LCEBR	Yes	Stable
MoWTe ₄	27	6.3.1144	0.88	C2DB	rectangular	nHSP-SOC	nHSP	0.30	LCEBR	/	Stable
AllnTe ₃	32	6.3.1239	0.75	C2DB	rectangular	/	nHSP	0.30	LCEBR	/	Stable
GaFTe	32	6.3.1276	2.07	C2DB	rectangular	Γ -SOC	nHSP	0.29	LCEBR	/	Stable
PdAsTe	16	3.3.75	0.50	C2DB	rectangular	/	nHSP	0.27	OAI	/	Stable
OsSe ₂	15	3.3.67	0.61	C2DB	rectangular	nHSP	Γ	0.26	OAI	/	Stable
Al ₂ Se ₃	32	6.3.1240	2.19	C2DB	rectangular	/	nHSP	0.25	LCEBR	/	Stable
CdSn ₂ Br ₂ O ₂	18	6.3.943	2.49	C2DB	rectangular	nHSP	/	0.24	LCEBR	/	Stable
ZrCl ₂	15	6.3.688	0.59	C2DB	rectangular	nHSP	nHSP	0.24	LCEBR	/	Stable
HgPb ₂ Br ₂ O ₂	18	6.3.946	2.39	C2DB	rectangular	Y	nHSP	0.23	LCEBR	/	Stable
OsS ₂	15	3.3.66	0.55	C2DB	rectangular	nHSP	Γ	0.23	OAI	/	Stable
GeO	32	6.3.1286	2.70	C2DB	rectangular	nHSP	/	0.23	LCEBR	/	Stable
SnO	32	6.3.1320	2.51	C2DB	rectangular	nHSP	nHSP-SOC	0.22	LCEBR	Yes	Stable
HgPb ₂ Cl ₂ O ₂	18	6.3.962	2.67	C2DB	rectangular	Y	nHSP	0.19	LCEBR	/	Stable
InTiCl ₄	14	6.3.589	2.98	C2DB	rectangular	/	nHSP	0.19	LCEBR	/	Stable
AllnS ₃	32	6.3.1237	2.37	C2DB	rectangular	/	nHSP	0.17	LCEBR	/	Stable
IrBrO	46	6.3.1442	0.26	C2DB	rectangular	Γ	nHSP	0.16	LCEBR	/	Stable
AlGaS ₃	32	6.3.1233	2.82	C2DB	rectangular	/	nHSP	0.10	LCEBR	/	Stable

TABLE S90: Computationally unstable materials with valley type: rectangular-nHSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
SnS ₂	18	3.4.20	0.89	C2DB	rectangular	nHSP	Y	0.59	OAI	/	Unstable
AlF	46	6.4.312	0.90	C2DB	rectangular	nHSP	/	0.53	LCEBR	/	Unstable
NbCl ₂ N	35	6.4.295	0.77	C2DB	rectangular	nHSP	nHSP-SOC	0.53	LCEBR	/	Unstable
OTe	11	6.4.83	0.60	C2DB	rectangular	Y-SOC	nHSP	0.52	LCEBR	/	Unstable
GaBrS ₂	13	6.4.106	1.22	C2DB	rectangular	nHSP	Γ	0.49	LCEBR	/	Unstable
CdSe ₂	18	3.4.12	1.36	C2DB	rectangular	Γ	nHSP	0.47	OAI	/	Unstable
GaLiS ₄	14	3.4.3	0.68	C2DB	rectangular	/	nHSP	0.47	OAI	/	Unstable
SnSe ₂	18	3.4.21	0.48	C2DB	rectangular	nHSP	Y	0.46	OAI	/	Unstable
CdTe ₂	18	3.4.13	1.08	C2DB	rectangular	nHSP	Y	0.46	OAI	/	Unstable
CaF ₂ Se ₂	18	6.4.172	1.57	C2DB	rectangular	nHSP	Γ	0.45	LCEBR	/	Unstable
MgF ₂ Se ₂	18	6.4.179	1.24	C2DB	rectangular	nHSP	Γ	0.45	LCEBR	/	Unstable
CdS ₂	18	3.4.11	1.74	C2DB	rectangular	Γ	nHSP	0.43	OAI	/	Unstable
ScBrS ₂	13	6.4.115	1.70	C2DB	rectangular	/	nHSP	0.41	LCEBR	/	Unstable
MgF ₂ Te ₂	18	6.4.180	0.73	C2DB	rectangular	nHSP	Γ	0.40	LCEBR	/	Unstable
GeS ₂	18	3.4.15	0.27	C2DB	rectangular	nHSP	Y	0.40	OAI	/	Unstable
CdHfSeTe	11	6.4.63	0.82	C2DB	rectangular	nHSP	nHSP-SOC	0.40	LCEBR	/	Unstable
FSb	18	1.4.13	0.33	C2DB	rectangular	nHSP	nHSP	0.39	SEBR	/	Unstable
CaF ₂ S ₂	18	6.4.170	1.92	C2DB	rectangular	nHSP	Γ	0.38	LCEBR	/	Unstable
SiTe	32	6.4.289	0.35	C2DB	rectangular	nHSP	/	0.31	LCEBR	/	Unstable
As ₂ O ₂ S	10	6.4.35	1.87	C2DB	rectangular	nHSP	Γ	0.31	LCEBR	/	Unstable
CIOsb	46	6.4.321	1.89	C2DB	rectangular	/	nHSP	0.31	LCEBR	/	Unstable
SnBr ₂	18	6.4.168	2.08	C2DB	rectangular	/	nHSP	0.27	LCEBR	/	Unstable
As ₂ OS ₂	10	6.4.37	0.68	C2DB	rectangular	nHSP	Γ	0.24	LCEBR	/	Unstable
SnCl ₂	18	6.4.176	2.77	C2DB	rectangular	/	nHSP	0.16	LCEBR	/	Unstable
AlFTe	32	6.4.252	2.90	C2DB	rectangular	Γ -SOC	nHSP	0.14	LCEBR	/	Unstable

d. nHSP-SOC

TABLE S91: Experimental materials with valley type: rectangular-nHSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
SnS	32	6.1.2	1.43	C2DB	rectangular	nHSP	nHSP-SOC	0.40	LCEBR	Yes	Exp.M.Exfo
SnSe	32	6.1.4	0.89	C2DB	rectangular	nHSP	nHSP-SOC	0.36	LCEBR	Yes	Exp.M.Exfo

TABLE S92: Computationally exfoliable materials with valley type: rectangular-nHSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
PbSnS ₂	11	6.2.313	1.05	MC2D	rectangular	nHSP	nHSP-SOC	0.45	LCEBR	Yes	Comp.Exfo
GeS	32	6.2.721	1.61	MC2D	rectangular	nHSP	nHSP-SOC	0.35	LCEBR	Yes	Comp.Exfo
WCl ₂ O ₂	29	6.2.678	2.02	MC2D	rectangular	/	nHSP-SOC	0.30	LCEBR	Yes	Comp.Exfo
Tl ₂ S ₃ Te	29	6.2.684	0.92	MC2D	rectangular	/	nHSP-SOC	0.30	LCEBR	Yes	Comp.Exfo

TABLE S93: Computationally stable materials with valley type: rectangular-nHSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
PdZnI ₂	13	6.3.564	1.28	C2DB	rectangular	Γ -SOC	nHSP-SOC	0.58	LCEBR	/	Stable
AgClGeTe	23	6.3.1062	1.19	C2DB	rectangular	nHSP-SOC	Γ	0.56	LCEBR	/	Stable
SrGeS ₂	11	6.3.482	1.21	C2DB	rectangular	nHSP	nHSP-SOC	0.56	LCEBR	/	Stable
PbGeSSe	11	6.3.481	0.99	C2DB	rectangular	nHSP-SOC	nHSP-SOC	0.54	LCEBR	/	Stable
HgF ₂ S	13	6.3.548	1.81	C2DB	rectangular	/	nHSP-SOC	0.51	LCEBR	/	Stable
BaSnTe ₂	11	6.3.443	0.74	C2DB	rectangular	nHSP-SOC	nHSP-SOC	0.50	LCEBR	/	Stable
Bi ₂ Cl ₂ SSe	11	6.3.444	1.08	C2DB	rectangular	/	nHSP-SOC	0.45	LCEBR	/	Stable
Sn ₂ SSe	11	6.3.508	1.07	C2DB	rectangular	nHSP-SOC	nHSP-SOC	0.44	LCEBR	/	Stable
PbSnSe ₂	11	6.3.504	1.46	C2DB	rectangular	/	nHSP-SOC	0.43	LCEBR	/	Stable
MoWSe ₄	27	6.3.1143	1.29	C2DB	rectangular	nHSP-SOC	/	0.43	LCEBR	/	Stable
PbI ₂ Se	13	6.3.563	1.62	C2DB	rectangular	nHSP-SOC	/	0.42	LCEBR	/	Stable
IOSb	46	6.3.1556	1.17	C2DB	rectangular	nHSP-SOC	/	0.42	LCEBR	/	Stable
MoWS ₄	27	6.3.1142	1.55	C2DB	rectangular	nHSP-SOC	nHSP	0.40	LCEBR	/	Stable
As ₂ S ₂ Te	10	6.3.372	0.82	C2DB	rectangular	/	nHSP-SOC	0.39	LCEBR	/	Stable
MoWTe ₄	27	6.3.1144	0.88	C2DB	rectangular	nHSP-SOC	nHSP	0.39	LCEBR	/	Stable
YBrS	23	6.3.1097	1.30	C2DB	rectangular	nHSP-SOC	Γ	0.38	LCEBR	/	Stable
BiIO	46	6.3.1426	1.40	C2DB	rectangular	nHSP-SOC	/	0.38	LCEBR	/	Stable
CrMoS ₄	27	6.3.1133	1.04	C2DB	rectangular	nHSP-SOC	nHSP	0.37	LCEBR	/	Stable
WBr ₂ O ₂	29	6.3.1221	1.20	C2DB	rectangular	/	nHSP-SOC	0.37	LCEBR	/	Stable
CrWS ₄	27	6.3.1136	0.97	C2DB	rectangular	nHSP-SOC	nHSP	0.36	LCEBR	/	Stable
WF ₂ O ₂	29	6.3.1225	2.38	C2DB	rectangular	X	nHSP-SOC	0.36	LCEBR	/	Stable
AgGaBr ₂	13	6.3.519	2.32	C2DB	rectangular	nHSP-SOC	Y	0.35	LCEBR	/	Stable
CrMoSe ₄	27	6.3.1134	0.84	C2DB	rectangular	nHSP-SOC	/	0.34	LCEBR	/	Stable
SnSbTe	20	6.3.1034	1.20	C2DB	rectangular	/	nHSP-SOC	0.33	LCEBR	/	Stable
GeS	32	6.3.1288	1.71	C2DB	rectangular	nHSP	nHSP-SOC	0.32	LCEBR	Yes	Stable
CrWSe ₄	27	6.3.1137	0.78	C2DB	rectangular	nHSP-SOC	/	0.32	LCEBR	/	Stable
PtGeS ₂	13	6.3.552	0.61	C2DB	rectangular	nHSP-SOC	nHSP-SOC	0.31	LCEBR	/	Stable
Ge ₂ STe	11	6.3.479	0.92	C2DB	rectangular	nHSP	nHSP-SOC	0.31	LCEBR	/	Stable
ISSb	46	6.3.1561	0.75	C2DB	rectangular	nHSP-SOC	/	0.30	LCEBR	/	Stable
CrWTe ₄	27	6.3.1138	0.51	C2DB	rectangular	nHSP-SOC	/	0.26	LCEBR	/	Stable
WCl ₂ O ₂	29	6.3.1223	2.23	C2DB	rectangular	/	nHSP-SOC	0.25	LCEBR	Yes	Stable
TlI	18	6.3.981	2.66	C2DB	rectangular	nHSP-SOC	/	0.22	LCEBR	/	Stable
MoF ₂ O ₂	29	6.3.1224	2.83	C2DB	rectangular	X	nHSP-SOC	0.20	LCEBR	/	Stable

