Supplementary Information for

Atomic-scale one-dimensional materials identified from graph theory

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Catalog

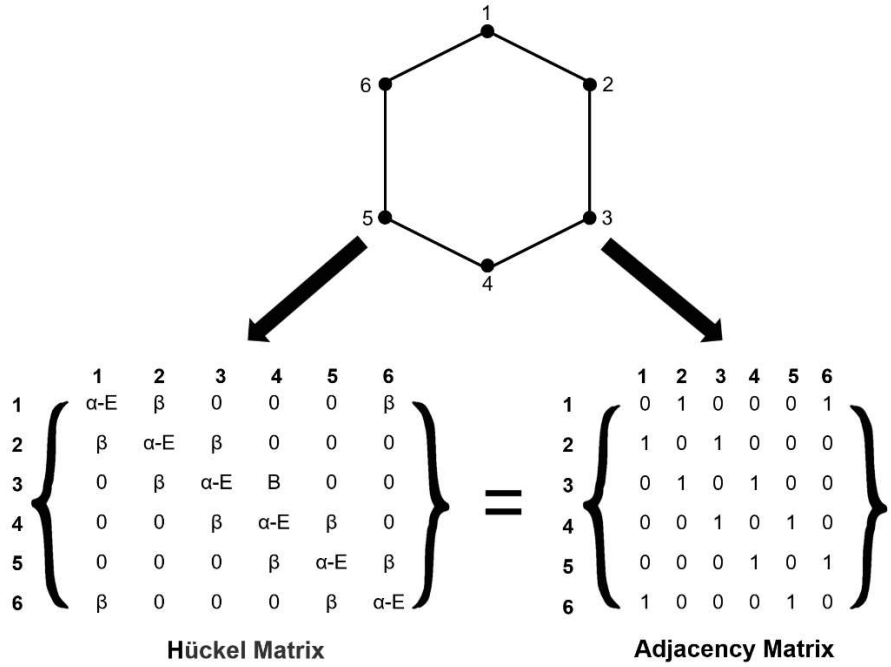
1 Discovery of low-dimensional materials via graph theory

1.1 A brief introduction to graph theory and structure graphs

Graph theory is one of the branches of mathematics that deals with the way of connectivity for objects. In 1736, Euler provided the solution to a celebrated problem, known as Königsberg Bridge Problem – that is, whether it is possible to walk over all the seven bridges on the river Pregel in Königsberg just once while not retracing one's footsteps. Euler reduced the question to a problem of graph theory and since then, the discipline of graph theory has been advanced continually and exploited in various fields of natural science.

The basic element in graph theory – *graph*, was first introduced to the chemical world in the latter half of the eighteenth century.[1] These graphs are called *chemical graphs*, which pertained to the description of internal structures of substances and the short-range forces between them. However, due to the lack of knowledge on the fundamental nature of matter, these chemical graphs in that time period expressed merely a fictitious quantification of the imagined interaction between substances. It was not until the early nineteenth century that the first attempt was made to use chemical graphs for the visualization of spatial arrangement of atoms in molecules. Then, the nomenclature for chemical species in a ball-and-stick model, where atoms were treated as hard spheres and molecules were represented as ensembles of atoms with interatomic forces, began to be adopted by the scientific community in the mid part of the century. Several decades later, the advent of quantum theory led to a revolution in our understanding of the nature of chemical bonds. The interactions between atoms were found to be so complexed that new mathematical tools had to be developed to describe the behavior of electrons in molecules. For example, to study the π-electrons in unsaturated molecules such as benzene, Hückel proposed that the molecular orbital energies of these organic molecules can be approximated by solving the determinants parameterized by two variables, a Coulomb integral α and a resonance integral β. The determinant assumes the form shown in Supplementary Fig. 1. A few years later, researchers found that this determinant is isomorphic to the *adjacency matrix* of the chemical graph of benzene. As a result, the eigenvectors of both matrices will be identical, and the energy levels

derived from the Hückel determinant will be linearly correlated with the eigenvalues of the adjacency matrix. This provides a clear example that the concepts in graph theory can be ideally suited to applications in chemical context. It can therefore be speculated that the underlying topology of a molecule influences its intrinsic properties in a decisive way.



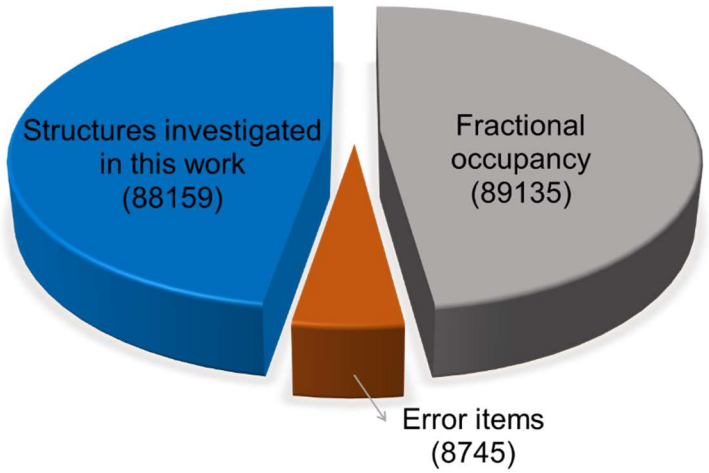
Supplementary Fig. 1 | The Hückel and adjacency matrices for benzene molecule[1].

The above realization has compelled researchers to look beyond the use of graph theory in molecules and adapt the concept of chemical graph to apply to periodic crystal systems. Pioneering work in this area was done by Isayev et al in 2017[2], who employed the Voronoi tessellation method to assign the nearest neighbors to each atom, and constructed the structure graphs for infinite periodic crystal structures. Later on, Xie and Grossman[3] used a combination of Voronoi tessellation and bond length thresholds to identify the atomic connectivity. Crystal graphs were generated with multiple edges between the same pair of end nodes so as to reproduce the characteristics of periodic crystals. In 2019, our group[4] established a database of structure graphs for a total of 626,772 inorganic compounds and developed a graph-theory-based algorithm for automatic deduplication of crystal structures in the database. The current version of graph-theory-based algorithm extends our previous work in that the threshold for atomic connectivity is more precisely determined based on Pauling's rules, and that the

chemically bonded manifolds, i.e. the structural blocks in bulk crystals, are unambiguously identified by the adjacency matrix of a supercell.

1.2 Database of existing bulk compounds

The database of bulk compounds used in this study is obtained from the Inorganic Crystal Structure Database (ICSD, version 2019), with a total of 186,039 data entries. Among them, 89,135 compounds with fractional occupancy at lattice sites are excluded from the calculations. We find that some of the data entries contain contradictory information in chemical composition, while some others have missing atoms in the atomic-coordinate data block. These entries are considered as error items and therefore filtered out from the database of bulk compounds (Supplementary Fig. 2). Moreover, there are several compounds whose crystal structures experience dramatic changes after structural optimization using density functional theory (DFT) calculations. To prevent the inconsistency between the structures of low-dimensional materials (LDMs) and their parent bulk crystals, the graph-theory-based algorithm for structural block identification is carried out after the DFT structural optimization of the corresponding bulk compounds.



