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Symmetry classification of 2D materials: layer groups versus space groups

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Abstract

The symmetry of a crystal structure with a three-dimensional (3D) lattice can be classified by one of the 230 space group types. For some types of crystals, e.g. crystalline films, surfaces, or planar interfaces, it is more appropriate to assume a two-dimensional (2D) lattice. With this assumption the structure can be classified by one of the 80 layer group types. We have implemented an algorithm to determine the layer group type of a 3D structure with a 2D lattice, and applied it to more than 15 000 monolayer structures in the Computational 2D Materials Database (C2DB). We compare the classification of monolayers by layer groups and space groups, respectively. The latter is defined as the space group of the 3D bulk structure obtained by repeating the monolayer periodically in the direction perpendicular to the 2D lattice (AA-stacking). By this correspondence, nine pairs of layer group types are mapped to the same space group type due to the inability of the space group to distinguish the in-plane and out-of-plane axes. In total 18% of the monolayers in the C2DB belong to one of these layer group pairs and are thus not properly classified by the space group type. Our results show that symmetry classification of 2D materials should be based on layer groups rather than the commonly used space groups.

1. Introduction

The classification of periodic solids by means of symmetry groups is fundamental to our understanding and description of crystalline materials. In addition to providing a unique classification scheme for crystal structures, the symmetry group can be used to derive important qualitative information about the physical properties of a material before they are measured or calculated. For example, the symmetry group dictates the possible degrees of degeneracy of energy levels, governs the selection rules for electronic and vibronic transitions [1], determines the possible topological phases [2], and relates different spatial components of response tensors of crystals [3].

The symmetry of a three-dimensional (3D) crystal structure with 3D translation periodicity, i.e. a 3D lattice, is described by one of the 230 space group

types (from hereon we shall for simplicity use the more common term 'space group' in place of 'space group type', see appendix A.4). For a 3D crystal structure with a two-dimensional (2D) lattice, for example a crystalline film, the relevant symmetry group is represented by the layer group. There exist a total of 80 layer groups in contrast to the 230 space groups. For the point group operations of the layer group, the symmetry axis of the operations must be either parallel or perpendicular to the 2D lattice plane. Moreover, the direction of the translation part of the symmetry operations must be parallel to the lattice plane.

Materials with a 2D lattice and a thickness of only a few atoms are generally referred to as 2D materials. This class of materials has attracted enormous attention from a broad range of scientific communities due to their unique and easily tunable properties, their extreme thinness, and their good device

integration potential [4–8]. Despite of this interest, the symmetry characterization of 2D materials has not received the attention it deserves, and is often restricted to specification of the point group or the space group of some related layered bulk structures. This holds in particular for all the computational databases of 2D materials, e.g. the Computational 2D Materials Database (C2DB) [9, 10], the Materials Cloud [11], and the 2DMatPedia [12], which hold the atomic structures of thousands of monolayers. Similar to the vast majority of studies on 2D materials, these databases have classified the monolayers by the space group of the bulk structure obtained by repeating the monolayer periodically in the direction normal to the 2D lattice plane, i.e. the space group of the AA-stacked bulk crystal. An important reason for this state of affairs has been the lack of a readily accessible software tool to determine the layer group of a general 2D atomic structure.

Here we report on a numerical algorithm to determine the layer group of a 3D crystal structure with a 2D lattice. The algorithm has been implemented and made available as part of the open source space group and magnetic space group symmetry analysis library *Spglib* [13, 14], which is widely used in the computational materials science community. We use the algorithm to obtain the layer groups of the 15 733 crystal structures currently contained in the C2DB database. A statistical analysis of the data reveals a rather inhomogeneous distribution with a number of layer group types being either very scarcely represented or not represented at all. We also show that the classification of a monolayer by the space group of its AA-stacked bulk structure is incomplete. In fact, for 18% of the monolayers in C2DB, the space group of the AA-stacked bulk crystal does not uniquely determine the layer group.

2. Method

In this paper, we use *layer system* to refer to the collection of a layer group crystallographic coordinate system and the atomic structure defined in this coordinate system. Following [13, 15], **a**, **b** and **c** represent basis vectors of the system, with two of the basis vectors being lattice vectors. Without loss of generality, we take the lattice vectors to be **a** and **b**. Furthermore, we denote the basis vectors in different unit cells by (**a**_i, **b**_i, **c**_i), (**a**_p, **b**_p, **c**_p), and (**a**_c, **b**_c, **c**_c), where the subscripts refer to the input cell, primitive cell, and conventional cell, respectively. Atom coordinates in the unit cell basis, i.e. fractional coordinates, are denoted by **x**. When necessary, the subscript i, p or c is used to indicate the type of unit cell. For layer groups, the role of **c** is only to provide a basis vector for representing the atomic positions. Nevertheless, the current implementation follows the crystallographic space group convention which requires the rotation part of symmetry transformations to be represented

by integer matrices under the primitive cell basis (see section 2.2). Hence the choice of **c**-basis can affect the point group and thus layer group. In this paper, we fix the non-lattice vector **c**_i to be orthogonal to **a**_i and **b**_i to obtain the highest symmetry.

For crystals with periodicity along the three basis axes, the distance between two atoms with positions **x** and **x'** respectively is defined by

$$d(\mathbf{x}, \mathbf{x}') = \|(\mathbf{a}, \mathbf{b}, \mathbf{c})(\Delta\mathbf{x} - \lfloor \Delta\mathbf{x} \rfloor)\|. \quad (1)$$

Here (**a**, **b**, **c**) denotes the coordinate matrix of the unit cell basis vectors, $\Delta\mathbf{x} = \mathbf{x} - \mathbf{x}'$, and $\lfloor \cdot \rfloor$ rounds components of a vector to the nearest integer. Layer systems do not have periodicity in the direction along the non-lattice vector **c**, and the rounding operation in equation (1) is not applied to this coordinate. To account for small distortions or numerical noise, *Spglib* determines the equality of two atom positions by the condition

$$d(\mathbf{x}, \mathbf{x}') < \epsilon, \quad (2)$$

where ϵ is a small tolerance parameter (called ‘sym-prec’) set by the user.

A symmetry operation maps the crystal structure onto itself. The operation is denoted (**W**, **w**), where the linear part **W** is a 3×3 integer matrix, and the translation part **w** is a 3×1 column vector. By the symmetry operation, an atom with position **x** will be sent to

$$\tilde{\mathbf{x}} = \mathbf{W}\mathbf{x} + \mathbf{w}. \quad (3)$$

Symmetry requires the position **x'** of one and only one atom with the same species to be equal to $\tilde{\mathbf{x}}$ in the sense of equation (2).

Our algorithm for determining the layer group of a layer system is illustrated in figure 1. The algorithm follows the one already implemented in *Spglib* for space groups and documented elsewhere [13]; thus we mainly focus on the aspects that are specific to layer groups. The lower part of figure 1 shows the main steps required to determine the layer/space group while the upper part details the criteria used to select the conventional unit cell for the various crystal systems. In addition to determining the point group and space/layer group, the algorithm also determines the site symmetry group for each atom and the occupied Wyckoff positions, and symmetrizes the input structure.

2.1. Primitive cell

The input cell will be transformed to a provisional primitive cell to reduce the computational complexity. To determine the primitive cell, the first step is to check whether the input cell can be reduced to a smaller unit that generates the crystal. Specifically, the algorithm searches for symmetry operations that are pure translations, i.e. $\mathbf{W}_i = \mathbf{I}$ and $\mathbf{w}_i \neq 0$. The three

3D Crystal system	Triclinic	Monoclinic		Orthorhombic	Tetragonal	Trigonal	Hexagonal	Cubic
Bulk crystal	Niggli cell	b : ± 2 -fold axis $a = \gamma = 90^\circ$ a, c : Delaunay basis		a, b, c : ± 2 -fold axis $a = \beta = \gamma = 90^\circ$ $n_1 = 2: a \leq b$ Bulk only: $n_1 = 3: a \leq b, a \leq c$ $n_1 = 6: a \leq b \leq c$	c : ± 4 -fold axis $a = \beta = \gamma = 90^\circ$ $a = b$	c : ± 3 -fold axis $a = \beta = 90^\circ$ $\gamma = 120^\circ$ $a = b$	Same as trigonal	a, b, c : $\pm N$ -fold axis $N = 2 \text{ or } 4$ $a = \beta = \gamma = 90^\circ$ $a = b = c$
Layer system Non-lattice vector c	(Rotated) Niggli cell	c : ± 2 -fold axis $a = \beta = 90^\circ$ a, b : Delaunay basis	a : ± 2 -fold axis $\beta = \gamma = 90^\circ$ b, c : (partially) Delaunay reduced					X
2D Bravais system	Oblique		Rectangular		Square	Hexagonal		