SnO	32	6.3.1320	2.51	C2DB	rectangular	nHSP	nHSP-SOC	0.19	LCEBR	Yes	Stable
As ₂ OSe ₂	10	6.3.370	0.49	C2DB	rectangular	nHSP-SOC	Γ -SOC	0.17	LCEBR	/	Stable
P ₂ Se ₂ Te	10	6.3.400	0.36	C2DB	rectangular	nHSP-SOC	Γ	0.13	LCEBR	/	Stable
PbTe ₃	9	6.3.355	0.32	C2DB	rectangular	/	nHSP-SOC	0.11	LCEBR	/	Stable
SnTe ₃	9	6.3.357	0.23	C2DB	rectangular	/	nHSP-SOC	0.10	LCEBR	/	Stable

TABLE S94: Computationally unstable materials with valley type: rectangular-nHSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
HfZnS ₂	11	6.4.70	1.28	C2DB	rectangular	nHSP-SOC	nHSP-SOC	0.58	LCEBR	/	Unstable
NbCl ₂ N	35	6.4.295	0.77	C2DB	rectangular	nHSP	nHSP-SOC	0.52	LCEBR	/	Unstable
PdScBrS ₂	13	6.4.114	0.72	C2DB	rectangular	/	nHSP-SOC	0.48	LCEBR	/	Unstable
PbBrIS	13	6.4.112	1.59	C2DB	rectangular	nHSP-SOC	/	0.45	LCEBR	/	Unstable
TaClIN	11	6.4.66	0.51	C2DB	rectangular	Γ	nHSP-SOC	0.43	LCEBR	/	Unstable
PS ₃ Sb	13	6.4.136	1.15	C2DB	rectangular	/	nHSP-SOC	0.40	LCEBR	/	Unstable
CdHfSeTe	11	6.4.63	0.82	C2DB	rectangular	nHSP	nHSP-SOC	0.40	LCEBR	/	Unstable
InFTe	32	6.4.276	1.88	C2DB	rectangular	nHSP-SOC	Γ	0.38	LCEBR	/	Unstable
PbO	23	6.4.239	0.22	C2DB	rectangular	/	nHSP-SOC	0.36	LCEBR	/	Unstable
As ₂ O ₂ Se	10	6.4.36	1.85	C2DB	rectangular	nHSP-SOC	Γ	0.34	LCEBR	/	Unstable
InBrTe	32	6.4.264	1.69	C2DB	rectangular	nHSP-SOC	Γ -SOC	0.33	LCEBR	/	Unstable
SnBrIO	11	6.4.62	0.24	C2DB	rectangular	nHSP-SOC	X	0.32	LCEBR	/	Unstable
InClTe	32	6.4.273	1.87	C2DB	rectangular	nHSP-SOC	Γ -SOC	0.31	LCEBR	/	Unstable
NbBrClN	13	6.4.105	0.67	C2DB	rectangular	nHSP-SOC	nHSP-SOC	0.31	LCEBR	/	Unstable
NbBSt ₂	13	6.4.97	0.27	C2DB	rectangular	Γ -SOC	nHSP-SOC	0.26	LCEBR	/	Unstable
TiGeTe ₂	13	6.4.127	0.44	C2DB	rectangular	nHSP-SOC	/	0.26	LCEBR	/	Unstable
P ₂ S ₂ Te	10	6.4.50	0.35	C2DB	rectangular	nHSP-SOC	Γ	0.19	LCEBR	/	Unstable
OP ₂ Te ₂	10	6.4.49	0.36	C2DB	rectangular	nHSP-SOC	Γ -SOC	0.16	LCEBR	/	Unstable

5. Oblique lattice

a. HSP

TABLE S95: Computationally exfoliable materials with valley type: oblique-HSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
Na ₂ TiH ₄ O ₅	2	6.2.125	1.69	MC2D	oblique	Γ	B	0.43	LCEBR	Yes	Comp.Exfo
CuI	2	6.2.97	1.98	MC2D	oblique	Γ	Γ	0.30	LCEBR	Yes	Comp.Exfo
VH ₂ O ₃	2	3.2.50	0.40	MC2D	oblique	/	Γ	0.12	OAI	Yes	Comp.Exfo
AgNO ₂	1	6.2.3	1.61	MC2D	oblique	B	A	0.55	LCEBR	Yes	Comp.Exfo
ISbTe	2	6.2.148	0.72	MC2D	oblique	nHSP	Y	0.45	LCEBR	Yes	Comp.Exfo
AgCO ₂	2	3.2.20	2.32	MC2D	oblique	/	B	0.34	OAI	Yes	Comp.Exfo

TABLE S96: Computationally stable materials with valley type: oblique-HSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
ReO ₂	2	3.3.40	1.35	C2DB	oblique	Γ	/	0.46	OAI	/	Stable
AgCuBr ₂	2	6.3.90	2.32	C2DB	oblique	A	Γ	0.32	LCEBR	/	Stable
AgF	1	6.3.1	0.52	C2DB	oblique	A	Γ	0.20	LCEBR	/	Stable
AsI	2	1.3.1	1.33	C2DB	oblique	Γ	nHSP	0.38	NLC	/	Stable

ScPSe ₄	2	6.3.208	1.17	C2DB	oblique	/	Γ	0.37	LCEBR	/	Stable
AgO ₃ P	2	6.3.89	2.56	C2DB	oblique	/	Γ	0.37	LCEBR	/	Stable
ScAsSe ₄	2	6.3.96	0.62	C2DB	oblique	/	Γ	0.28	LCEBR	/	Stable
ScPS ₄	2	6.3.207	1.91	C2DB	oblique	/	Γ	0.27	LCEBR	Yes	Stable
CuYCl ₄	2	6.3.141	2.32	C2DB	oblique	/	Y	0.36	LCEBR	/	Stable
GaTe	3	6.3.220	0.29	C2DB	oblique	B	B-SOC	0.38	LCEBR	/	Stable

TABLE S97: Computationally unstable materials with valley type: oblique-HSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
BClSiTe	1	6.4.3	1.13	C2DB	oblique	B-SOC	Γ	0.55	LCEBR	/	Unstable
CdS ₂	2	3.4.1	1.39	C2DB	oblique	B	B	0.60	OAI	/	Unstable
HgO ₂	2	6.4.19	0.49	C2DB	oblique	B	/	0.31	LCEBR	/	Unstable

b. HSP-SOC

TABLE S98: Computationally stable materials with valley type: oblique-HSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
Cd ₂ I ₂ Te	1	6.3.54	1.92	C2DB	oblique	/	Γ-SOC	0.43	LCEBR	/	Stable
AuHgTe	3	6.3.215	0.76	C2DB	oblique	nHSP-SOC	B-SOC	0.50	LCEBR	/	Stable
GaTe	3	6.3.220	0.29	C2DB	oblique	B	B-SOC	0.38	LCEBR	/	Stable

TABLE S99: Computationally unstable materials with valley type: oblique-HSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
BClSiTe	1	6.4.3	1.13	C2DB	oblique	B-SOC	Γ	0.57	LCEBR	/	Unstable

c. nHSP

TABLE S100: Computationally exfoliable materials with valley type: oblique-nHSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
SnS	1	6.2.19	1.42	MC2D	oblique	nHSP	nHSP-SOC	0.36	LCEBR	Yes	Comp.Exfo
AgClO ₂	1	6.2.2	0.30	MC2D	oblique	nHSP	/	0.35	LCEBR	Yes	Comp.Exfo
ISbTe	2	6.2.148	0.72	MC2D	oblique	nHSP	Y	0.34	LCEBR	Yes	Comp.Exfo
AgBrO ₂	1	6.2.1	0.34	MC2D	oblique	nHSP	/	0.28	LCEBR	Yes	Comp.Exfo

TABLE S101: Computationally stable materials with valley type: oblique-nHSP.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
AsI	2	1.3.1	1.33	C2DB	oblique	Γ	nHSP	0.45	NLC	/	Stable
SnAsFS ₃	5	6.3.227	1.56	C2DB	oblique	/	nHSP	0.39	LCEBR	/	Stable
ZrPSe ₃	2	3.3.42	0.54	C2DB	oblique	nHSP	/	0.24	OAI	/	Stable

d. nHSP-SOC

TABLE S102: Computationally exfoliable materials with valley type: oblique-nHSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
---------	----	----	-----	----------	---------	------------	------------	-------------	----------	------	-----------

SnS	1	6.2.19	1.42	MC2D	oblique	nHSP	nHSP-SOC	0.37	LCEBR	Yes	Comp.Exfo
-----	---	--------	------	------	---------	------	----------	------	-------	-----	-----------

TABLE S103: Computationally stable materials with valley type: oblique-nHSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
AuHgITe	3	6.3.215	0.76	C2DB	oblique	nHSP-SOC	B-SOC	0.32	LCEBR	/	Stable
InTe ₂	1	6.3.77	0.55	C2DB	oblique	/	nHSP-SOC	0.30	LCEBR	Yes	Stable
PbFPS ₃	5	6.3.252	2.27	C2DB	oblique	/	nHSP-SOC	0.17	LCEBR	/	Stable

TABLE S104: Computationally unstable materials with valley type: oblique-nHSP-SOC.