Supplementary Fig. 2 | Database of bulk compounds from ICSD.

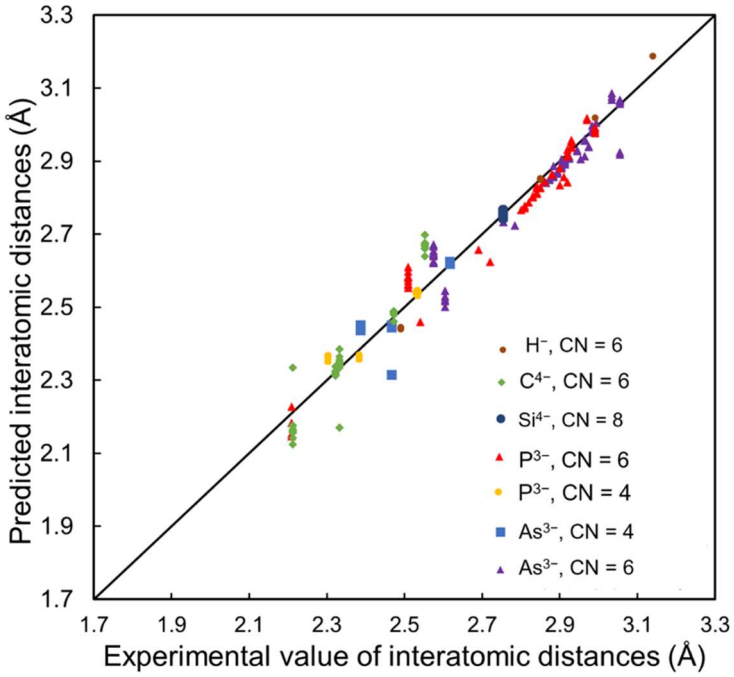
1.3 Criterion for atomic connectivity

The chemical bonding character of each pair of neighboring atoms is determined by their electronegativity. If both atoms are nonmetal elements with electronegativity of no less than 1.98 (the value of Si), we use covalent radii to assess their connectivity. When both are metal elements, metallic radii are employed. The rest of the cases correspond to ionic bonding, in which ionic radii are adopted. Note that any nonmetal atom could only be negatively charged when forming ionic bond with a metal atom, and that the positively charged nonmetal atoms will appear in the covalent bonding cases according to the above protocol. Supplementary Table 1 tabulates the covalent, metallic and ionic radii used in this work, which are extracted from literature[5-7]. It should be pointed out that although the ionic radii can vary with the valence states, here we only employ the maximum value for the evaluation of atomic connectivity. Since the ionic radii of H, C, Si, P and As are unavailable in the literature, we carry out systematic searches in ICSD for ionic compounds containing these elements, and establish empirical ionic radii for them on the basis of interatomic distances and the known radii of other elements. Supplementary Fig. 3 shows the comparison between the predicted interatomic distances using the deduced atomic radii of the above elements and the corresponding experimental data. The chemical bond of an atom pair is heuristically identified when the interatomic distance is smaller than the sum of radii multiplied by 1.1, which is essential for including the effect of bond-length fluctuations while not introducing too much empirical input.

Supplementary Table 1 | Covalent, metallic and ionic radii for all elements

Element	Covalent radius (Å)	Metallic radius (Å)	Ionic radius (Å)	Element	Covalent radius (Å)	Metallic radius (Å)	Ionic radius (Å)
H	0.37	/	1.33	**Li**	1.23	1.52	1.06
Be	0.89	1.13	0.59	**C**	0.77	/	1.47
B	0.83	/	1.47	**N**	0.7	/	1.32
O	0.66	/	1.28	**F**	0.64	/	1.19
Ne	1.31	/	/	**Na**	1.57	1.54	1.53
Mg	1.36	1.60	1.03	**Al**	1.25	1.43	0.68
Si	1.17	/	2.04	**P**	1.10	/	1.80
S	1.04	/	1.70	**Cl**	0.99	/	1.67

Ar	1.74	/	/	**K**	2.03	2.28	1.78
Ca	1.74	1.97	1.40	**Sc**	1.44	1.61	1.01
Ti	1.32	1.45	1.00	**V**	1.22	1.32	0.93
Cr	1.17	1.25	0.94	**Mn**	1.17	1.24	1.10
Fe	1.17	1.24	1.06	**Co**	1.16	1.25	1.04
Ni	1.15	1.25	0.83	**Cu**	1.17	1.28	0.91
Zn	1.25	1.33	1.04	**Ga**	1.25	1.22	0.76
Ge	1.22	1.23	0.87	**As**	1.21	1.25	1.86
Se	1.17	/	1.84	**Br**	1.14	/	1.82
Kr	1.89	/	/	**Rb**	2.16	2.48	1.97
Sr	1.92	2.15	1.58	**Y**	1.62	1.81	1.22
Zr	1.45	1.60	1.03	**Nb**	1.34	1.43	0.93
Mo	1.29	1.36	0.87	**Tc**	/	1.36	0.79
Ru	1.24	1.33	0.82	**Rh**	1.25	1.35	0.81
Pd	1.28	1.38	1.00	**Ag**	1.34	1.44	1.42
Cd	1.41	1.49	1.45	**In**	1.50	1.63	1.06
Sn	1.40	1.41	0.95	**Sb**	1.41	1.41	0.94
Te	1.37	1.43	2.07	**I**	1.33	/	2.06
Xe	2.09	/	0.62	**Cs**	2.35	2.61	2.02
Ba	1.98	2.17	1.75	**La**	1.69	1.88	1.50
Ce	1.64	1.83	1.48	**Pr**	1.65	1.83	1.32
Nd	1.64	1.82	1.49	**Pm**	/	1.81	1.28
Sm	1.66	1.80	1.46	**Eu**	1.85	2.04	1.49
Dy	1.56	1.77	1.33	**Gd**	1.61	1.80	1.25
Ho	1.58	1.77	1.26	**Tb**	1.59	1.78	1.24
Er	1.57	1.76	1.20	**Hf**	1.44	1.56	0.97
Tm	1.56	1.75	1.23	**Ta**	1.34	1.43	0.88
Yb	1.70	1.94	1.28	**W**	1.30	1.37	0.8
Lu	1.56	1.73	1.17	**Re**	1.28	1.37	0.77
Au	1.34	1.44	1.51	**Os**	1.26	1.34	0.77
Hg	1.44	1.60	1.33	**Ir**	1.26	1.36	0.82
Tl	1.55	1.70	1.84	**Pt**	1.29	1.38	0.94
Pb	1.54	1.75	1.63	**Ac**	/	1.88	1.26
Bi	1.52	1.55	1.31	**Th**	/	1.80	1.35
Po	1.53	1.67	1.22	**Pa**	/	1.61	1.18
At	/	/	0.76	**U**	/	1.36	1.31
Fr	/	2.70	1.94	**Np**	/	1.31	1.24
Ra	/	2.20	1.84	**Pu**	/	1.51	1.14
Am	/	1.84	1.45	**Cf**	/	/	1.09
Cm	/	/	1.11	**No**	/	/	1.24
Bk	/	/	1.10				