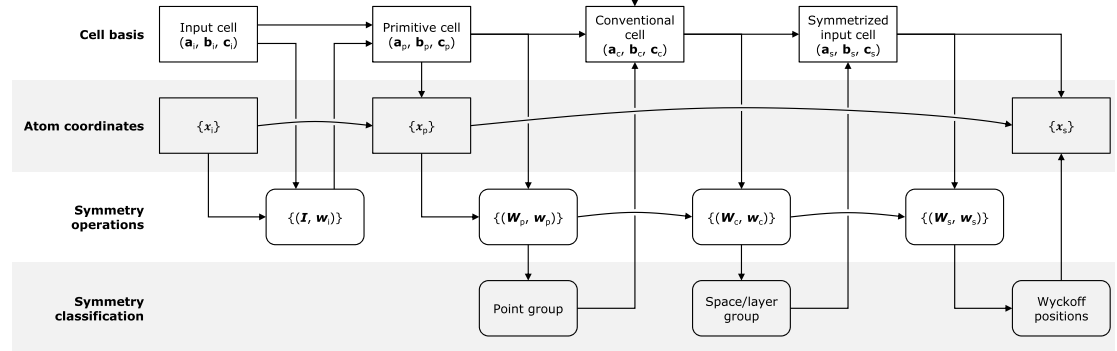


Figure 1. Upper: the criteria (rotation axes and metric conditions) used by `Spglib` to determine a standardized conventional cell of a bulk crystal (3D lattice) and a layer system (2D lattice). The criteria are listed for each of the seven crystal systems. The layer system can be additionally classified by the Bravais system of its lattice, which is listed in the last row of the table. For triclinic and monoclinic crystal systems, the criteria specific to bulk and layer systems are listed in the second and third rows, respectively. Monoclinic crystal systems with oblique and rectangular lattices have different criteria, and are separately listed with different colors. For orthorhombic systems, the bulk and layer systems share most of the conditions. For the tetragonal, trigonal and hexagonal crystal systems, the bulk and layer systems share all the same criteria, and the rows for these systems are combined. The cubic crystal system does not exist for layer groups, and is left blank in the table. The criteria include axis choices for selecting $\mathbf{a}_c$, $\mathbf{b}_c$ and $\mathbf{c}_c$ from the symmetry operation with certain types, and metric parameters. The remaining conditions are additional metric rules used by `Spglib` when the standard choices defined in [15, 18] cannot uniquely determine the shape and/or setting of the conventional cells. Details of the rules are described in appendix C. Lower: workflow used by the algorithm to determine the point group, space/layer group, Wyckoff positions, and more.

vectors among the found $\mathbf{w}$ s and the input cell basis $\mathbf{a}_i$, $\mathbf{b}_i$ and $\mathbf{c}_i$ which form the cell with smallest non-zero volume are the primitive cell basis vectors. For layer systems, the non-lattice vector $\mathbf{c}_i$ will always be chosen as the primitive basis vector $\mathbf{c}_p$. The obtained primitive cell will further be transformed to the Delaunay cell [16]. The shape of the Delaunay primitive cell belongs to one of the 24 symmetric varieties [16, 17]. Matrix elements of the linear part $\mathbf{W}_p$ are 0, 1 or -1 under the Delaunay reduced basis. Note that this procedure may not be fully applicable to a layer system as it can transform the lattice vectors into linear combinations of the original lattice and non-lattice vectors. Thus the Delaunay reduction requires special care for layer systems as discussed in detail in appendix B.

2.2. Symmetry operations

After obtaining the primitive cell, the algorithm searches for the matrix-column pairs $(\mathbf{W}_p, \mathbf{w}_p)$ of all symmetry operations in the Delaunay reduced primitive cell basis $(\mathbf{a}_p, \mathbf{b}_p, \mathbf{c}_p)$. For space group operations, $\mathbf{W}_p$ consists of 0 and ± 1 satisfying $\det(\mathbf{W}_p) = \pm 1$. For layer groups, preservation of the 2D lattice prohibits mixing the non-periodic component into the lattice vectors, e.g. $\mathbf{a}' = \mathbf{a} + \mathbf{c}$. For layer systems, 'A'-face, 'B'-face, body-, and face centered conventional cells do not exist. Consequently, these conventional cells are

not considered. the algorithm searches for operations with the matrix pattern

$$\mathbf{W}_{\text{layer}} = \begin{pmatrix} W_{11} & W_{12} & 0 \\ W_{21} & W_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix} \quad W_{ij} = 0, \pm 1. \quad (4)$$

With this matrix pattern, any operation with rotation order higher than two must have the rotation axis perpendicular to the lattice plane. Consequently, point groups belonging to the cubic crystal system are not allowed for layer systems. In addition, any ± 2 -fold rotations must have the rotation axis either parallel or perpendicular to the lattice plane. Furthermore, equation (1) rules out the possibility of finding screw rotation or glide reflection with a non-lattice component in the translation part $\mathbf{w}$. To find the symmetry operations of a layer system, the algorithm searches for all transformations $(\mathbf{W}, \mathbf{w})$ with $\mathbf{W}$ of the form (4) satisfying $d(\tilde{\mathbf{x}}, \mathbf{x}') < \epsilon$, where $d(\cdot, \cdot)$ is defined in equation (1), $\tilde{\mathbf{x}} = \mathbf{W}\mathbf{x} + \mathbf{w}$, and $\mathbf{x}$ and $\mathbf{x}'$ are the position of atoms of the same type.

2.3. Point group

The linear part $\mathbf{W}$ of all found symmetry operations $(\mathbf{W}, \mathbf{w})$ compose the crystallographic point group $\mathcal{P}$ in the primitive cell basis. The type of the point group is determined by counting the number of the

ten different rotation orders ($\pm 1, \pm 2, \pm 3, \pm 4, \pm 6$) appearing in $\mathcal{P}$ (see table V in [13]). Once the point group type has been determined, the search for the space/layer group can be narrowed down accordingly.

2.4. Standardized conventional cell

To determine the space/layer group type from the symmetry operations they must be compared with those already stored in `Spglib`. However, a direct comparison requires that the same crystallographic coordinate systems (CCSs), i.e. origin position and basis vectors (including their order), are employed. For each space group, reference [18] lists the possible conventional CCSs and designates one of them as the standard choice. A standard CCS for layer systems is defined by [15].

`Spglib` adopts Hall symbols [19] to distinguish the different choices of CCS. A table of all the Hall symbols for space groups can be found in table A1.4.2.7 of [20]. `Spglib` contains a database with all $(\mathbf{W}, \mathbf{w})$ matrix-column pairs generated using Hall symbols. For layer groups, we are not aware of a complete table of Hall symbols. Thus we have produced one corresponding to the different choices of CCSs listed in [15], see appendix D.

2.5. Layer group

The crystallographic point group determines the type of the Bravais lattice and puts some constraints on the metric parameters of the conventional cell (relations between basis vector lengths and angles), see upper panel of figure 1 and appendix C. Generally, one of the basis vectors $\mathbf{a}_c$, $\mathbf{b}_c$ and $\mathbf{c}_c$ is chosen as the symmetry axes of a specific symmetry operation, as shown in the first line for each criteria in figure 1. The shortest two vectors in the perpendicular plane that satisfy the metric conditions are chosen for the remaining two basis vectors. The $\mathbf{W}$ matrices will retain integer elements under this basis.

When the basis vector choices are the same as the standard CCS of the relevant space/layer group, $\mathbf{W}$ will match the standard counterparts stored in `Spglib`. Still, $\mathbf{w}$ may differ from the stored ones by a shift of the origin. The origin shift is determined following the algorithm in [13, 21] except the distances in the algorithm are measured by equation (1).