Formula	LG	ID	Gap	Database	Lattice	VBM valley	CBM valley	Twist score	Topology	Bulk	Mat. type
BiCdBrTe	1	6.4.4	0.91	C2DB	oblique	nHSP-SOC	/	0.49	LCEBR	/	Unstable
BiPS ₃	5	6.4.27	1.30	C2DB	oblique	/	nHSP-SOC	0.34	LCEBR	/	Unstable
BiAsS ₃	5	6.4.23	1.55	C2DB	oblique	/	nHSP-SOC	0.31	LCEBR	/	Unstable
S ₃ Sb ₂	5	6.4.31	1.89	C2DB	oblique	/	nHSP-SOC	0.25	LCEBR	/	Unstable

Appendix VII: Band Structures of Twistable Materials

In the following two sections, we present the monolayer band structures of promising twistable semimetals and insulators. The materials included are selected based on the following criteria: (i) they are either experimentally reported in monolayer or few-layer form, computationally exfoliable, or computationally stable with corresponding bulk materials; (ii) a cutoff twist score of 0.25 is applied for semimetals, and 0.4 for insulators; and (iii) a maximum of 10 materials are included for each class.

The complete catalog of twistable materials, along with their detailed electronic properties, can be accessed at Topological 2D Materials Database.

VIII. BAND PLOTS OF TWISTABLE SEMIMETALS

A. Hexagonal lattice

1. Γ -SOC, computationally exfoliable

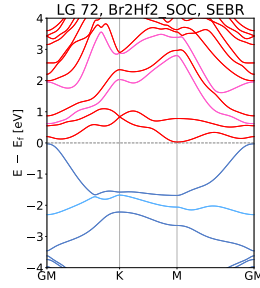


FIG. S1: 1.2.104

2. Γ -SOC, computationally stable

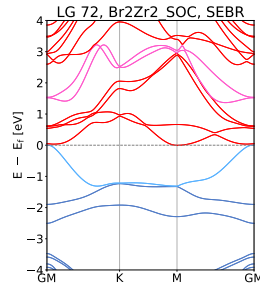


FIG. S2: 1.3.213

3. K , experimental

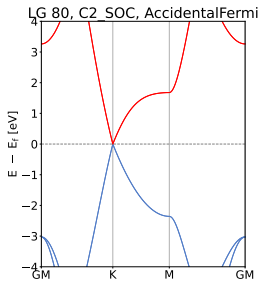


FIG. S3: 5.1.3

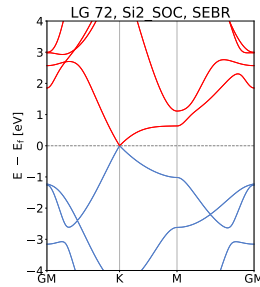


FIG. S4: 5.1.2

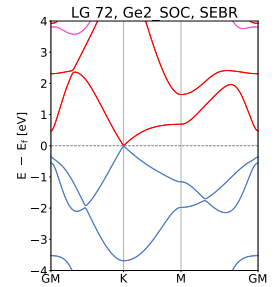


FIG. S5: 1.1.15

4. K -SOC, experimental

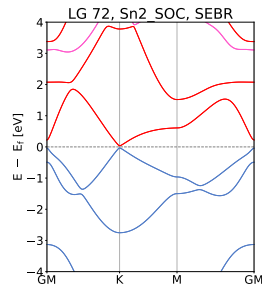


FIG. S6: 1.1.17

5. *K*-SOC, computationally exfoliable

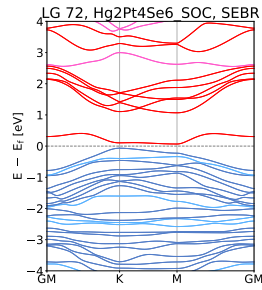


FIG. S7: 1.2.121

B. Square lattice

C. Rectangular lattice

1. *n*HSP, computationally exfoliable

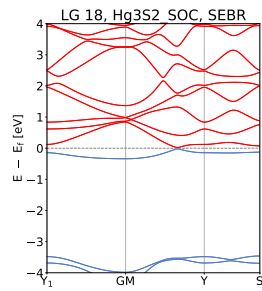


FIG. S8: 1.2.29

2. *n*HSP-SOC, experimental

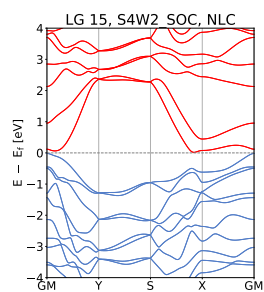


FIG. S9: 1.3.24

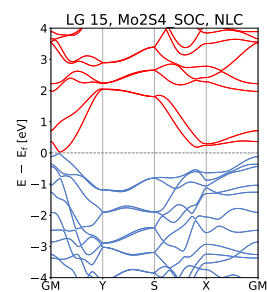


FIG. S10: 1.1.1

3. *nHSP-SOC, computationally exfoliable*

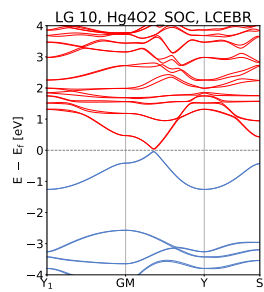


FIG. S11: 6.2.307

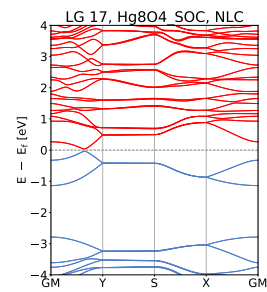


FIG. S12: 1.2.25

IX. BAND PLOTS OF TWISTABLE INSULATORS

A. Hexagonal lattice

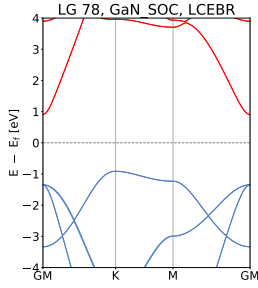