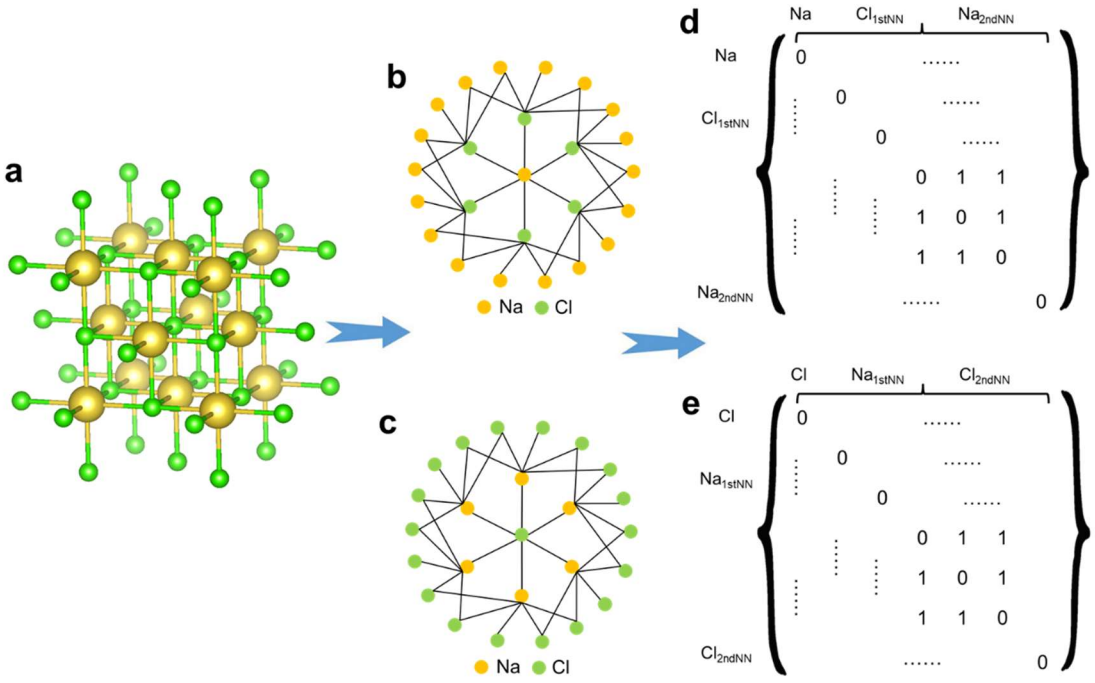


Supplementary Fig. 3 | Comparison between the predicted and experimental values of interatomic distances for atom pairs containing H, C, Si, P and As anions with different coordination number (CN).

1.4 Identification and categorization of structural blocks

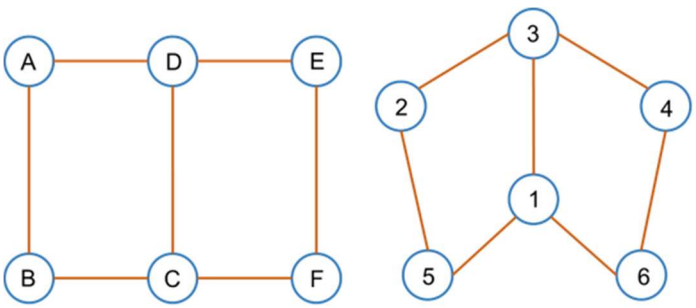
The topological structure of any bulk compound can be depicted by a simple undirected graph. Atoms are represented by small circles, and chemical bonds by lines that connect the corresponding circles. Here, the structure graph of NaCl is exemplified (Supplementary Fig. 4). Both Na and Cl atoms in a unit cell are taken as the starting point for constructing the subgraphs, which merge into a complete graph where all atoms in the unit cell are involved. The shortest path between any two nodes is called a geodesic and its length defines the distance between nodes. Atoms linked to the original Na/Cl have a distance of 1 to the central atoms, and are therefore described as the first nearest neighbors (1st NN). Atoms with distance of 2, 3 and so on are the 2nd NN, the 3rd NN and so on. Each structure graph is represented by an adjacency matrix defined as follows

$$\boldsymbol{A}_{jk} = \begin{cases} 0 & \ldots \text{if } j = k \\ 1 & \ldots \text{if } j \text{ and } k \text{ are connected} \\ 0 & \ldots \text{if } j \text{ and } k \text{ are not connected} \end{cases} \quad (1)$$



Supplementary Fig. 4 | Construction of structure graph for NaCl. a, Structure of NaCl. **b, c,** Na-centered (**b**) and Cl-centered (**c**) subgraphs. **d, e,** Adjacency matrices of the subgraphs.

This matrix is used for evaluating the isomorphism among different structures. Supplementary Fig. 5 shows the example of two isomorphic graphs. Two structures may be considered as topologically identical whenever there is a bijective mapping between their structure graphs. This mapping is performed on all the subgraphs via the algorithm shown in Supplementary Fig. 6. The application of this algorithm to the database of bulk compounds can assist in the automatic deduplication of crystal structures. When applied to LDMs, this algorithm makes possible the classification of structural prototypes, which only takes into account the topological information of materials.



Original Node	Mapping Node
A	2
B	5
C	1
D	3
E	4
F	6

Supplementary Fig. 5 | Isomorphic graphs.

Input: structure A, B

Output: True or False (if A and B are isomorphic)

```
a=generateGraph(A)
b=generateGraph(B)
flagA=[False*A's atom number]
for each atom atom_a ∈A do:
    Ga(V,E)=constructgraph(a,atom_a)
    InDepthOrder=[0,1,.....A_Natom]
    for each atom atom_b ∈B do:
        Gb(V,E)=constructgraph(b,atom_b)
        result=graphIsomorphic(Ga,Gb,InDepthOrder)
    flagA[atom_a]=(if any result is True)
flagB=[False*B_Natom]
exchange(A,B)
repeatJudgeProcess()
return (if flagA is all True && flagB is all True)
```

Subroutine graphIsomorphic(Ga,Gb,InDepthOrder)

```
if(InDepthOrder is finish)
    Ga is isomorphic to Gb
    return True
else if(InDepthOrder is not finish && Gb's all node is used)
    Ga is not isomorphic to Gb
    return False
else
    for each unused node target in Gb do:
        if(InDepthOrder[i],target connectivity is same)
            InDepthOrder moves next
            return graphIsomorphic(Ga,Gb,InDepthOrder)
        else
            Backtrack for InDepthOrder previous status or next target
```