2.6. Symmetrization

The site symmetry group of each atom is determined using the distance measure in equations (1) and (2). Each atom is further assigned a Wyckoff position. Finally, the atomic structure is symmetrized by applying all of the site symmetry operations separately to each atom and performing an average over the resulting positions. The standardized conventional cell is

symmetrized such as to satisfy the lattice metric conditions in figure 1(upper) exactly to obtain the symmetrized input cell $(\mathbf{a}_s, \mathbf{b}_s, \mathbf{c}_s)$ and the standard primitive cell. For the standard conventional cells with primitive lattice, the standard primitive cells are the conventional cells. While for 'C'-face centered standard conventional cells, the standard primitive cell $(\mathbf{a}_{sp}, \mathbf{b}_{sp}, \mathbf{c}_{sp}) = (\mathbf{a}_{sc}, \mathbf{b}_{sc}, \mathbf{c}_{sc})\mathbf{P}_C$, where

$$\mathbf{P}_C = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (5)$$

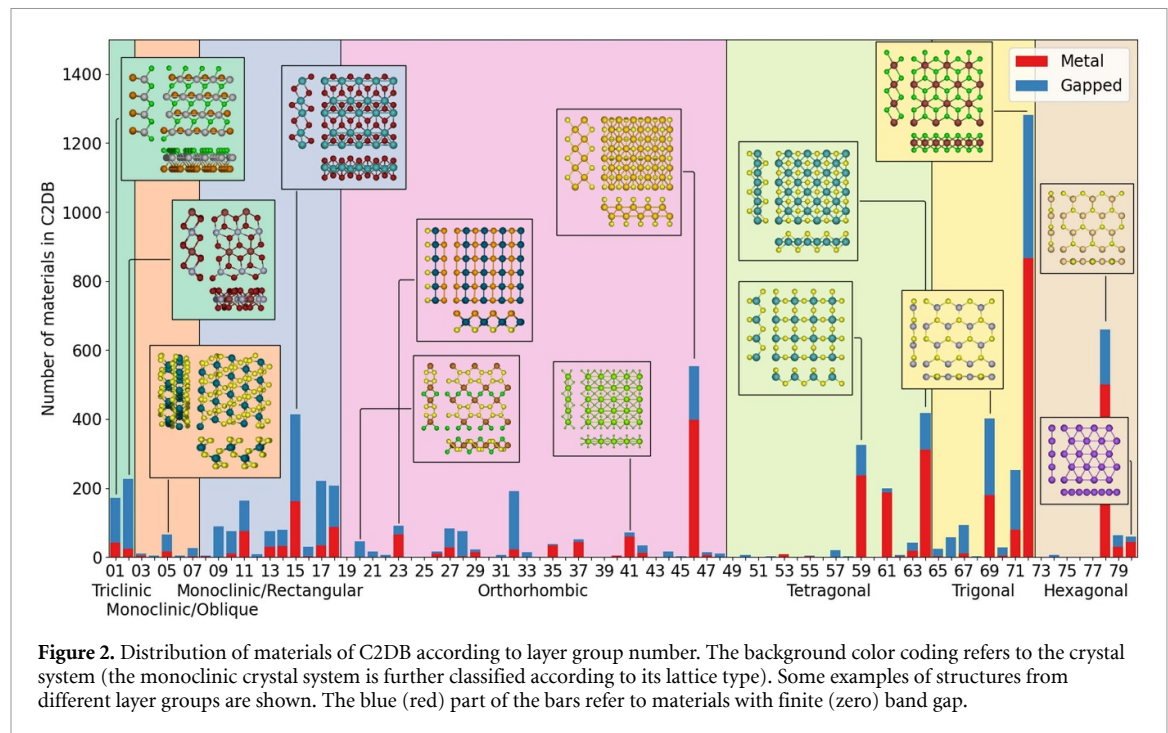
3. Results

The C2DB currently contains 15 735 2D materials. Most of the structures have been generated by computational exfoliation of experimentally known layered bulk crystals followed by systematic lattice decoration (atomic substitution) of the thus obtained monolayers [9, 10]. Recently, the data set was amended by monolayers created by a deep generative model [22]. All the monolayers in C2DB have been relaxed using density functional theory with the Perdew Burke Ernzerhof (PBE) exchange-correlation functional [23].

We have determined the layer group of all the monolayers in C2DB alongside the space group of the corresponding AA-stacked bulk structures (see next section). Figure 2 shows the distribution of the C2DB monolayers according to the layer group. The distribution shown has been limited to the subset of monolayers for which the band gap has been calculated (7201 materials), and the materials have been divided into metallic and non-metallic compounds. The background color is used to indicate the different crystal systems (along with Bravais system if necessary). Examples of crystal structures from selected layer groups are shown.

The most frequently occurring layer group is number 72 ($p\bar{3}m1$) with 1231 occurrences. It should be noted, that the distribution of materials by layer group number is highly non-uniform, with several completely empty bins accompanied by several with just a few materials. In particular, there are no materials in C2DB with layer group numbers 19, 24, 25, 30, 38, 39, 43, 49, 54, 56, 60, 73, 75, 76 and 77 (using a tolerance parameter 'symprec' = 0.1 Å).

There is a tendency that insulating behavior (blue bars) is more pronounced among the materials with lower layer group numbers while metallic behavior (red bars) is dominant in materials with high layer group numbers. This is due to the fact that, as a rough rule, layer groups with smaller numbers contain fewer symmetry transformations. The less symmetric crystals will have energy bands of lower degeneracy and



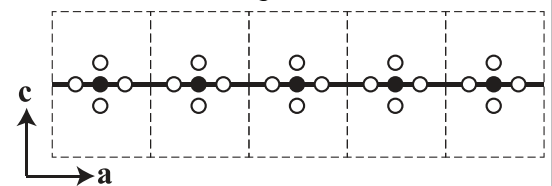
therefore a higher chance of all bands being either fully occupied or empty. On the other hand, more symmetric crystals will have energy bands of higher degeneracy and consequently a higher chance of partially occupied, i.e. metallic, bands.

3.1. Layer group versus space group

When discussing the layer group of a 2D material, we model the material as an ideal crystal with finite thickness along the c direction and infinite periodicity along the a and b directions, as shown in figure 3(a). On the other hand, as mentioned in the introduction, 2D materials have so far mainly been classified using space groups. The use of space groups implies a 3D lattice and thus an artificial periodicity must be imposed along the c direction. Therefore, the space group actually represents the symmetry of a 3D crystal consisting of the 2D material repeated periodically along the c direction. For simplicity, we assume c to be perpendicular to the ab lattice plane and refer to the resulting bulk crystal as the ‘AA-stacking model’, see figure 3(b). When a sufficiently large vacuum region is used to separate the 2D layers along c , the AA-stacking model corresponds to the structures used to simulate 2D materials in periodic plane wave density functional theory calculations. Perhaps for this reason the space group of the AA-stacking model has been widely used to represent the symmetry of 2D materials. In this section we compare the two classification schemes and highlight possible pitfalls arising when using the AA-stacking model and the corresponding space group to describe a 2D material.

(a) 2D material model

Periodic along a and b , but not c



(b) AA-stacking model

Periodic along a , b , and c

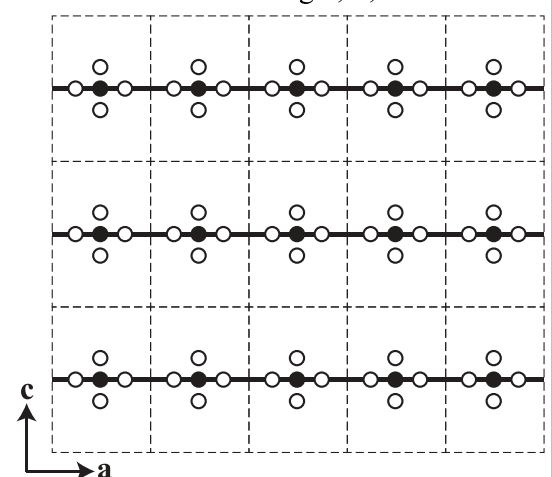


Figure 3. (a) The 2D material is periodic along the a and b axes, but not along the c axis. (b) In the AA-stacking model, the 2D material is periodically repeated along the out-of-plane c axis, extending it to the domain of space groups and making it compatible with computational plane wave codes, which require periodic boundary conditions in all directions.