 1. Γ , experimental


FIG. S13: 6.1.78

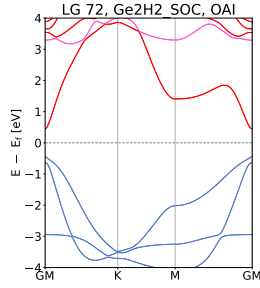


FIG. S14: 3.1.18

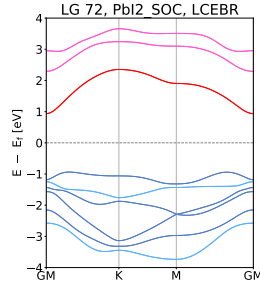


FIG. S15: 6.1.54

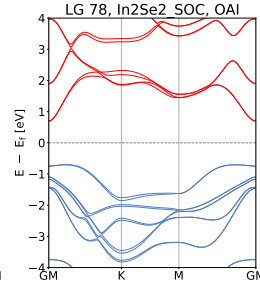


FIG. S16: 3.1.37

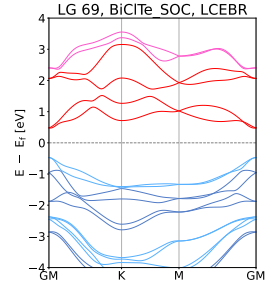


FIG. S17: 6.3.1963

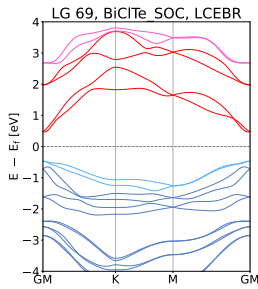


FIG. S18: 6.1.11

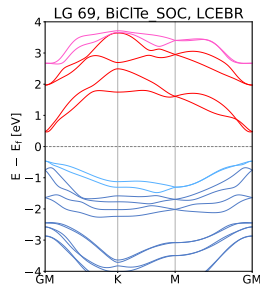


FIG. S19: 6.1.12

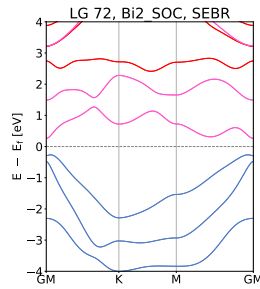


FIG. S20: 1.1.10

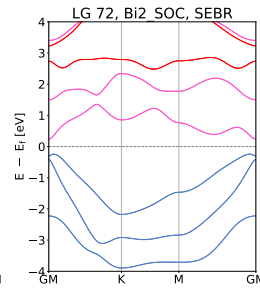


FIG. S21: 1.1.9

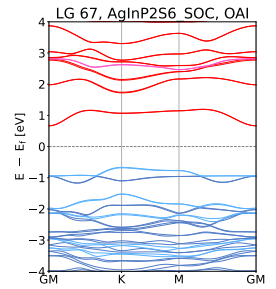


FIG. S22: 3.3.222

 2. Γ , computationally exfoliable

Band plots of twistable insulators

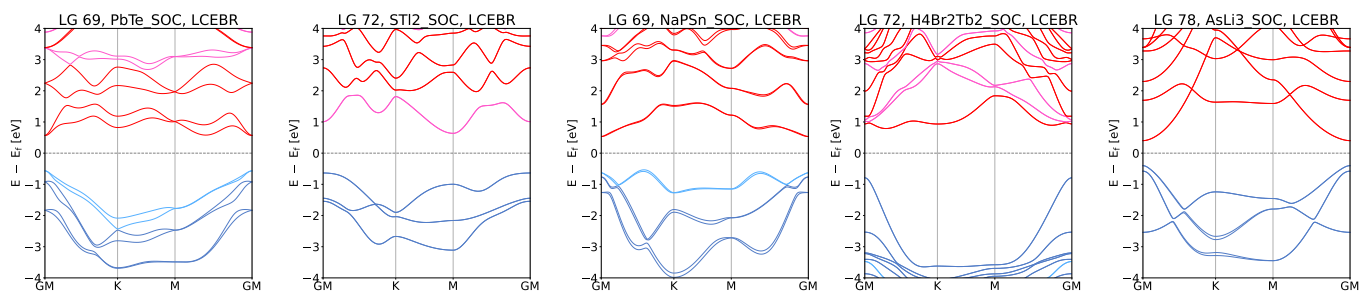


FIG. S23: 6.2.1129

FIG. S24: 6.2.1302

FIG. S25: 6.2.1128

FIG. S26: 6.2.1255

FIG. S27: 6.2.1312

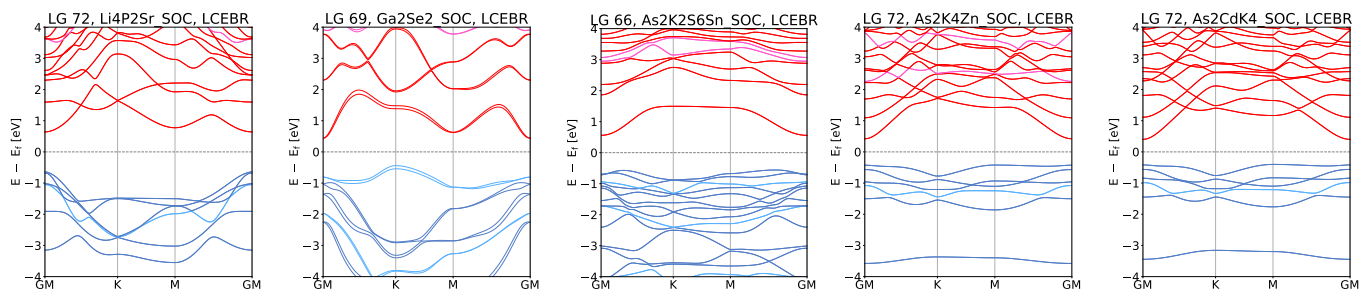


FIG. S28: 6.2.1277

FIG. S29: 6.2.1106

FIG. S30: 6.2.1064

FIG. S31: 6.2.1171

FIG. S32: 6.2.1168

3. Γ , computationally stable

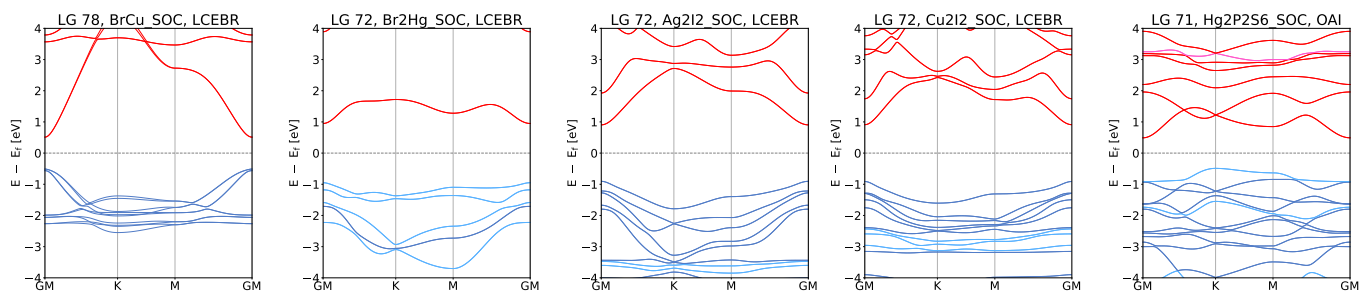


FIG. S33: 6.3.2619

FIG. S34: 6.3.2320

FIG. S35: 6.1.17

FIG. S36: 6.1.41

FIG. S37: 3.3.334

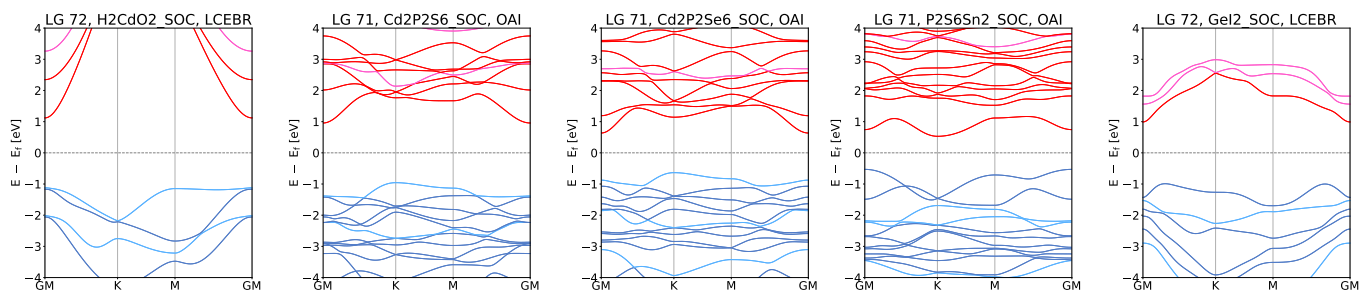


FIG. S38: 6.3.2466

FIG. S39: 3.3.314

FIG. S40: 3.3.315

FIG. S41: 3.3.356

FIG. S42: 6.3.2453

4. Γ -SOC, experimental

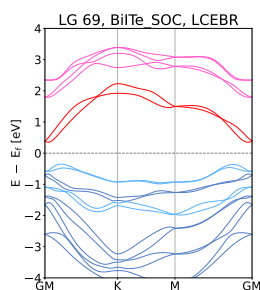


FIG. S43: 6.1.13

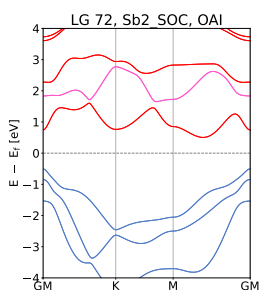


FIG. S44: 3.1.25

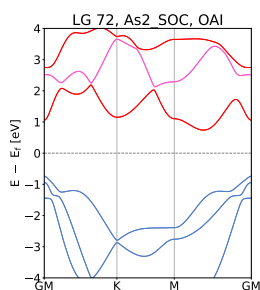


FIG. S45: 3.1.11

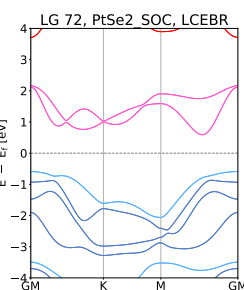


FIG. S46: 6.1.58

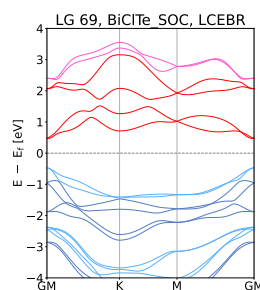


FIG. S47: 6.3.1963

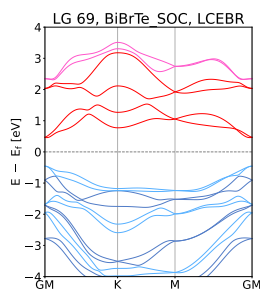


FIG. S48: 6.1.10

5. Γ -SOC, computationally exfoliable

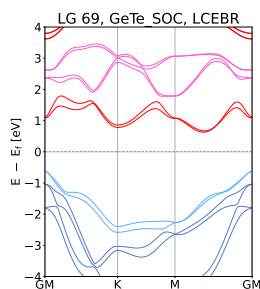


FIG. S49: 6.2.1108

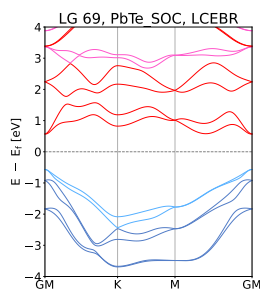


FIG. S50: 6.2.1129

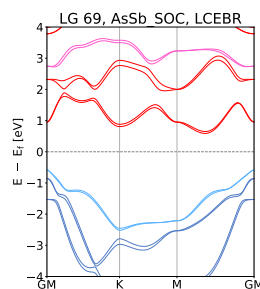


FIG. S51: 6.2.1090

6. Γ -SOC, computationally stable

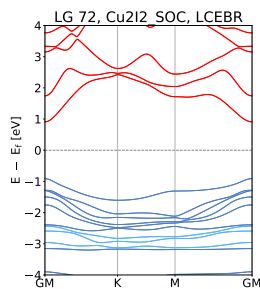


FIG. S52: 6.1.41

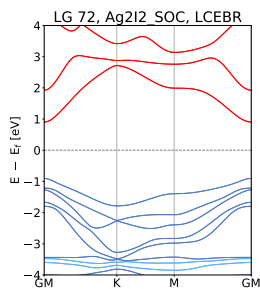


FIG. S53: 6.1.17

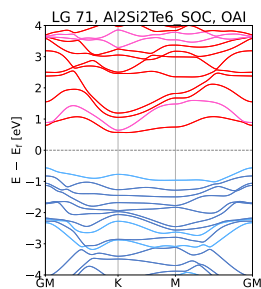


FIG. S54: 3.3.304

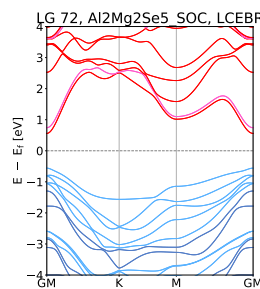


FIG. S55: 6.3.2266

7. K , experimental

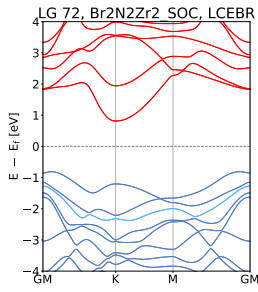


FIG. S56: 6.3.2323