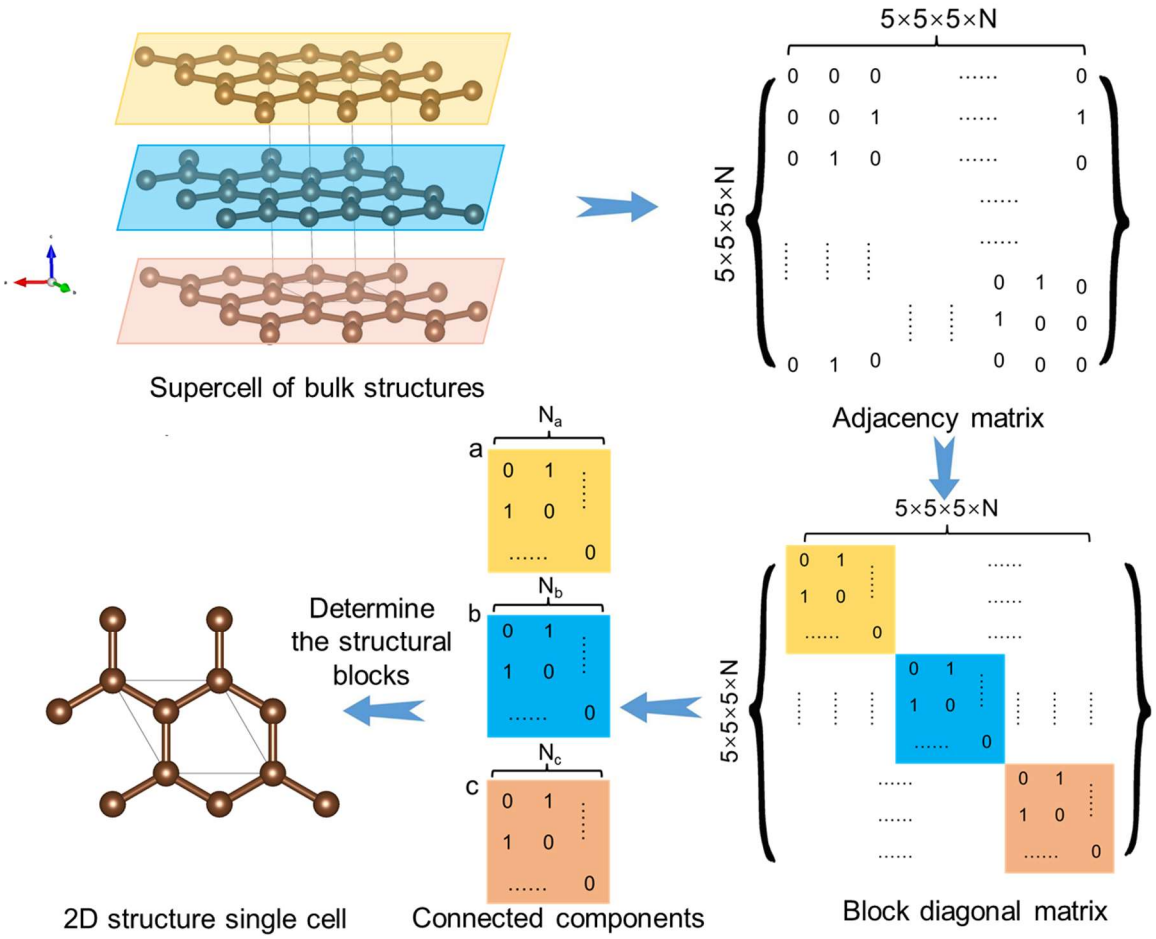
Supplementary Fig. 6 | Pseudo-code for determining the isomorphism of two structures.

To determine the chemically connected structural blocks in bulk materials, a structure graph based on the 5×5×5 supercell of the compound is employed. All atoms in the supercell are included as nodes. The corresponding adjacency matrix can be transformed into block diagonal matrix. For example, if matrix $\boldsymbol{A}$ can be blocked into three smaller square matrices $\boldsymbol{A_1'}$, $\boldsymbol{A_2'}$ and $\boldsymbol{A_3'}$, with zero matrices $\mathbf{0}$, then we have:

$$\boldsymbol{A'} = \boldsymbol{Q}^{-1}\boldsymbol{A}\boldsymbol{Q} = \begin{pmatrix} \boldsymbol{A_1}' & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{A_2}' & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \boldsymbol{A_3}' \end{pmatrix} \tag{2}$$

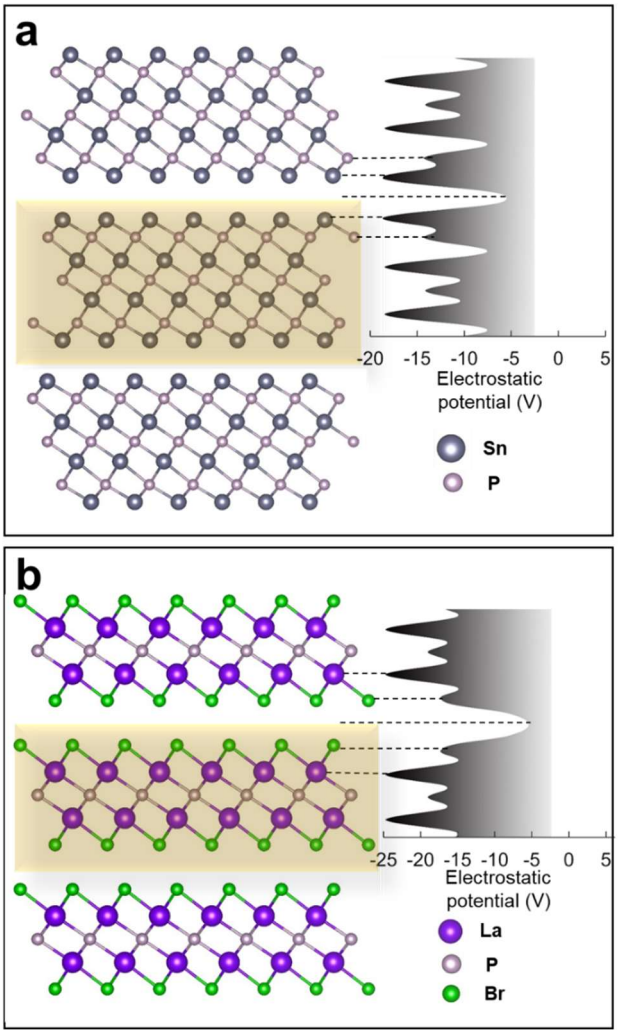
From the reduced matrices $\boldsymbol{A_1'}$, $\boldsymbol{A_2'}$ and $\boldsymbol{A_3'}$, we can identify the structural blocks and determine their dimensionality. We consider an example where graphene is extracted from the structure of graphite, as shown in Supplementary Fig. 7. Supercell is built and converted into a different structure graph from

that of the unit cell. The new structure graph is represented by an adjacency matrix of order 5×5×5×N (N is the number of atoms per unit cell). After matrix transformations, a block diagonal matrix is obtained, in which each block corresponds to an assembly of chemically connected atoms in the supercell. The structural blocks can be uniquely constructed according to the matrix and are isolated into low-dimensional structures. It is worth noting that there exist cases where the structural blocks are off-stoichiometric with respect to the parent bulk compounds. The derived LDMs tend to undergo significant structural reconstruction due to the change in valency. Therefore, in order to avoid unrealistic predictions, these cases are left out of consideration in the present work.



Supplementary Fig. 7 | Identification of structural blocks using the structure graph of supercell. Based on the adjacency matrix, the structure of 2D graphene can be extracted from supercell structure graph of graphite.