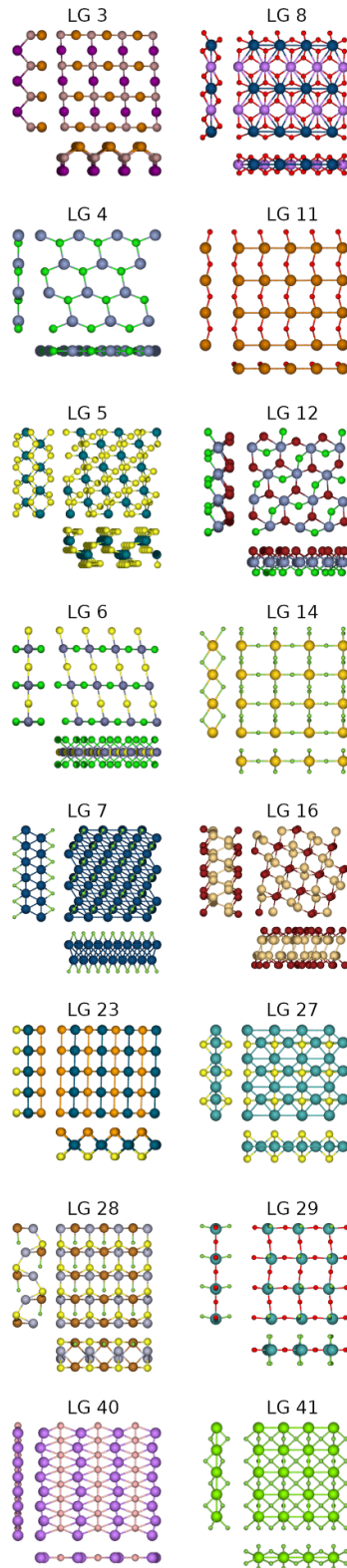


Figure 4. Examples of structures that are incompletely classified by the space group of their AA-stacked bulk, see table 1. Each row shows a pair of 2D crystal structures belonging to distinct layer groups, but with the same space group (of the AA-stacked bulk). Structures from the layer group pair (24, 31) are not shown as the C2DB contains no monolayers from layer group 24.

Table 1. List of all cases where two different layer groups are mapped to the same space group upon AA stacking of the 2D material. The number of monolayers in the C2DB is indicated in parenthesis after the Hermann–Mauguin symbol of each layer group with tolerance parameter set to 10^{-1} Å. In figure 4 some illustrative examples of crystal structures from the relevant layer groups are shown.

Layer group pairs		Space group
3: $p112$ (46)	8: $p211$ (11)	3: $P2$
4: $p11m$ (59)	11: $pm11$ (591)	6: Pm
5: $p11a$ (201)	12: $pb11$ (11)	7: Pc
6: $p112/m$ (30)	14: $p2/m11$ (230)	10: $P2/m$
7: $p112/a$ (51)	16: $p2/b11$ (88)	13: $P2/c$
23: $pmm2$ (375)	27: $pm2m$ (186)	25: $Pmm2$
28: $pm2_1b$ (245)	29: $pb2_1m$ (24)	26: $Pmc2_1$
24: $pma2$ (0)	31: $pm2a$ (10)	28: $Pma2$
40: $pmam$ (5)	41: $pmma$ (154)	51: $Pmma$

First, on a general note, it has been shown that for each layer group L with point group $\mathcal{P}$ and translation lattice $\mathbf{L}_L$, there exists a symmorphic representative which is the 3D space group S that shares the same point group and symmetry diagram [24, 25]. The lattice of the symmorphic representative

$$\mathbf{L}_S = \mathbf{L}_L \oplus \mathbf{L}_R \quad (6)$$

is the direct sum of the 2D lattice of the layer group L and the 1D lattice $\mathbf{L}_R$ of a symmorphic rod group R with point group $\mathcal{P}$. The layer group and its symmorphic representative can be represented by the same Hermann–Mauguin symbol which only differ by the upper and lowercase of the first letter [25]. However, for some types of the space groups, the splitting of the lattice $\mathbf{L}_S$ into two $\mathcal{P}$ -invariant sub-lattices is not unique. Consequently, one symmorphic representatives may correspond to multiple layer groups with different types. Ambiguity thereupon arises.

To be more specific, the symmorphic space group representatives of the 80 layer groups belong to 71 different space groups. Only 62 of these 71 space groups have a one-to-one mapping with the corresponding layer groups, while each of the remaining nine space groups are related to two different layer groups. In table 1, we list these nine non-injective mappings. The numbers in parenthesis represent the number of materials in C2DB with the specific layer group. Examples of concrete structures from the relevant layer groups are provided in figure 4. Note that only eight cases are shown in figure 4 as C2DB currently does not include any structures from layer group 24. As illustrated in table 1, a total of 2848 of the monolayers in C2DB (18%) belong to one of the layer groups in table 1, and thus are not uniquely classified by the space group of the AA-stacked structure.

Inspection of the structures/layer groups in figure 4 and table 1 shows that the first five pairs

are examples where the two layer groups belong to the monoclinic crystal systems with oblique and rectangular Bravais systems, respectively. In these cases one of the structures has an in-plane ± 2 -fold symmetry, which is replaced by an out-of-plane ± 2 -fold symmetry in the other structure. The last four pairs of layer groups all belong to the orthorhombic crystal system. For each pair of the examples, the out-of-plane rotation, mirror reflection or glide translation is exchanged with an in-plane symmetry that has a different type. For example, the out-of-plane two-fold rotation and one of the in-plane mirror reflections of layer group 23 ($pmm2$) becomes an out-of-plane mirror reflection and in-plane two-fold rotation for layer group 27 ($pm2m$). These distinctions cannot be made by the space group of the AA-stacking model.

The ability of the layer groups to differentiate structures of the same space group (defined via the AA-stacking model) is not without practical value. For example, Ji *et al* showed how layer groups can be used as a tool to determine possible outcomes of ferroelectricity when two monolayers are stacked to form a bilayer [26]. They further divided the layer groups into distinct polar types, according to whether polarization is allowed in-plane, out-of-plane, or both. An example is given by figure 4, where layer group 4 ($p11m$) is polar in-plane and layer group 11 ($pm11$) is polar out-of-plane, while both share the space group 6 (Pm). Many other properties of 2D materials, e.g. classification of electronic [27, 28] and topological [29–31] phases are also governed by the layer group symmetry. We note that useful crystallographic and Brillouin-zone databases for layer groups are available on the Bilbao crystallographic server [32].

The results of this section show that a symmetry classification of 2D materials based on space groups, such as the AA-stacking model, is less precise and more coarse grained than one based on layer groups. Consequently, to ensure a more accurate and unambiguous description of 2D crystal symmetries it is our recommendation that the 2D materials community abandons the use of space groups and uses layer groups instead.

4. Conclusions

We have introduced an algorithm to determine the layer group of a crystal structure with a 2D periodic lattice, and applied it to 15 000+ atomically thin crystals stored in the C2DB. A symmetry analysis of the 2D materials in C2DB revealed a rather inhomogeneous distribution of layer groups with several layer groups only sparsely populated and 15 groups not represented at all. It would be interesting for future

2D materials discovery projects to explore crystals from these layer groups.

We compared two different symmetry classification schemes for 2D materials based, respectively, on the layer group of the 2D crystal and the space group of the 3D bulk crystal obtained by repeating the 2D material periodically in the direction normal to the 2D plane (AA-stacking model). We showed that because the latter scheme does not distinguish between the in-plane and out-of-plane directions, it is less accurate and unable to distinguish between some 2D crystals with different layer groups. This problem occurs for 18% of the crystals in the C2DB. On this basis we conclude that symmetry classification of 2D materials should be based on layer groups rather than space groups.

The method to determine the layer group is available as part of the open source Spglib library. The algorithm will be useful for researchers working with 2D crystal structures in general, and will facilitate the application of various theories and concepts developed for 2D materials that build on the layer group symmetry.

Data availability statement

The data that support the findings of this study are openly available at the following URL/DOI: <https://github.com/spglib/spglib>.

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Appendix A. Classification of layer group

Below we summarize the mathematical structure and classification of the layer groups. We mainly follow the terminologies in references [15, 18]. We classify the layer groups according to the point groups (appendix A.1), Bravais lattice (appendix A.2), and both (appendix A.3).

A.1. Point group of layer group

Two point groups, $\mathcal{P}$ and $\mathcal{P}'$, belong to the same geometric crystal class if they are conjugate by an invertible matrix $\mathbf{P}$, i.e. $\mathbf{P}^{-1}\mathcal{P}\mathbf{P} = \mathcal{P}'$. Two layer groups,

Table 2. Classification of the point groups of layer groups. Names and symbols of the crystal systems and geometric crystal classes are based on table 3.2.1.4 of [18]. The Laue class classifies the geometric crystal classes by ignoring inversion.