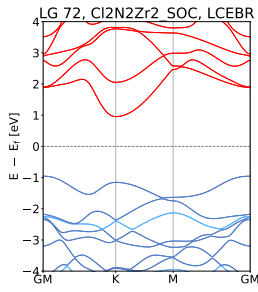


FIG. S57: 6.3.2408

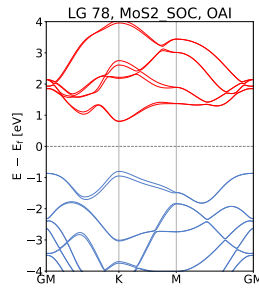


FIG. S58: 3.1.39

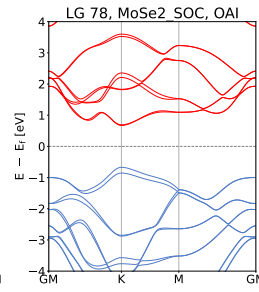


FIG. S59: 3.1.41

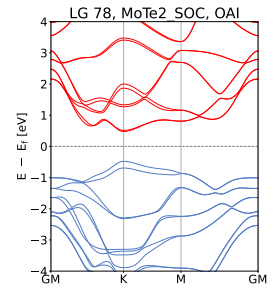


FIG. S60: 3.1.43

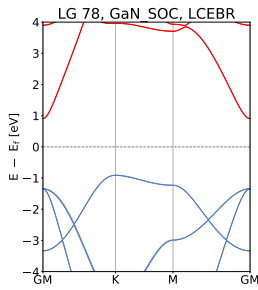


FIG. S61: 6.1.78

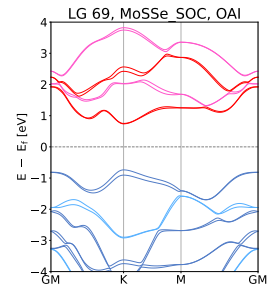


FIG. S62: 3.1.10

8. K , computationally exfoliable

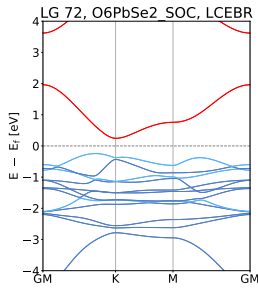


FIG. S63: 6.2.1287

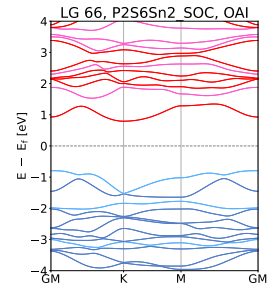


FIG. S64: 3.2.152

9. K , computationally stable

Band plots of twistable insulators

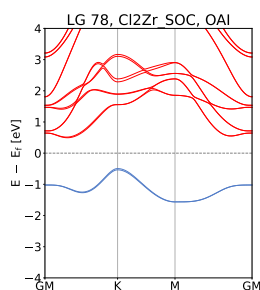


FIG. S65: 3.3.495

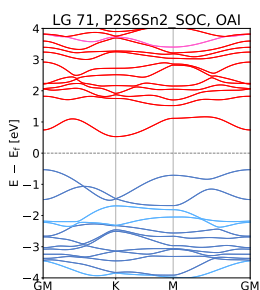


FIG. S66: 3.3.356

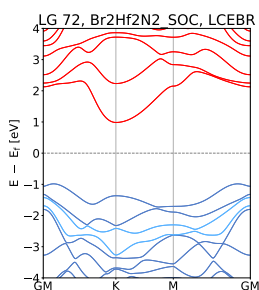


FIG. S67: 6.3.2318

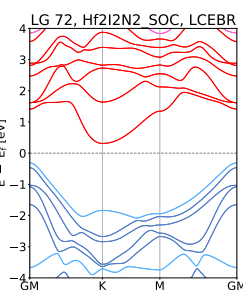


FIG. S68: 6.3.2492

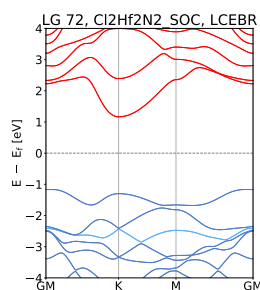


FIG. S69: 6.3.2403

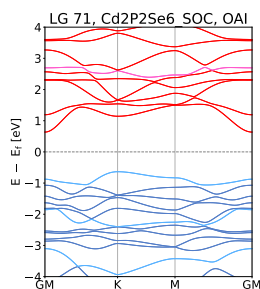


FIG. S70: 3.3.315

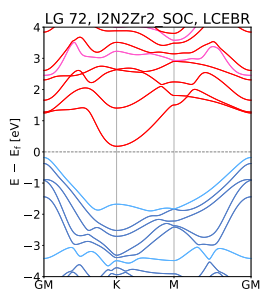


FIG. S71: 6.3.2502

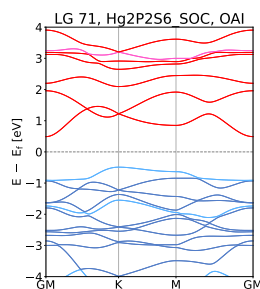


FIG. S72: 3.3.334

10. *K*-SOC, experimental

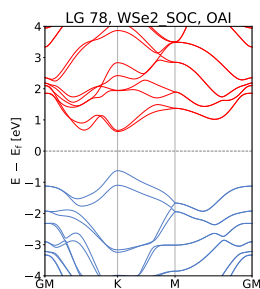


FIG. S73: 3.1.46

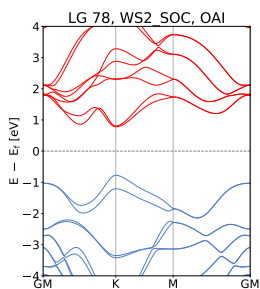


FIG. S74: 3.1.45

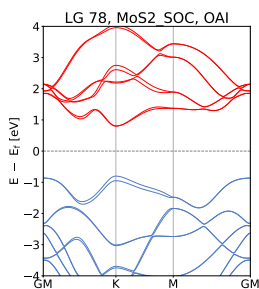


FIG. S75: 3.1.39

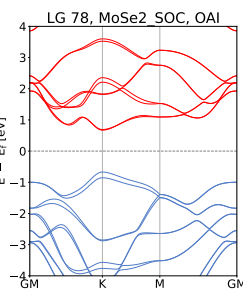


FIG. S76: 3.1.41

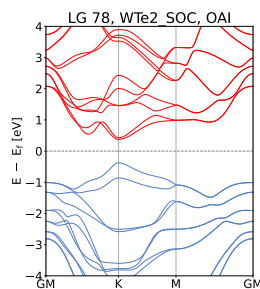


FIG. S77: 3.1.47

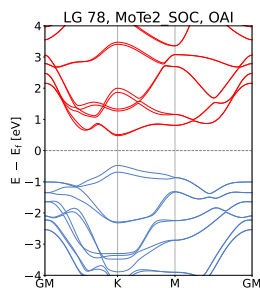


FIG. S78: 3.1.43

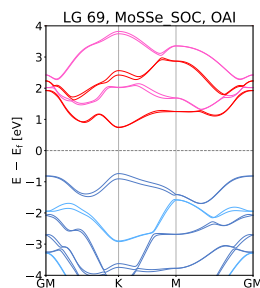


FIG. S79: 3.1.10

11. *K*-SOC, computationally exfoliable

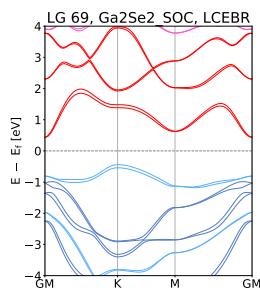


FIG. S80: 6.2.1106

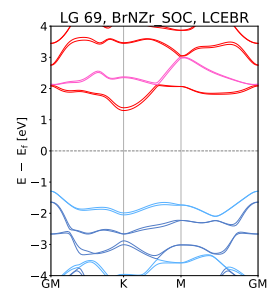


FIG. S81: 6.2.1099

12. *K*-SOC, computationally stable

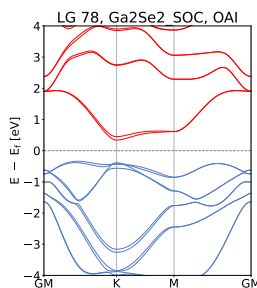


FIG. S82: 3.1.33

13. *M*, experimental

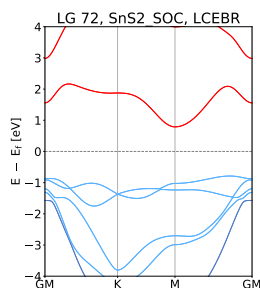


FIG. S83: 6.1.75

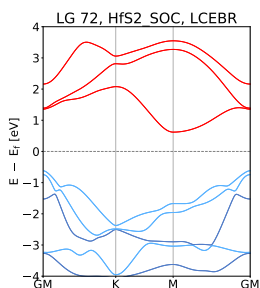


FIG. S84: 6.1.43

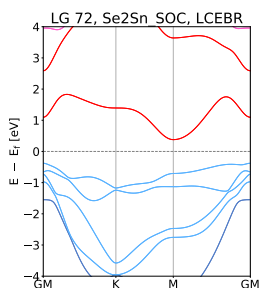


FIG. S85: 6.1.71

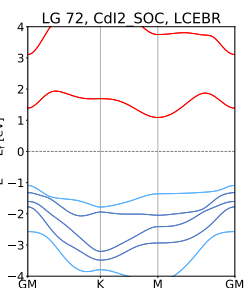


FIG. S86: 6.1.38

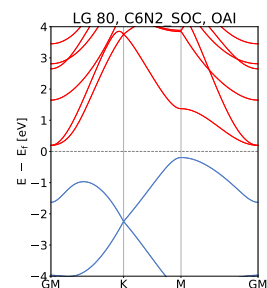


FIG. S87: 3.1.48

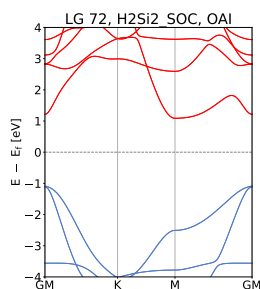


FIG. S88: 3.1.19

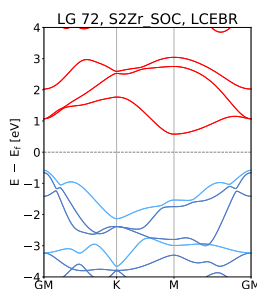


FIG. S89: 6.1.61