Sn_4P_3 and La_2PBr_2 (Supplementary Fig. 8) are two representative compounds that according to our calculations, exhibit the potential for exfoliation into 2D atomic layers, while not yet in the list of 2D compounds in previous studies. Conventional approaches rely on the van der Waals radii, which tend to classify the Sn-Sn and Br-Br bonds as connected[8], contradicting the DFT calculated electrostatic potentials (insets in Supplementary Fig. 8) which reveal a relatively weak interaction between neighboring structural blocks in both materials and suggest the possibility of exfoliation. We believe that a prior classification of covalent, ionic and metallic interactions between possible neighboring atoms can help determine the proper choice of atomic radii, thus yielding the bonding cutoff distances in a precise way.



Supplementary Fig. 8 | Structures of Sn_4P_3 and La_2PBr_2. a, b, Structural blocks of Sn_4P_3 (**a**) and La_2PBr_2 (**b**), and the corresponding plane-averaged electrostatic potentials along the layer normal.

2 Density functional theory calculations

2.1 Parameters setting

Structural optimization and energy calculations were performed via PWmat code[9,10], which is a plane wave pseudopotential package based on DFT and accelerated by GPU architecture. The Perdew–Burke–Ernzerhof (PBE)[11] generalized gradient approximation (GGA) functional and NCPP-SG15-PBE pseudopotential were used. The electron wave functions were expanded by plane waves with cutoff energies of 50 Ryd (680 eV). The convergence tolerance for total energy and residual force on each atom during structure relaxation were set to 10^{-5} eV and 0.02 eV/Å, respectively. In all the calculations, the Brillouin zone was sampled by Monkhorst-Pack *k*-point grid[12] with density of at least 1000/(the number of atoms per cell). To complement the deficiencies of DFT in treating dispersion interactions, a van der Waals correction term developed by Grimme[13] was adopted. Spin polarization was taken into consideration and the ferromagnetic configuration was set as the initial magnetic structure. To avoid spurious interactions between periodic images, a space vacuum of at least 8 Å was placed between atomic layers, while for atomic chains and clusters, the periodic images were at least 10 Å apart.

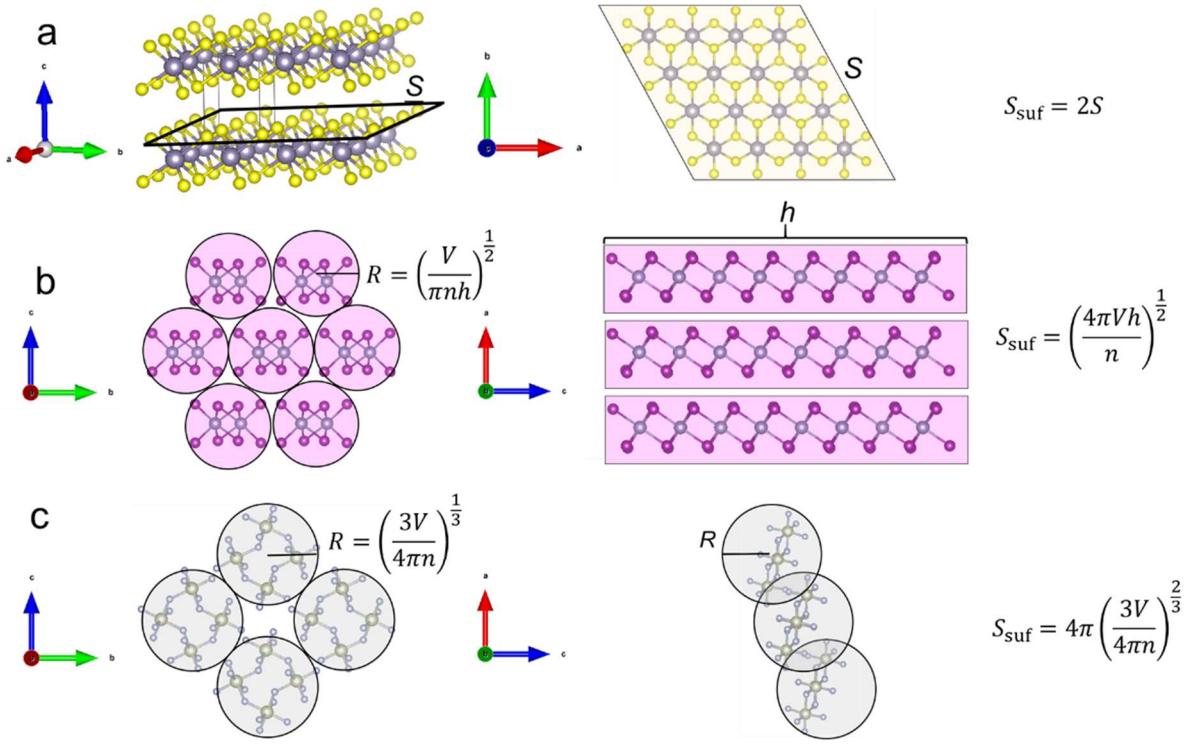
The calculations of Bader charge, electron density distribution and electron localization function were performed on Vienna ab initio simulation package (VASP)[14,15] using the plane-wave projector-augmented wave method[16] and GGA-PBE functional. Energy cutoff was set to 520 eV and the *k*-point sampling was the same as that in PWmat calculations. Based on the density of states (DOS) from VASP calculations, the crystal orbital Hamilton populations (COHP)[17,18] was calculated using Local Orbital Basis Suite Towards Electronic-Structure Reconstruction (LOBSTER) code[19,20].

2.2 Exfoliation energy

The exfoliation energy per surface area for the LDMs is calculated as follow:

$$E_{\mathrm{exf}} = \frac{E_{\mathrm{iso}} - E_{\mathrm{bulk}}/n}{S_{\mathrm{suf}}} \tag{3}$$

where E_{iso} is the total energy of the LDM per unit cell, E_{bulk} is the total energy of the parent bulk compound consisting of n structural blocks (each structural block corresponds to a unit cell of LDM), and S_{suf} is the effective surface area of the LDM. For 2D materials, the S_{suf} is defined as double the in-plane area (S) of the bulk unit cell. To calculate the effective surface area of 1D and 0D compounds, we treat an atomic chain as a cylinder and an atomic cluster as a sphere. Their volumes are estimated by dividing the volumes of their parent bulk compounds by n. The surface area is then derived according to the calculated volume, as shown in Supplementary Fig. 9.



Supplementary Fig. 9 | The effective surface area for 2D, 1D and 0D materials. a, 2D atomic layers. **b,** 1D atomic chains. **c,** 0D atomic clusters.

Supplementary Table 2 lists the calculated exfoliation energies of several well-known 2D atomic layers. The values obtained in this work are consistent with previous studies[8,21]. The threshold for potentially exfoliable LDMs is given by the upper bound of these values, i.e. 52.60 meV/Å^2, close to the threshold set by other researchers[8].