Crystal system	Laue class	Geometric crystal classes
Triclinic	$\bar{1}$	1, $\bar{1}$
Monoclinic	$2/m$	2, m , $2/m$
Orthorhombic	mmm	222, $2mm$, mmm
Tetragonal	$4/m$	4, $\bar{4}$, $4/m$
	$4/mmm$	422, $\bar{4}2m$, $4mm$, $4/mmm$
Trigonal	$\bar{3}$	3, $\bar{3}$
	$\bar{3}m$	32, $3m$, $\bar{3}m$
Hexagonal	$6/m$	6, $\bar{6}$, $6/m$
	$6/mmm$	622, $\bar{6}2m$, $6mm$, $6/mmm$

L and L' , with point groups $\mathcal{P}$ and $\mathcal{P}'$ belong to the same geometric crystal class if and only if $\mathcal{P}$ and $\mathcal{P}'$ belong to the same geometric crystal class. Because the point groups of layer groups are 3D, geometric crystal classes of layer groups are classified with the same notation as those of space groups.

Two point groups belong to the same crystal system if and only if the sets of Bravais type of lattices which these point groups leave invariant, coincide. Crystal systems of layer groups are also classified with the same notation as those of space groups: triclinic, monoclinic, orthorhombic, tetragonal, trigonal, and hexagonal. Note that a cubic crystal system does not exist for layer groups because the point groups of layer groups should preserve the 2D lattice plane (the point group of the cubic crystal system would contain an operation that rotates the structure out of the lattice plane). Table 2 shows the classification of point groups for layer groups.

A.2. Translation lattice of layer group

For a lattice L , a Bravais group $\mathcal{B}(L)$ is a set of isometry mappings that preserve L . Two lattices L and L' belong to the same Bravais type of lattices if and only if their Bravais groups are conjugate by a unimodular matrix P , i.e. $P^{-1}\mathcal{B}(L)P = \mathcal{B}(L')$. Because translation lattices of layer groups are two-dimensional, Bravais types of lattices of layer groups are classified with the same notation as those of plane groups.

Two lattices L and L' belong to the same lattice system if and only if their Bravais groups belong to the same geometric crystal class. The corresponding

Table 3. Classification of translation lattices of layer groups. Names and symbols of lattice systems are based on table 3.1.1.1 of [18]. Symbols of Bravais types of lattices are based on table 3.1.2.1 of [18].

Lattice system	Holohedry	Bravais type
Oblique (monoclinic) m	$2/m$	mp
Rectangular (orthorhombic) o	mmm	op
Square (tetragonal) t	$4/mmm$	tp
Hexagonal h	$6/mmm$	hp

point group for the geometric crystal class is called a holohedry. Lattice systems of layer groups are also classified with the same notation as those of plane groups: oblique, rectangular, square, and hexagonal. Table 3 shows the classification of translation lattices of layer groups.

A.3. Arithmetic-geometric crystal class

Let $\mathcal{T}_i$ and $\mathcal{P}_i$ be a translation subgroup and a point group of layer groups L_i ($i = 1, 2$). Two layer groups L_1 and L_2 belong to the same arithmetic-geometric crystal class [33] if $\mathcal{P}_1$ and $\mathcal{P}_2$ are conjugate by a basis transformation from $\mathcal{T}_1$ to $\mathcal{T}_2$ and a transformation along the non-periodic axis. Table 4 shows the classification of layer groups by the arithmetic-geometric crystal classes.

A.4. Layer group or layer group type?

Layer group type defines the equivalence relationship between different layer groups. Two layer groups L and L' belong to the same layer group type if they are conjugate by an orientation-preserving transformation (P, p) , i.e. $(P, p)^{-1}L(P, p) = L'$ and $\det(P) > 0$.

The terminologies ‘group’ and ‘group type’ are often mixed by material scientists. For example, sentence like ‘the layer group of graphene is $p6/mmm$ ’ is commonly used in research paper. However, this is not accurate, because $p6/mmm$ is in fact the type of the layer group. The layer group is the group containing six-fold rotation, mirror reflection, translation symmetry and etc. The layer group of a graphene before and after we stretch it isotropically are different, because the lattice constant changes, and the translation symmetry in the group alters accordingly, while its layer group type keeps to be $p6/mmm$.

Table 4. Arithmetic-geometric crystal classes for layer groups. Each arithmetic-geometric crystal class is represented by a layer group in ITE whose sequential number is the smallest among the belonging arithmetic-geometric crystal class.

Crystal class/lattice system	Geometric crystal class	Arithmetic-geometric crystal class
Triclinic/oblique	1	$p1$ (1)
	$\bar{1}$	$p\bar{1}$ (2)
Monoclinic/oblique	2	$p112$ (3)
	m	$p11m$ (4)
	$2/m$	$p112/m$ (6)
Monoclinic/rectangular	2	$p211$ (8)
		$c211$ (10)
	m	$pm11$ (11)
		$cm11$ (13)
	$2/m$	$p2/m11$ (14)
Orthorhombic/rectangular		$c2/m11$ (18)
	222	$p222$ (19)
		$c222$ (22)
	$mm2$	$pmm2$ (23)
		$cmm2$ (26)
	$(m2m)$	$pm2m$ (27)
		$cm2m$ (35)
	mmm	$pmmm$ (37)
Tetragonal/square		$cmmm$ (47)
	4	$p4$ (49)
	$\bar{4}$	$p\bar{4}$ (50)
	$4/m$	$p4/m$ (51)
	422	$p422$ (53)
	$4mm$	$p4mm$ (55)
	$\bar{4}2m$	$p\bar{4}2m$ (57)
	$(\bar{4}m2)$	$p\bar{4}m2$ (59)
	$4/mmm$	$p4/mmm$ (61)
Trigonal/hexagonal	3	$p3$ (65)
	$\bar{3}$	$p\bar{3}$ (66)
	312	$p312$ (67)
	(321)	$p321$ (68)
	$3m1$	$p3m1$ (69)
	$(31m)$	$p31m$ (70)
	$\bar{3}1m$	$p\bar{3}1m$ (71)
	$(\bar{3}m1)$	$p\bar{3}m1$ (72)
Hexagonal/hexagonal	6	$p6$ (73)
	$\bar{6}$	$p\bar{6}$ (74)
	$6/m$	$p6/m$ (75)
	622	$p622$ (76)
	$6mm$	$p6mm$ (77)
	$\bar{6}m2$	$p\bar{6}m2$ (78)
	$(\bar{6}2m)$	$p\bar{6}2m$ (79)
	$6/mmm$	$p6/mmm$ (80)

Appendix B. Delaunay reduction

where

Given an n -dimensional (nD) lattice, the goal of Delaunay reduction is to find the shortest basis vectors $\mathbf{b}_i (1 \leq i \leq n)$ spanning the lattice. In practice the algorithm achieves that by minimizing

$$\sum_{i=1}^{n+1} \mathbf{b}_i^2, \quad (\text{B1})$$

$$\mathbf{b}_{n+1} = -\sum_{i=1}^n \mathbf{b}_i. \quad (\text{B2})$$

For $n = 2$, we start by selecting two basis vectors $\mathbf{b}_1$ and $\mathbf{b}_2$. The extended basis $\mathbf{b}_3 = -\mathbf{b}_1 - \mathbf{b}_2$. Check the three scalar products $\mathbf{b}_i \cdot \mathbf{b}_j (i \neq j)$ one after the other. Any time $\mathbf{b}_i \cdot \mathbf{b}_j > 0$, the transformation