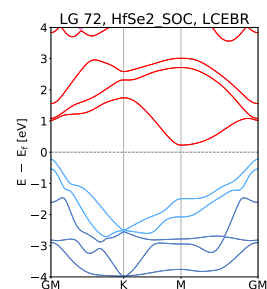


FIG. S90: 6.1.44

14. M , computationally exfoliable

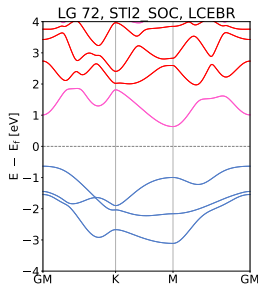


FIG. S91: 6.2.1302

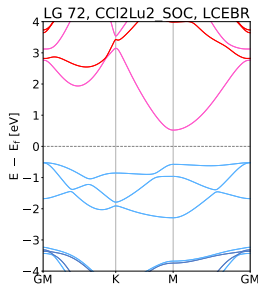


FIG. S92: 6.2.1199

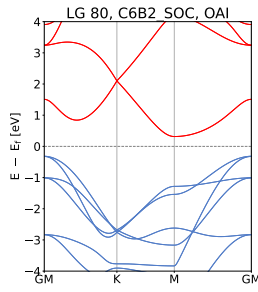


FIG. S93: 3.2.206

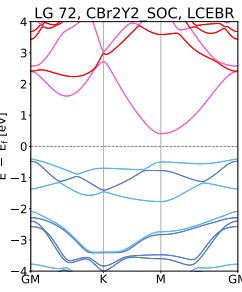


FIG. S94: 6.2.1198

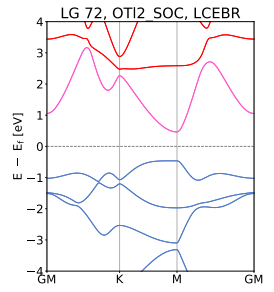


FIG. S95: 6.2.1288

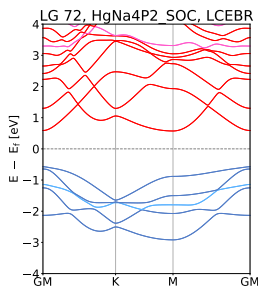


FIG. S96: 6.2.1261

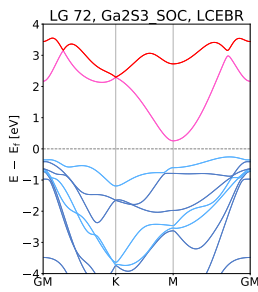


FIG. S97: 6.2.1237

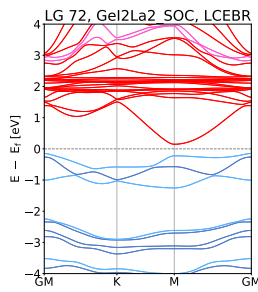


FIG. S98: 6.2.1240

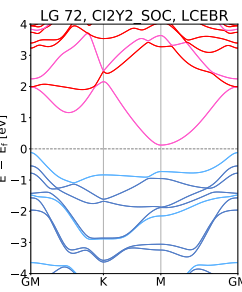


FIG. S99: 6.2.1201

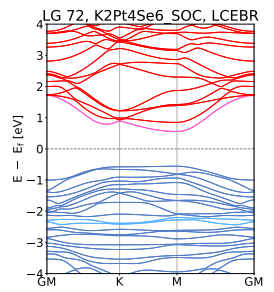


FIG. S100: 6.2.1276

15. M , computationally stable

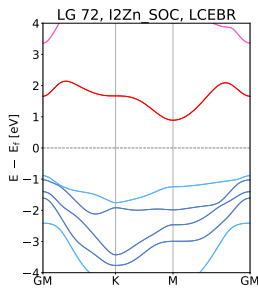


FIG. S101: 6.3.2510

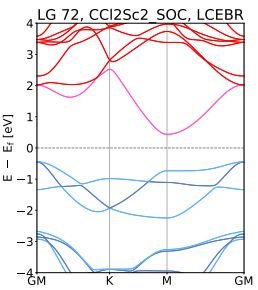


FIG. S102: 6.3.2355

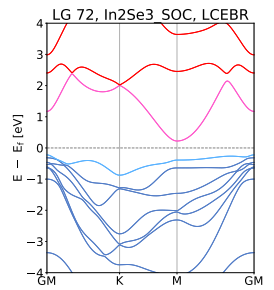


FIG. S103: 6.3.2527

16. M -SOC, experimental

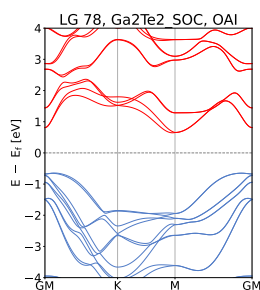


FIG. S104: 3.1.35

17. *nHSP, experimental*

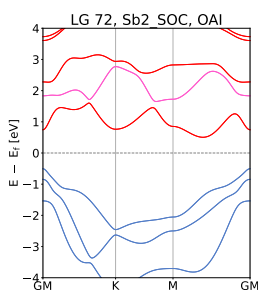


FIG. S105: 3.1.25

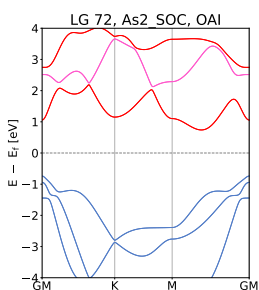


FIG. S106: 3.1.11

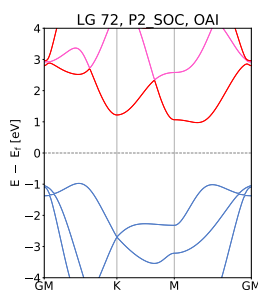


FIG. S107: 3.1.23

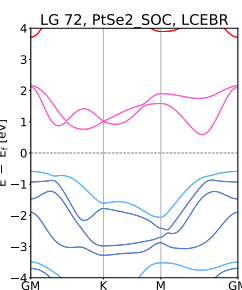


FIG. S108: 6.1.58

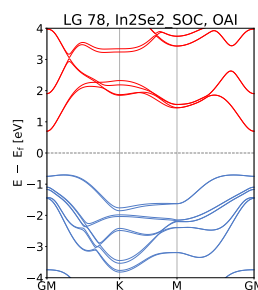


FIG. S109: 3.1.37

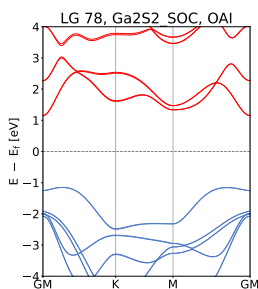


FIG. S110: 3.1.30

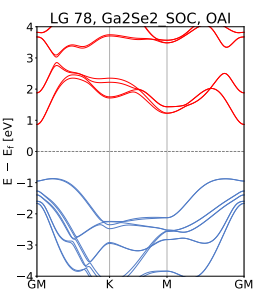


FIG. S111: 3.1.32

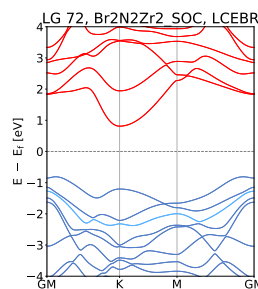


FIG. S112: 6.3.2323

18. *nHSP, computationally exfoliable*

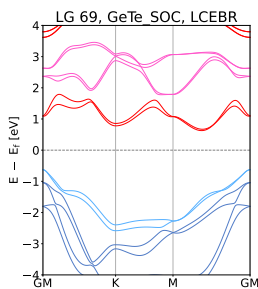


FIG. S113: 6.2.1108

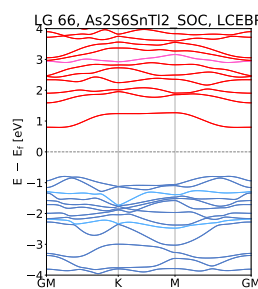


FIG. S114: 6.2.1065

19. *nHSP, computationally stable*

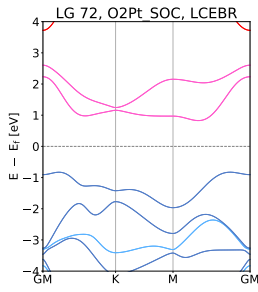


FIG. S115: [6.3.2546](#)

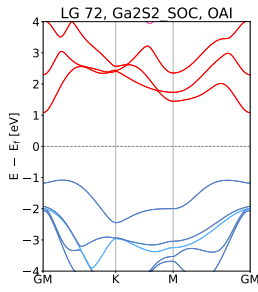


FIG. S116: [3.3.432](#)

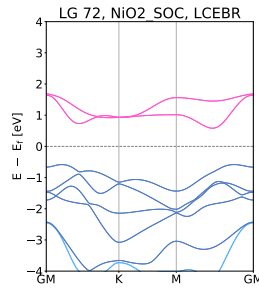


FIG. S117: [6.3.2540](#)

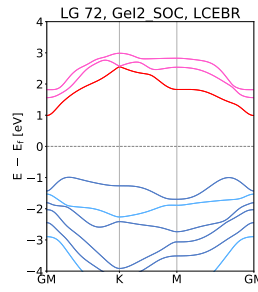


FIG. S118: [6.3.2453](#)

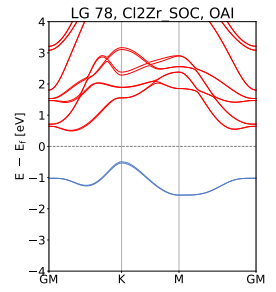


FIG. S119: [3.3.495](#)

20. *nHSP-SOC, computationally exfoliable*

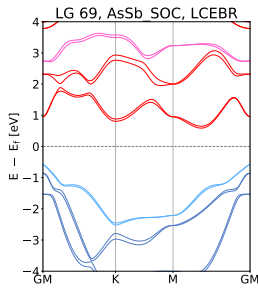


FIG. S120: [6.2.1090](#)

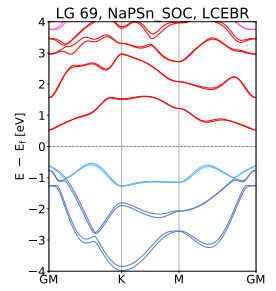


FIG. S121: [6.2.1128](#)