Supplementary Table 2 | Exfoliation energy of typical 2D materials

2D materials	Exfoliation energy (meV/Å^2)
C (graphene)	13.11
P (phosphorene)	12.63
BN	11.95
MoS_2	6.70
GaS	52.60
$PtSe_2$	22.04

2.3 Electronic structure

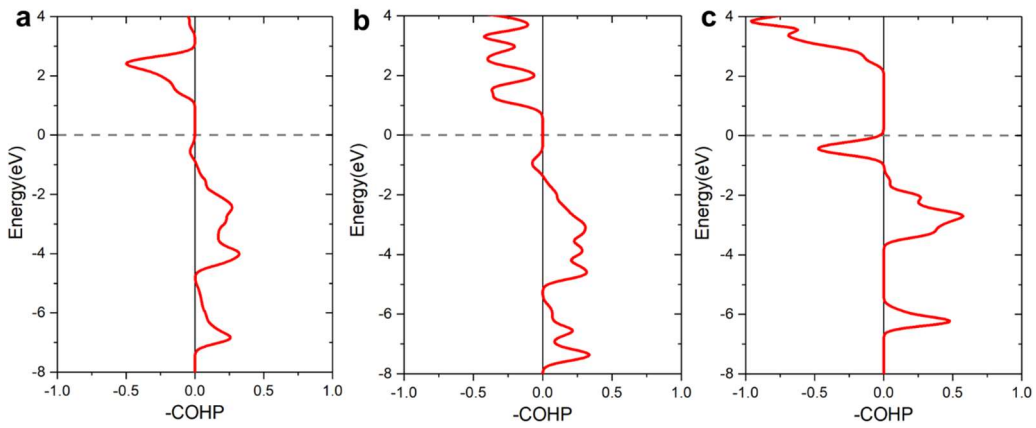
Bader charges of Sn, S and Br ions are tabulated in Supplementary Table 3. The calculated charges on Sn ion fall into two classes: 0.8~1.1 and ~1.5. Given that the change transfer is generally underestimated by the Bader analysis, the above values are expected to correspond to Sn^{2+} and Sn^{4+}.

Supplementary Table 3 | Bader charge of different ions in SnS_2, Sn_2S_3 and $SnBr_2$

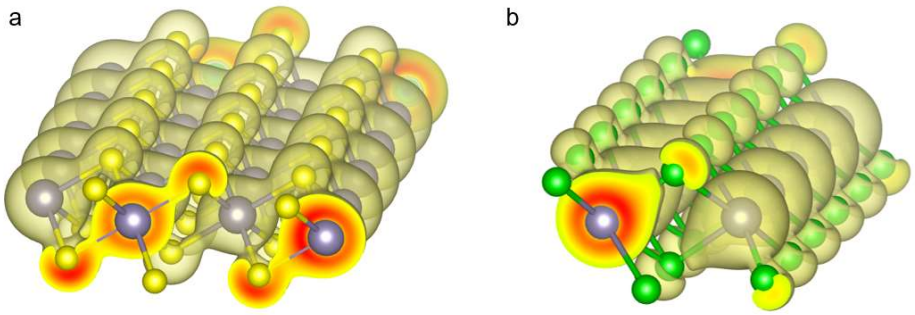
Bader charge (*e*)					
2D SnS_2		**1D Sn_2S_3**		**1D $SnBr_2$**	
Sn	1.54	$Sn^{(1)}$	0.88	Sn	1.09
S	−0.77	$Sn^{(2)}$	1.54	Br	−0.55
		$S^{(1)}$	−0.83		
		$S^{(1)}$	−0.79		

COHP analysis is essential to assess the bonding character between Sn and anions. We follow the conventional denotation of bonding (positive values) and antibonding (negative values) states and present –COHP in Supplementary Fig. 10. It is noted that for Sn_2S_3 and $SnBr_2$, the Sn-*s* and S/Br-*p* orbitals overlap in the energy range of −7 ~ −5 eV where the –COHP is positive, indicating bonding interaction between Sn and anions. A relatively strong orbital overlap is also observed near the valence band maximum, which presents antibonding character. Hence, there appears to be a strong coupling

between the Sn *s* and anion *p* states. This conclusion is also substantiated by the charge density between −7 and −5 eV shown in Supplementary Fig. 11.



Supplementary Fig. 10 | COHP for Sn-anion bonds. a, Sn-S in SnS_2. **b,** Sn-S in Sn_2S_3. **c,** Sn-Br in $SnBr_2$. Energies are referenced to the Fermi level.



Supplementary Fig. 11 | Charge density of states between −7 and −5 eV vs. the Fermi energy. a, Sn_2S_3. **b,** $SnBr_2$. Color code: Sn grey, S yellow, and Br green.

2.4 Electron localization function

Electron localization function (ELF)[22] is a measure of the conditional probability of finding an electron in the neighborhood of another electron with the same spin. The extent of spatial localization of electrons can be estimated using this approach. That is to say, the electron pair probability in multi-electronic systems can be rigorously mapped and quantified. ELF is calculated as follows:

$$\mathrm{ELF} = \frac{1}{1+(D/D^0)^2} \tag{4}$$

$$D = \frac{1}{2}\sum_i^{occ}|\nabla\varphi_i|^2 - \frac{|\nabla\rho|^2}{8\rho} \tag{5}$$

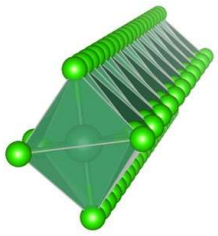
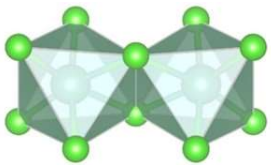
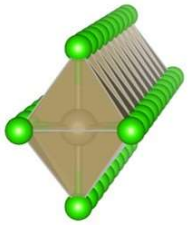
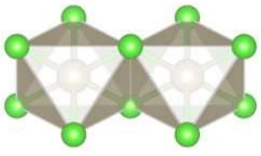
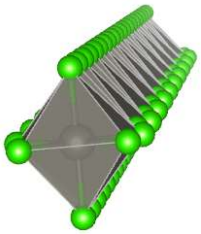
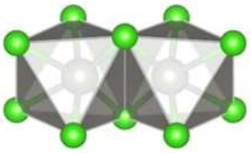
$$D^0 = \frac{3}{10}(3\pi^2)^{5/3}\rho^{5/3} \tag{6}$$