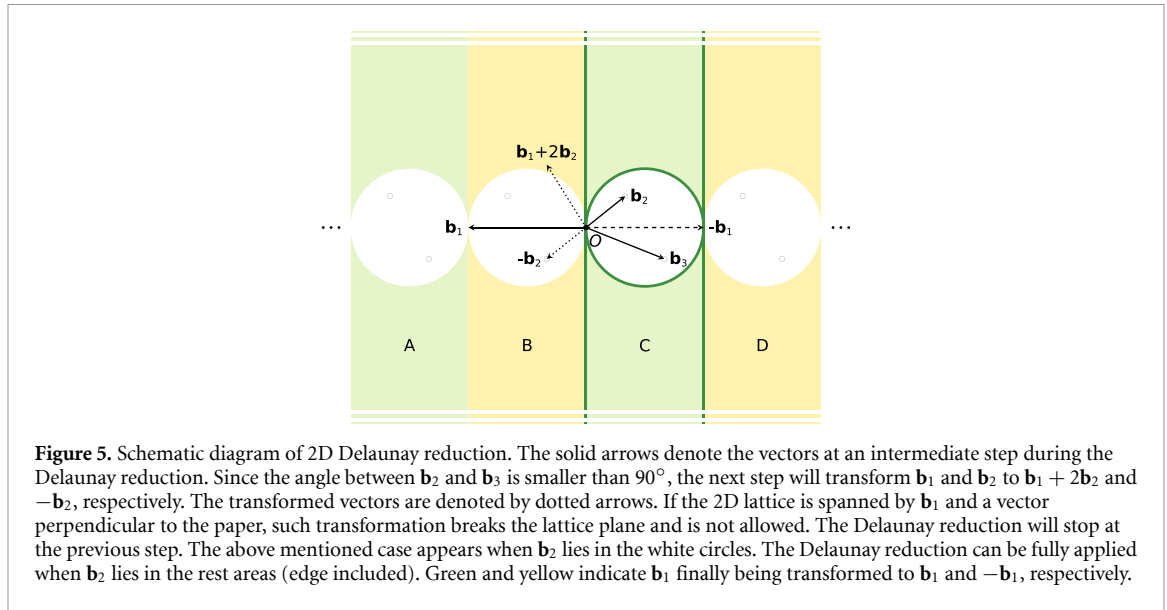


Figure 5. Schematic diagram of 2D Delaunay reduction. The solid arrows denote the vectors at an intermediate step during the Delaunay reduction. Since the angle between $\mathbf{b}_2$ and $\mathbf{b}_3$ is smaller than 90° , the next step will transform $\mathbf{b}_1$ and $\mathbf{b}_2$ to $\mathbf{b}_1 + 2\mathbf{b}_2$ and $-\mathbf{b}_2$, respectively. The transformed vectors are denoted by dotted arrows. If the 2D lattice is spanned by $\mathbf{b}_1$ and a vector perpendicular to the paper, such transformation breaks the lattice plane and is not allowed. The Delaunay reduction will stop at the previous step. The above mentioned case appears when $\mathbf{b}_2$ lies in the white circles. The Delaunay reduction can be fully applied when $\mathbf{b}_2$ lies in the rest areas (edge included). Green and yellow indicate $\mathbf{b}_1$ finally being transformed to $\mathbf{b}_1$ and $-\mathbf{b}_1$, respectively.

$$\begin{aligned} \mathbf{b}'_i &= -\mathbf{b}_i \\ \mathbf{b}'_j &= \mathbf{b}_j \\ \mathbf{b}'_k &= \mathbf{b}_k + 2\mathbf{b}_i \end{aligned} \quad (\text{B3})$$

is performed, where $k \neq i, j$. After the transformation, $\sum \mathbf{b}'_i \cdot \mathbf{b}'_j = \sum \mathbf{b}_i \cdot \mathbf{b}_j - 4\mathbf{b}_i \cdot \mathbf{b}_j < \sum \mathbf{b}_i \cdot \mathbf{b}_j$. Then we check $\mathbf{b}'_1 \cdot \mathbf{b}'_2$, $\mathbf{b}'_1 \cdot \mathbf{b}'_3$ and $\mathbf{b}'_2 \cdot \mathbf{b}'_3$, and so on. The loop stops when all $\mathbf{b}_i \cdot \mathbf{b}_j \leq 0$, i.e. the angles between $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ all become non-acute. 2D Delaunay reduction is applied to the basis vectors forming the oblique face of a monoclinic cell and works well on bulk systems. For the monoclinic/oblique cell, the target vectors to be reduced are the lattice vectors $\mathbf{a}$ and $\mathbf{b}$, and the procedure has no difference from the bulk case. However, the oblique face of a monoclinic/rectangular cell is composed of $\mathbf{b}_1 = \mathbf{b}$ and $\mathbf{b}_2 = \mathbf{c}$. As shown in figure 5, the basis vectors of the periodic plane are $\mathbf{b}_1$ and the unique axis $\mathbf{a}$ which is vertical to the paper. Allowed transformations for $\mathbf{b}_1$ are $\mathbf{b}_1 \rightarrow \mathbf{b}_1$ and $\mathbf{b}_1 \rightarrow -\mathbf{b}_1$. When the angle between $\mathbf{b}_2$ and $\mathbf{b}_3$ is acute, Delaunay reduction requires $\mathbf{b}_1 \rightarrow \mathbf{b}_1 + 2\mathbf{b}_2$ and $\mathbf{b}_2 \rightarrow -\mathbf{b}_2$. The new vectors break the lattice plane, which is not permitted (dotted arrows in figure 5). For certain input cell, candidates for $\mathbf{b}_2, \mathbf{b}_3$ are predetermined (represented by hollow points in figure 5). When the points lay on the colored areas (including edges), $\forall \mathbf{b}_i \cdot \mathbf{b}_j \leq 0$ fulfills after Delaunay reduction. $\mathbf{b}_2$ with initial position at the green areas will be sent to the green area of region C. $\mathbf{b}_2$ in the yellow areas will finally deposit in region B, with $\mathbf{b}_1$ being switched to $-\mathbf{b}_1$. If the input $\mathbf{b}_2$ lies in any of the white circles, at least one angle between the vectors will be acute. In Spglib, it is the one between $\mathbf{b}_2$ and $\mathbf{b}_3$. After reduction, the non-lattice vector $\mathbf{c}$ and the shortest two vectors among $\mathbf{b}_1, \mathbf{b}_2$ and $\mathbf{b}_3$ are selected to build the bulk or monoclinic/oblique cell. While for a monoclinic/rectangular cell, one of $\pm \mathbf{b}_1$ must be

chosen to maintain the periodic plane. The other two vectors are $\mathbf{a}$ and the shortest in $\mathbf{b}_2$ and $\mathbf{b}_3$.

The workflow for $n = 3$ is similar. The transformation for $\mathbf{b}_i \cdot \mathbf{b}_j > 0$ ($i, j = 1, \dots, 4$; $i \neq j$) reads

$$\begin{aligned} \mathbf{b}'_i &= -\mathbf{b}_i \\ \mathbf{b}'_j &= \mathbf{b}_j \\ \mathbf{b}'_k &= \mathbf{b}_k + \mathbf{b}_i \\ \mathbf{b}'_l &= \mathbf{b}_l + \mathbf{b}_i. \end{aligned} \quad (\text{B4})$$

For layer systems, when the non-lattice vector $\mathbf{c}$ lies in the intersection of an infinitely long prism and a sphere, the Delaunay reduction cannot be fully applied. The angle between $\mathbf{b}_3$ and $\mathbf{b}_4$ will be less than 90° . The two basis vectors that form the cross section of the prism are

$$\begin{aligned} \mathbf{p}_1 &= \frac{(\mathbf{b}_1 + \mathbf{b}_2) \cdot \mathbf{b}_2}{(\mathbf{b}_2 \times \mathbf{b}_1) \cdot \mathbf{e}_z} (\mathbf{e}_z \times \mathbf{b}_1) \text{ and,} \\ \mathbf{p}_2 &= \frac{(\mathbf{b}_1 + \mathbf{b}_2) \cdot \mathbf{b}_1}{(\mathbf{b}_2 \times \mathbf{b}_1) \cdot \mathbf{e}_z} (\mathbf{e}_z \times \mathbf{b}_2), \end{aligned} \quad (\text{B5})$$

where $\mathbf{e}_z = (0, 0, 1)$, $\mathbf{p}_1 \perp \mathbf{b}_1$, $\mathbf{p}_2 \perp \mathbf{b}_2$, and $\mathbf{p}_1 + \mathbf{p}_2 = -\mathbf{b}_1 - \mathbf{b}_2$. The prism is infinite along the $\pm z$ direction. The origin of the sphere is $-\frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2)$ and the radius is $-\frac{1}{2}|\mathbf{b}_1 + \mathbf{b}_2|$.

Appendix C. Conventional cells

The standard crystallographic coordinate system (CCS) choices defined in [15, 18] impose constraints on the choices and the orientations of the basis vectors, and are firstly consulted for building the conventional cells. Additional metric rules are added when the standard choices cannot uniquely determine the cell. The criteria used by Spglib are summarized in figure 1.