B. Square lattice

1. Γ , *computationally exfoliable*

Band plots of twistable insulators

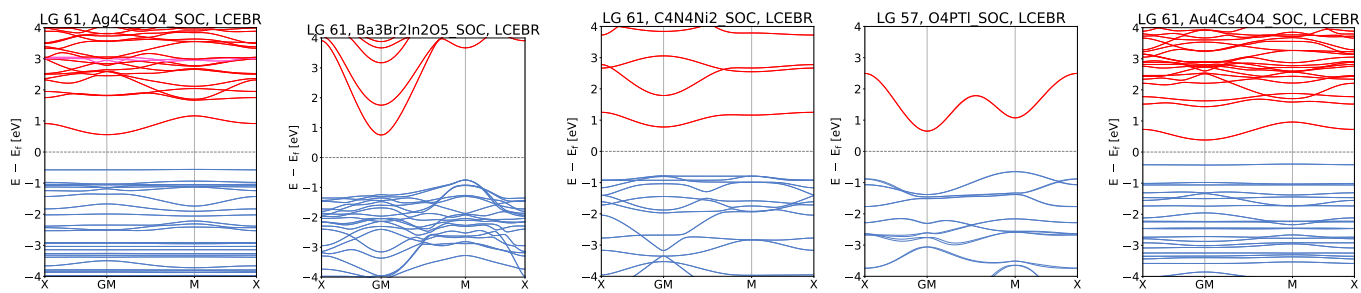


FIG. S122: 6.2.944

FIG. S123: 6.2.946

FIG. S124: 6.2.949

FIG. S125: 6.2.931

FIG. S126: 6.2.945

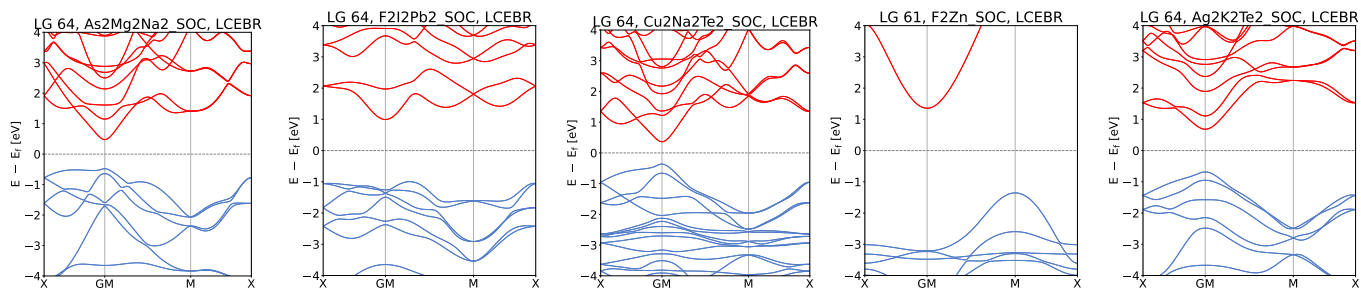


FIG. S127: 6.2.972

FIG. S128: 6.2.1017

FIG. S129: 6.2.1008

FIG. S130: 6.2.956

FIG. S131: 6.2.970

2. Γ , computationally stable

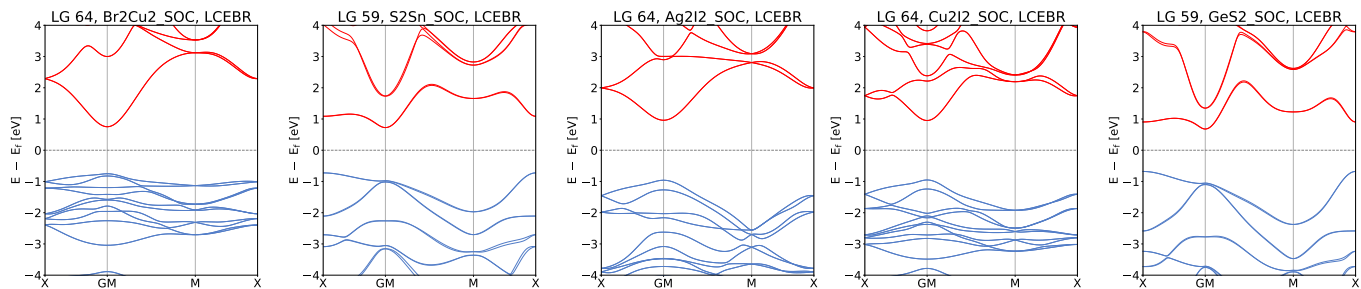


FIG. S132: 6.3.1738

FIG. S133: 6.3.1685

FIG. S134: 6.3.1724

FIG. S135: 6.3.1761

FIG. S136: 6.3.1660

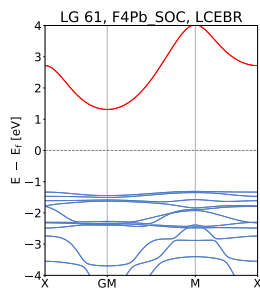


FIG. S137: 6.3.1699

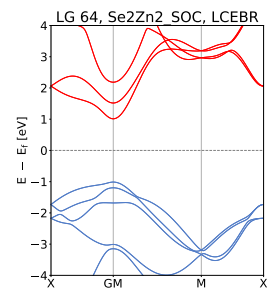


FIG. S138: 6.3.1812

3. Γ -SOC, computationally exfoliable

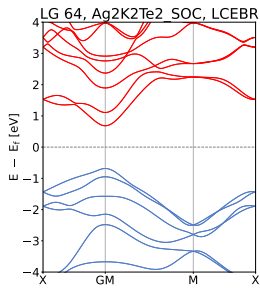


FIG. S139: 6.2.970

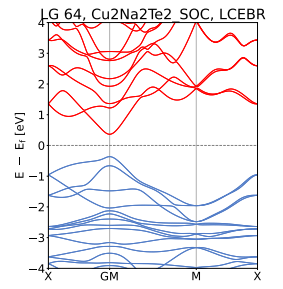


FIG. S140: 6.2.1008

4. Γ -SOC, computationally stable

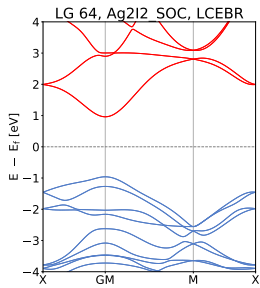


FIG. S141: 6.3.1724

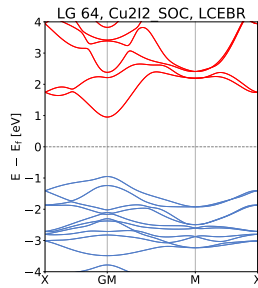


FIG. S142: 6.3.1761

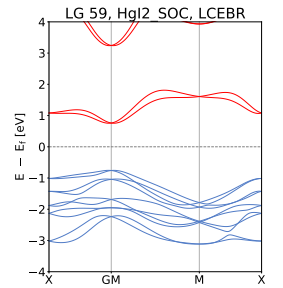


FIG. S143: 6.3.1669

5. M , computationally exfoliable

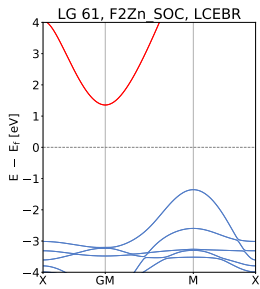


FIG. S144: 6.2.956

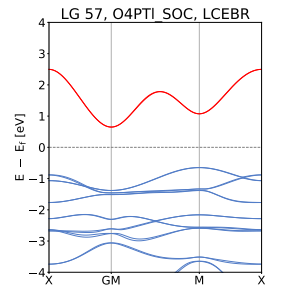


FIG. S145: 6.2.931

6. X , computationally stable

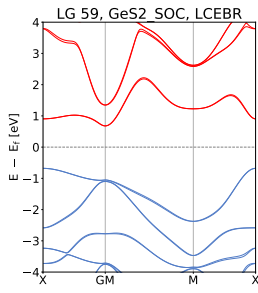


FIG. S146: 6.3.1660

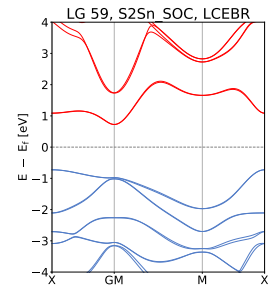


FIG. S147: 6.3.1685

7. *nHSP, computationally exfoliable*

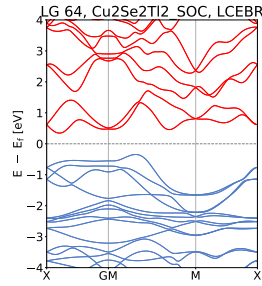


FIG. S148: 6.2.1010

8. *nHSP, computationally stable*

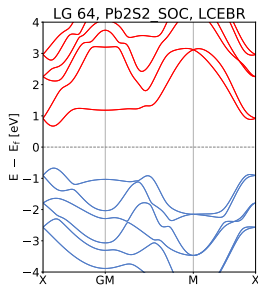


FIG. S149: 6.3.1807

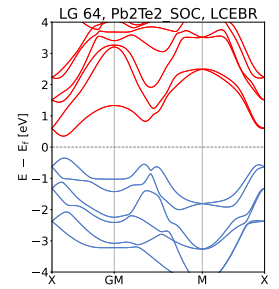


FIG. S150: 6.3.1809

C. Rectangular lattice

1. *HSP, experimental*

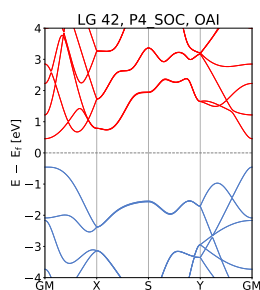


FIG. S151: 3.1.7

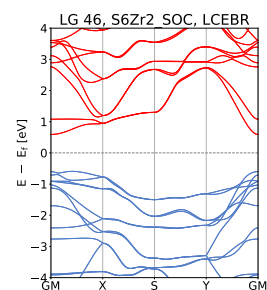


FIG. S152: 6.1.6

2. HSP, computationally exfoliable

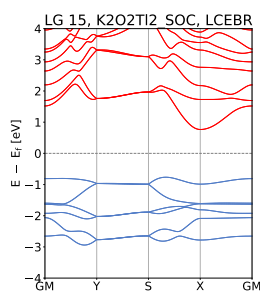


FIG. S153: 6.2.416

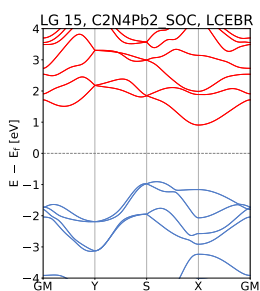


FIG. S154: 6.2.365

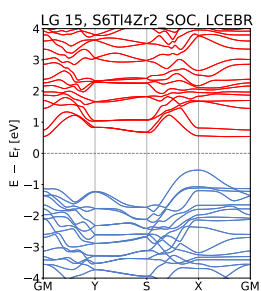


FIG. S155: 6.2.438

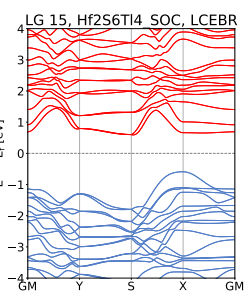


FIG. S156: 6.2.408

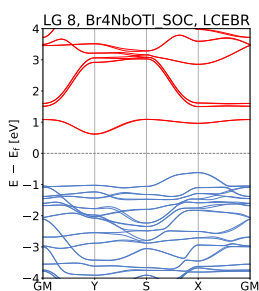


FIG. S157: 6.2.227

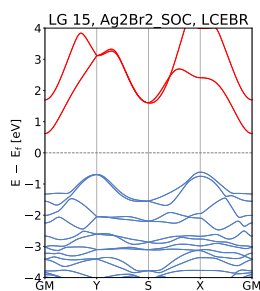