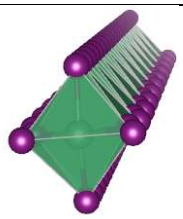
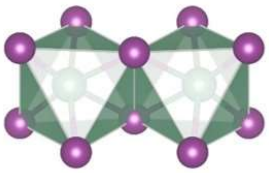
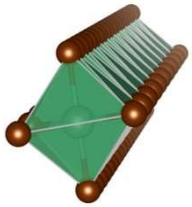
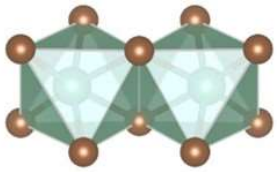
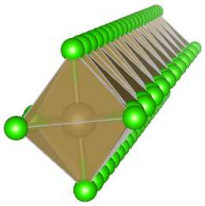
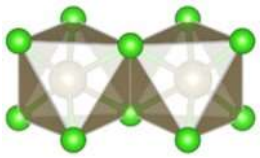
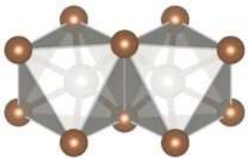
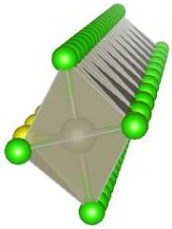
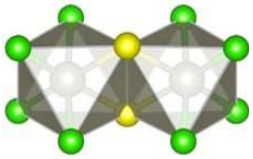
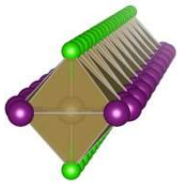
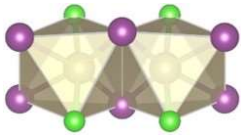
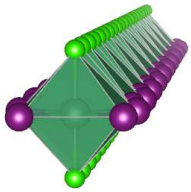
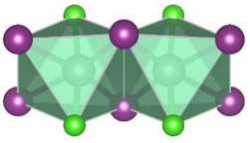
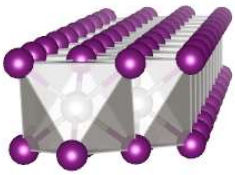
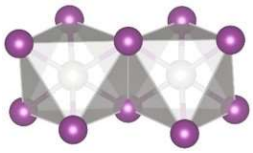
where φ_i denotes spin ortibal and ρ is the electron spin density. D^0 is the counterpart of D for non-interaction homogenous electron gas. ELF varies within the range of [0,1]. A higher ELF value corresponds to a more localized distribution of electrons, generally indicating that there is covalent bonding, a lone electron pair or the inner shell of an atom[22-24].

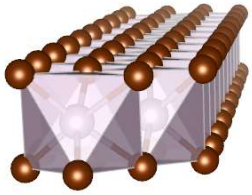
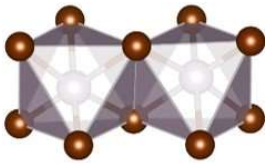
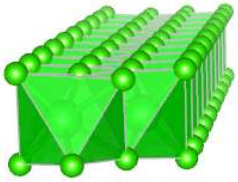
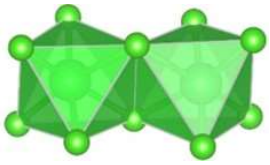
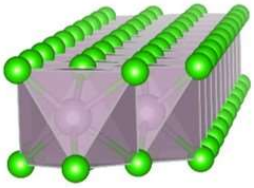
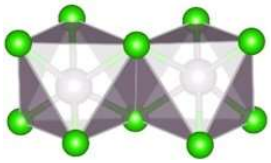
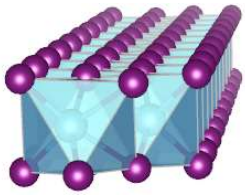
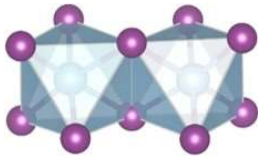
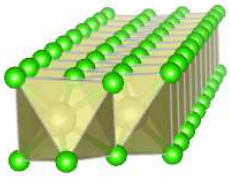
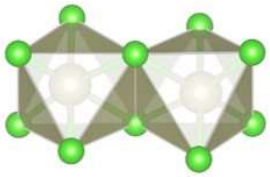
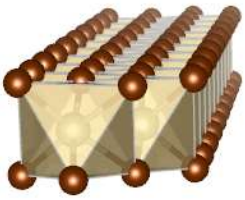
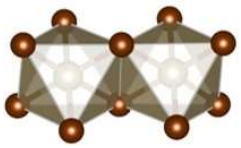
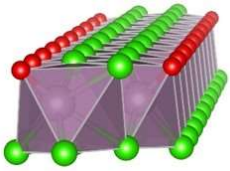
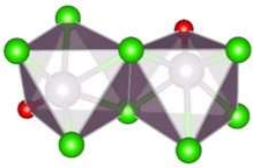
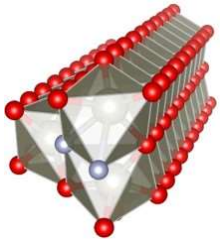
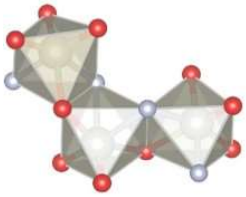
3 Representative 1D and 0D materials

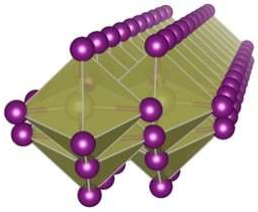
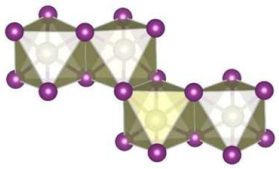
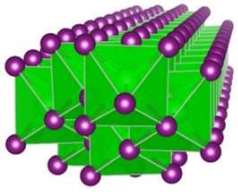
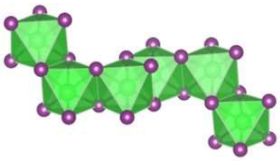
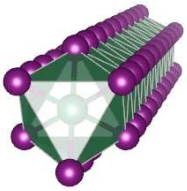
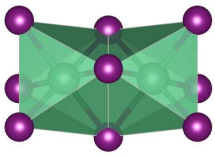
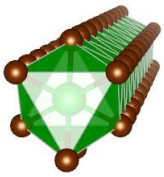
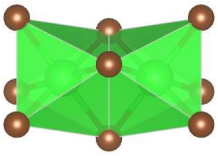
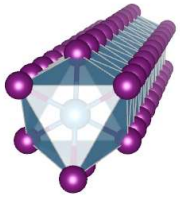
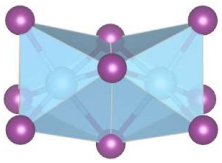
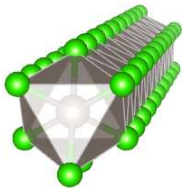
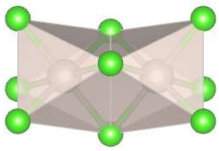
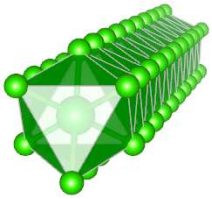
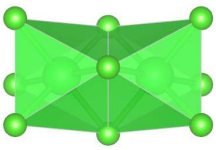
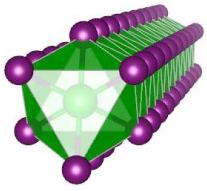
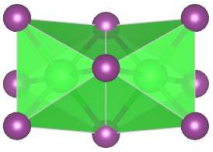
3.1 1D atomic chains