For triclinic lattices, a Niggli cell [34] is chosen to be the conventional cell by virtue of its uniqueness. For bulk crystals (3D lattice), the Niggli conditions include $|\mathbf{a}_c| \leq |\mathbf{b}_c| \leq |\mathbf{c}_c|$ and $|\mathbf{a}_c \cdot \mathbf{c}_c| \leq |\mathbf{a}_c \cdot \mathbf{b}_c|$ if $|\mathbf{b}_c| = |\mathbf{c}_c|$ for bulk systems. The Niggli reduction will swap $\mathbf{b}_c$ and $\mathbf{c}_c$ when the aforementioned conditions are not met. For layer systems with the non-lattice vector $\mathbf{c}_c$, such action is not allowed. In this case, the resulting cell will thus differ from the conventional Niggli cell by a rotation.

The monoclinic crystal system is subdivided into monoclinic/oblique and monoclinic/rectangular according to the 2D Bravais lattice. The unique two-fold axis is vertical to the plane and set to be parallel to $\mathbf{c}_c$ for the former, while for the latter the axis is in-plane and chosen to be along $\mathbf{a}_c$. 2D Delaunay reduction is conducted for the oblique face of the cell. As shown in appendix B, this procedure cannot be completely performed for the monoclinic/rectangular system. In this case, both the shape and the orientation of the resulting cell will differ from the conventional cell that would have been obtained for a monoclinic bulk crystal.

The conventional cells of the orthorhombic groups are cuboids. The standard CCS choice requires the axes of certain symmetry operations to be perpendicular to the faces of the cuboids. When multiple faces share same symmetry diagram up to an origin shift, permutation of the cell vectors will not influence the CCS choice. To find out which basis vectors can be swapped, the Euclidean normalizer of the space/layer group is utilized. The Euclidean normalizer of a group $\mathcal{G}$ is the group $\mathcal{N}_E(\mathcal{G})$ consisting of all Euclidean transformations which map $\mathcal{G}$ onto itself by conjugation

$$\mathcal{N}_E(\mathcal{G}) \equiv \{s \in \mathcal{E} \mid s^{-1}\mathcal{G}s = \mathcal{G}\}, \quad (\text{C1})$$

where $\mathcal{E}$ is the group of all Euclidean transformations [18]. $\mathcal{G}$ is a normal subgroup of $\mathcal{N}_E$, and the factor group $\mathcal{N}_E(\mathcal{G})/\mathcal{G}$ classifies the transformations. Each element $s\mathcal{G}$ of the factor group represents a different kind of CCS transformation (axis permutation, origin shift, etc) that does not alter the CCS choice. We are interested in all the $s\mathcal{G}$ which contains one of the six right-handed axis permutations **abc**, **ba $\bar{c}$** , **cab**, **c $\bar{b}$ a**, **bca** and **a $\bar{c}$ b**. They can be obtained by exploiting the group-subgroup relationship revealed in section 3.5.2.1 of [18]

$$\mathcal{G} \leq \mathcal{K}(\mathcal{G}) \leq \mathcal{L}(\mathcal{G}) \leq \mathcal{N}_E(\mathcal{G}), \quad (\text{C2})$$

where $\mathcal{K}(\mathcal{G})$ is an intermediate group that retains the linear part of $\mathcal{G}$ and the translation part of $\mathcal{N}_E(\mathcal{G})$. $\mathcal{L}(\mathcal{G}) = \mathcal{K}(\mathcal{G}) \otimes \{1, \bar{1}\}$ if $\mathcal{G}$ does not have inversion symmetry while $\mathcal{N}_E(\mathcal{G})$ is centrosymmetric, else $\mathcal{L}(\mathcal{G}) = \mathcal{K}(\mathcal{G})$. The group $\mathcal{N}_E(\mathcal{G})/\mathcal{L}(\mathcal{G})$ factors out choices related to origin shift and inversion which flips the handedness. The index $n_1 = |\mathcal{N}_E(\mathcal{G})/\mathcal{L}(\mathcal{G})|$ indicates the number of axes permutation types that preserves the CCS choice. For space groups, when

$n_1 = 6$, the six different axis permutations do not influence the CCS choice. The order of the three basis vectors can be arbitrarily chosen. Spglib requires $|\mathbf{a}_c| \leq |\mathbf{b}_c| \leq |\mathbf{c}_c|$. Space groups $P222$, $F222$, $Ibca$, etc belong to this case. Space group $Pbca$ is the only one with $n_1 = 3$, where **abc**, **cab** and **bca** preserves the standard CCS choice, while **ba $\bar{c}$** , **c $\bar{b}$ a** and **a $\bar{c}$ b** changes the choice to another. Spglib chooses $\mathbf{a}_c$ to be the shortest vector, the orientation of $\mathbf{b}_c$ and $\mathbf{c}_c$ will be settled accordingly. $n_1 = 2$ means the standard choice fixes certain symmetry axis being parallel to $\mathbf{c}_c$. $\mathbf{a}_c$ and $\mathbf{b}_c$ cannot be determined by symmetry. Spglib adds the constraint $|\mathbf{a}_c| \leq |\mathbf{b}_c|$. Typical space groups are $P22_1$, $C22_2$, etc. The rest orthorhombic space groups like $Pmc2_1$ have $n_1 = 1$, of which the standard choices uniquely determine the basis of the conventional cells. For layer groups, $n_1 \leq 2$ due to $\mathbf{c}_c$ being the non-lattice vector.

For bulk, table 3.5.2.4 of [18] lists n_1 for centrosymmetric $\mathcal{N}_E(\mathcal{G})$, and $n_k = |\mathcal{N}_E(\mathcal{G})/\mathcal{K}(\mathcal{G})|$ for noncentrosymmetric $\mathcal{N}_E(\mathcal{G})$. For simplicity, we use n_1 to denote the two symbols. Different metric parameter conditions may lead to different $\mathcal{N}_E(\mathcal{G})$, and the one with highest symmetry should be consulted. For layer, n_1 can be deduced from the table by consulting the line with highest symmetry under the metric conditions $a \neq c$ and $b \neq c$. It can also be found in [35].

For space groups, additional correction matrices must be applied for monoclinic and orthorhombic conventional cells with 'A', 'B' or body-centering types, as the standard choices only possess 'C' centering lattices. The correction matrices are listed in [13]. This step is not necessary for layer groups.

Appendix D. Hall symbols

Hall symbols are used to represent the different CCS choices of space and layer groups in Spglib. Comparing to Hermann–Mauguin symbols, Hall symbols take the origin of each symmetry operation into consideration. A unique symmetry group can be deduced from a Hall symbol without additional information. The 530 Hall symbols for different choices of space groups are tabulated in table A1.4.2.7 of [20]. As there does not exist a standard table for layer group Hall symbols, we have produced table 5 as a reference.

The first column of the table gives the layer group number. If there are multiple CCS choices for one layer group type, the group number is followed by the axis codes of the choice. The first row of each group number always corresponds to the standard choice defined in chapter 4 of [15]. The non-standard choices are generated according to table 1.2.6.1 and chapter 4 of [15]. The second to the fourth column lists the Hermann–Mauguin entries, Hall entries suitable for computer processing and the Hall symbols,

Table 5. Table of the layer group numbers along with possible axis codes, Hermann–Mauguin symbols, Hall entries and Hall symbols. The table follows the format of table A1.4.2.7 in [20]. The first row of each layer group number demonstrates the standard choice. All the choices are compatible with the symmetry diagrams in chapter 4 and table 1.2.6.1 of [15]. The first letter ‘p’ and ‘c’ of the Hall symbols are in lowercase to represent layer groups.