FIG. S158: 6.2.345

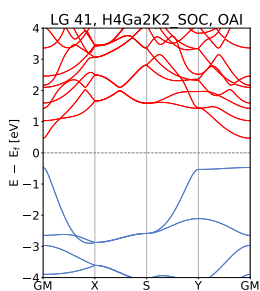


FIG. S159: 3.2.124

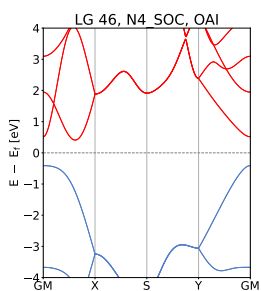


FIG. S160: 3.2.132

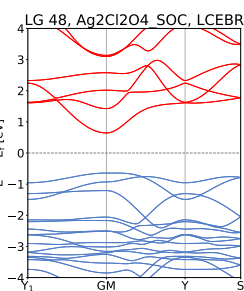


FIG. S161: 6.2.908

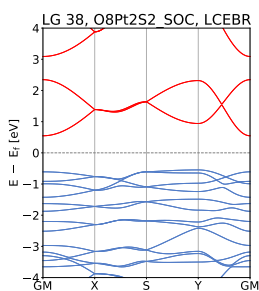


FIG. S162: 6.2.775

3. HSP, computationally stable

Band plots of twistable insulators

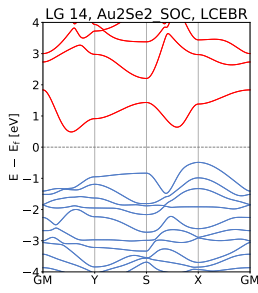


FIG. S163: 6.3.580

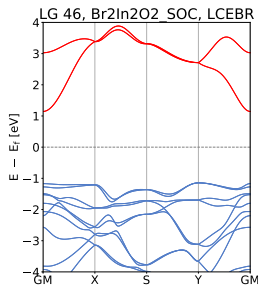


FIG. S164: 6.3.1439

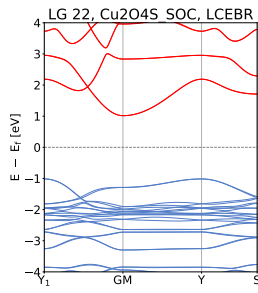


FIG. S165: 6.3.1057

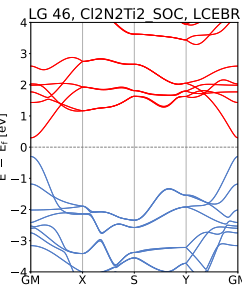


FIG. S166: 6.3.1488

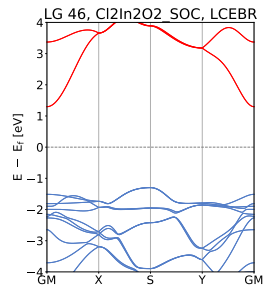


FIG. S167: 6.3.1478

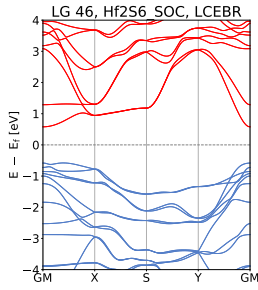


FIG. S168: 6.3.1543

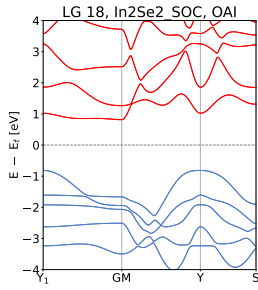


FIG. S169: 3.3.130

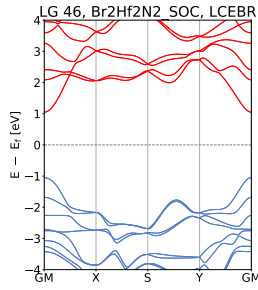


FIG. S170: 6.3.1438

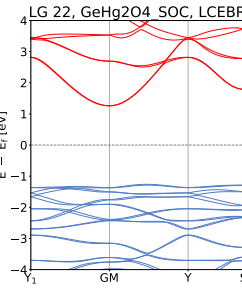


FIG. S171: 6.3.1058

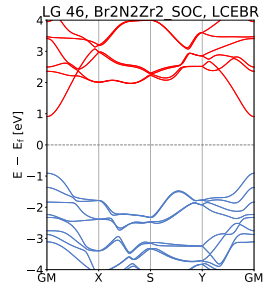


FIG. S172: 6.3.1450

4. *nHSP, experimental*

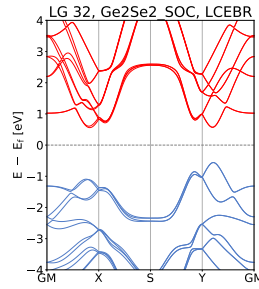


FIG. S173: 6.1.1

5. *nHSP, computationally exfoliable*

Band plots of twistable insulators

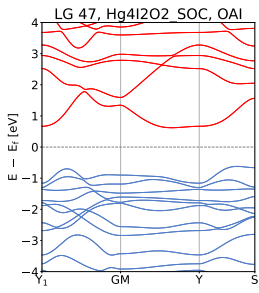


FIG. S174: [3.2.134](#)

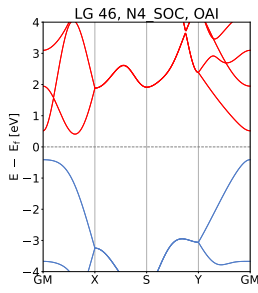


FIG. S175: [3.2.132](#)

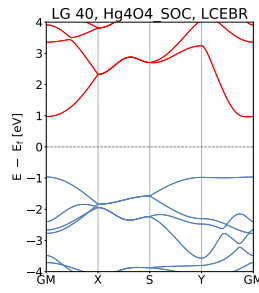


FIG. S176: [6.2.785](#)

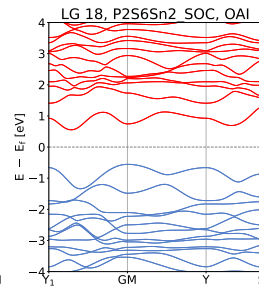


FIG. S177: [3.2.113](#)

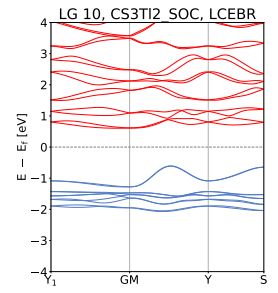


FIG. S178: [6.2.293](#)

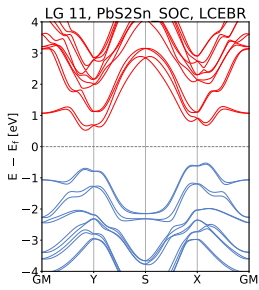


FIG. S179: [6.2.313](#)

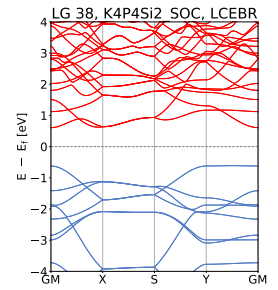


FIG. S180: [6.2.774](#)

6. *nHSP, computationally stable*

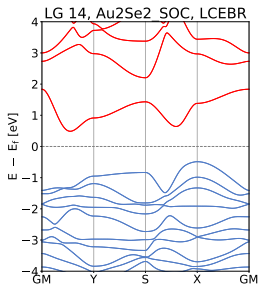


FIG. S181: [6.3.580](#)

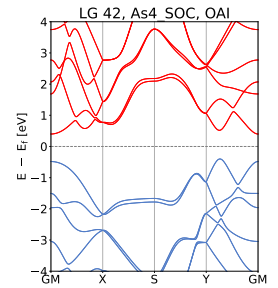


FIG. S182: [3.3.152](#)

7. *nHSP-SOC, experimental*

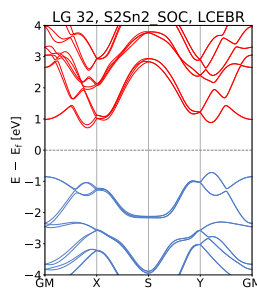


FIG. S183: [6.1.2](#)

8. *nHSP-SOC, computationally exfoliable*

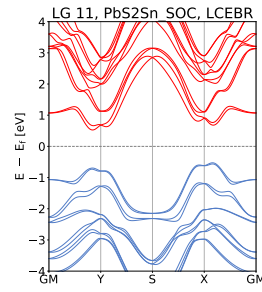


FIG. S184: 6.2.313

D. Oblique lattice

1. *HSP, computationally exfoliable*

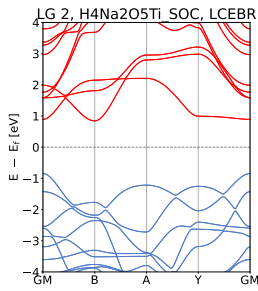


FIG. S185: 6.2.125

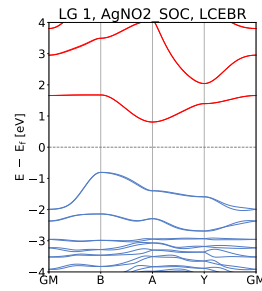


FIG. S186: 6.2.3

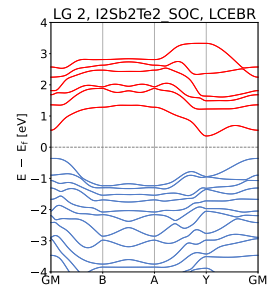


FIG. S187: 6.2.148