$n:c$	H–M entry	Hall entry	Hall symbol	$n:c$	H–M entry	Hall entry	Hall symbol
1	p 1	p 1	p 1	34:b-ac	p 2 a n	p -2ab 2	p $\bar{2}_{ab}$ 2
2	p -1	-p 1	$\bar{p}$ 1	35	c m 2 m	c -2 -2	c $\bar{2}$ $\bar{2}$
3:c	p 1 1 2	p 2	p 2	35:b-ac	c 2 m m	c -2 2	c $\bar{2}$ 2
4:c	p 1 1 m	p -2	p $\bar{2}$	36	c m 2 e	c -2a -2a	c $\bar{2}_a$ $\bar{2}_a$
5:c1	p 1 1 a	p -2a	p $\bar{2}_a$	36:b-ac	c 2 m e	c -2a 2	c $\bar{2}_a$ 2
5:c2	p 1 1 n	p -2ab	p $\bar{2}_{ab}$	37	p m m m	-p 2 2	$\bar{p}$ 2 2
5:c3	p 1 1 b	p -2b	p $\bar{2}_b$	38	p m a a	-p 2a 2	$\bar{p}$ 2a 2
6:c	p 1 1 2/m	-p 2	$\bar{p}$ 2	38:b-ac	p b m b	-p 2b 2b	$\bar{p}$ 2b 2b
7:c1	p 1 1 2/a	-p 2a	$\bar{p}$ 2a	39	p b a n	-p 2ab 2b	$\bar{p}$ 2ab 2b
7:c2	p 1 1 2/n	-p 2ab	$\bar{p}$ 2ab	40	p m a m	-p 2 2a	$\bar{p}$ 2 2a
7:c3	p 1 1 2/b	-p 2b	$\bar{p}$ 2b	40:b-ac	p b m m	-p 2 2b	$\bar{p}$ 2 2b
8:a	p 2 1 1	p 2x	p 2 ^x	41	p m m a	-p 2a 2a	$\bar{p}$ 2a 2a
8:b	p 1 2 1	p 2y	p 2 ^y	41:b-ac	p m m b	-p 2b 2	$\bar{p}$ 2b 2
9:a	p 2 1 1 1	p 2xa	p 2 ^x _a	42	p m a n	-p 2ab 2	$\bar{p}$ 2ab 2
9:b	p 1 2 1 1	p 2yb	p 2 ^y _b	42:b-ac	p b m n	-p 2ab 2ab	$\bar{p}$ 2ab 2ab
10:a	c 2 1 1	c 2x	c 2 ^x	43	p b a a	-p 2a 2b	$\bar{p}$ 2a 2b
10:b	c 1 2 1	c 2y	c 2 ^y	43:b-ac	p b a b	-p 2b 2ab	$\bar{p}$ 2b 2ab
11:a	p m 1 1	p -2x	p $\bar{2}^x$	44	p b a m	-p 2 2ab	$\bar{p}$ 2 2ab
11:b	p 1 m 1	p -2y	p $\bar{2}^y$	45	p b m a	-p 2a 2ab	$\bar{p}$ 2a 2ab
12:a	p b 1 1	p -2xb	p $\bar{2}_b^x$	45:b-ac	p m a b	-p 2b 2a	$\bar{p}$ 2b 2a
12:b	p 1 a 1	p -2ya	p $\bar{2}_a^y$	46	p m m n	-p 2ab 2a	$\bar{p}$ 2ab 2a
13:a	c m 1 1	c -2x	c $\bar{2}^x$	47	c m m m	-c 2 2	$\bar{c}$ 2 2
13:b	c 1 m 1	c -2y	c $\bar{2}^y$	48	c m m e	-c 2a 2	$\bar{c}$ 2a 2
14:a	p 2/m 1 1	-p 2x	$\bar{p}$ 2 ^x	49	p 4	p 4	p 4
14:b	p 1 2/m 1	-p 2y	$\bar{p}$ 2 ^y	50	p -4	p -4	p $\bar{4}$
15:a	p 2 1/m 1 1	-p 2xa	$\bar{p}$ 2 ^x _a	51	p 4/m	-p 4	$\bar{p}$ 4
15:b	p 1 2 1/m 1	-p 2yb	$\bar{p}$ 2 ^y _b	52:1	p 4/n:1	p 4 -1ab	p 4 $\bar{1}_{ab}$
16:a	p 2/b 1 1	-p 2xb	$\bar{p}$ 2 ^x _b	52:2	p 4/n:2	-p 4a	$\bar{p}$ 4a
16:b	p 1 2/a 1	-p 2ya	$\bar{p}$ 2 ^y _a	53	p 4 2 2	p 4 2	p 4 2
17:a	p 2 1/b 1 1	-p 2xab	$\bar{p}$ 2 ^x _{ab}	54	p 4 2 1 2	p 4 2ab	p 4 2ab
17:b	p 1 2 1/a 1	-p 2yab	$\bar{p}$ 2 ^y _{ab}	55	p 4 m m	p 4 -2	p 4 $\bar{2}$
18:a	c 2/m 1 1	-c 2x	$\bar{c}$ 2 ^x	56	p 4 b m	p 4 -2ab	p 4 $\bar{2}_{ab}$
18:b	c 1 2/m 1	-c 2y	$\bar{c}$ 2 ^y	57	p -4 2 m	p -4 2	p $\bar{4}$ 2
19	p 2 2 2	p 2 2	p 2 2	58	p -4 2 1 m	p -4 2ab	p $\bar{4}$ 2ab
20	p 2 1 2 2	p 2 2a	p 2 2 _a	59	p -4 m 2	p -4 -2	p $\bar{4}$ $\bar{2}$
20:b-ac	p 2 2 1 2	p 2 2b	p 2 2 _b	60	p -4 b 2	p -4 -2ab	p $\bar{4}$ $\bar{2}_{ab}$
21	p 2 1 2 1 2	p 2 2ab	p 2 2 _{ab}	61	p 4/m m m	-p 4 2	$\bar{p}$ 4 2
22	c 2 2 2	c 2 2	c 2 2	62:1	p 4/n b m:1	p 4 2 -1ab	p 4 2 $\bar{1}_{ab}$
23	p m m 2	p 2 -2	p 2 $\bar{2}$	62:2	p 4/n b m:2	-p 4a 2b	$\bar{p}$ 4a 2b
24	p m a 2	p 2 -2a	p 2 $\bar{2}_a$	63	p 4/m b m	-p 4 2ab	$\bar{p}$ 4 2ab
24:b-ac	p b m 2	p 2 -2b	p 2 $\bar{2}_b$	64:1	p 4/n m m:1	p 4 2ab -1ab	p 4 2ab $\bar{1}_{ab}$
25	p b a 2	p 2 -2ab	p 2 $\bar{2}_{ab}$	64:2	p 4/n m m:2	-p 4a 2a	$\bar{p}$ 4a 2a
26	c m m 2	c 2 -2	c 2 $\bar{2}$	65	p 3	p 3	p 3
27	p m 2 m	p -2 -2	p $\bar{2}$ $\bar{2}$	66	p -3	-p 3	$\bar{p}$ 3
27:b-ac	p 2 m m	p -2 2	p $\bar{2}$ 2	67	p 3 1 2	p 3 2	p 3 2
28	p m 2 1 b	p -2b -2	p $\bar{2}_b$ $\bar{2}$	68	p 3 2 1	p 3 2''	p 3 2''
28:b-ac	p 2 1 m a	p -2a 2a	p $\bar{2}_a$ 2a	69	p 3 m 1	p 3 -2''	p 3 $\bar{2}$ ''
29	p b 2 1 m	p -2 -2b	p $\bar{2}$ $\bar{2}_b$	70	p 3 1 m	p 3 -2	p 3 $\bar{2}$
29:b-ac	p 2 1 a m	p -2 2a	p $\bar{2}$ 2a	71	p -3 1 m	-p 3 2	$\bar{p}$ 3 2
30	p b 2 b	p -2b -2b	p $\bar{2}_b$ $\bar{2}_b$	72	p -3 m 1	-p 3 2''	$\bar{p}$ 3 2''
30:b-ac	p 2 a a	p -2a 2	p $\bar{2}_a$ 2	73	p 6	p 6	p 6
31	p m 2 a	p -2a -2a	p $\bar{2}_a$ $\bar{2}_a$	74	p -6	p -6	p $\bar{6}$
31:b-ac	p 2 m b	p -2b 2	p $\bar{2}_b$ 2	75	p 6/m	-p 6	$\bar{p}$ 6
32	p m 2 1 n	p -2ab -2	p $\bar{2}_{ab}$ $\bar{2}$	76	p 6 2 2	p 6 2	p 6 2
32:b-ac	p 2 1 m n	p -2ab 2ab	p $\bar{2}_{ab}$ 2ab	77	p 6 m m	p 6 -2	p 6 $\bar{2}$
33	p b 2 1 a	p -2a -2ab	p $\bar{2}_a$ $\bar{2}_{ab}$	78	p -6 m 2	p -6 2	p $\bar{6}$ 2
33:b-ac	p 2 1 a b	p -2b 2a	p $\bar{2}_b$ 2a	79	p -6 2 m	p -6 -2	p $\bar{6}$ $\bar{2}$
34	p b 2 n	p -2ab -2ab	p $\bar{2}_{ab}$ $\bar{2}_{ab}$	80	p 6/m m m	-p 6 2	$\bar{p}$ 6 2

respectively. The detailed meaning of the Hall symbols is described in [20], except we use symbols with the first letter upper and lowercase to distinguish the space and layer groups, respectively.

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