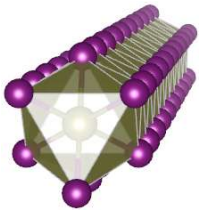
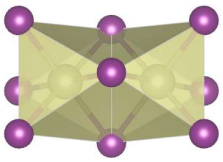
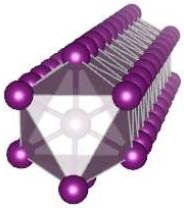
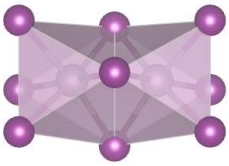
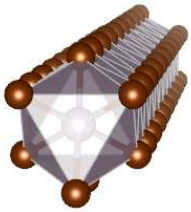
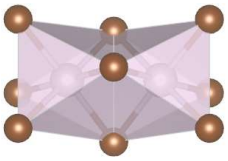
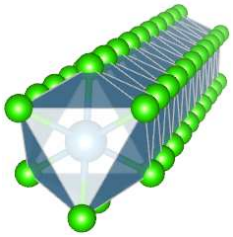
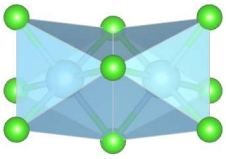
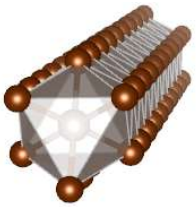
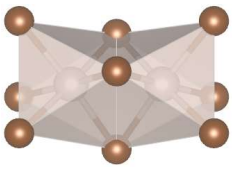
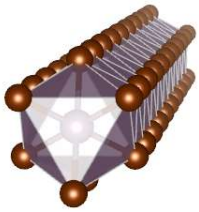
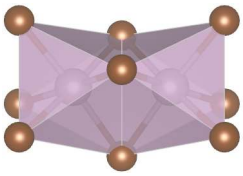
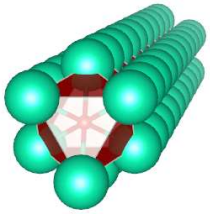
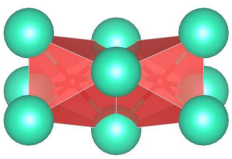
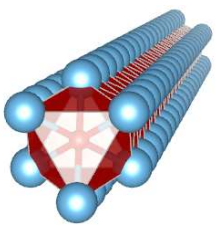
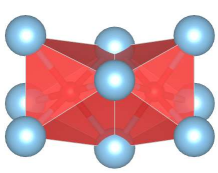
Supplementary Table 4 | The formula, structure, structure unit, and ICSD number (parent bulk crystal) of the representative 1D materials

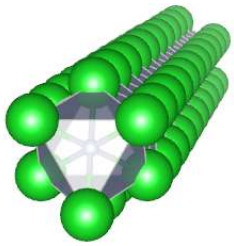
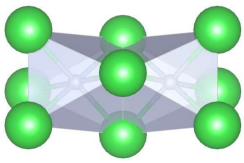
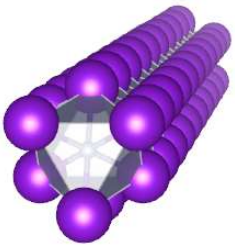
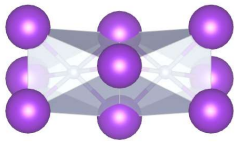
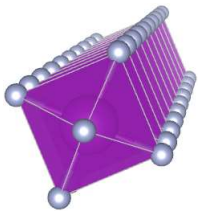
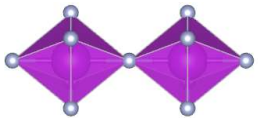
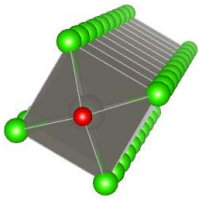
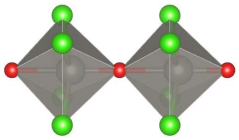
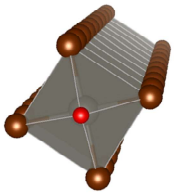
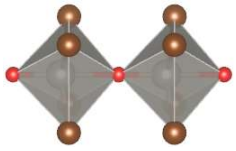
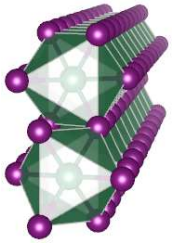
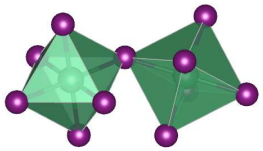
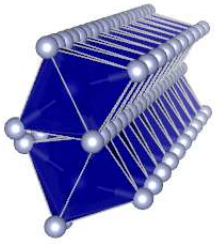
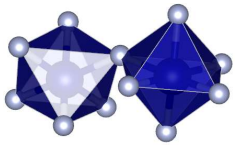
Type	Formula	Structure	Structure unit	Element	ICSD
1	$NbCl_4$			Nb Cl	1010
1	$OsCl_4$			Os Cl	1165
1	WCl_4			W Cl	165263

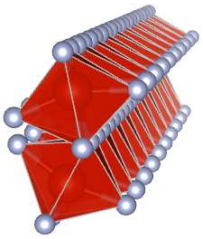
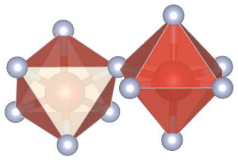
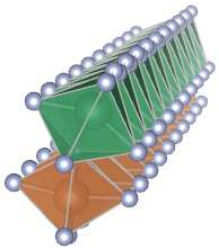
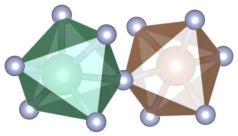
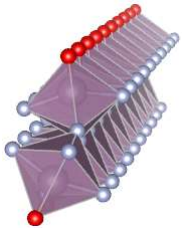
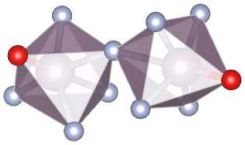
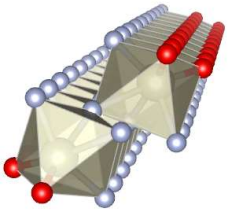
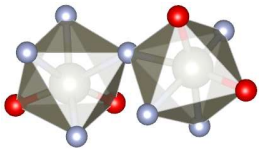
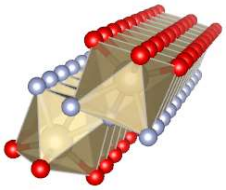
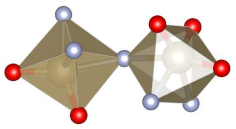
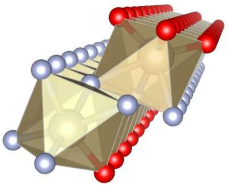
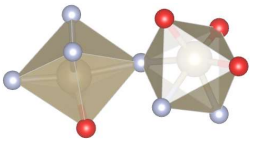
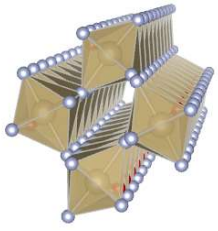
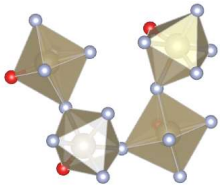
1	NbI_4			Nb I	23916
1	$NbBr_4$			Nb Br	239640
1	$TaCl_4$			Ta Cl	402406
1	WBr_4			W Br	423461
1	$ReSCl_3$			Re S Cl	429458
1	TaI_2Cl_2			Ta I Cl	69688
1	NbI_2Cl_2			Nb I Cl	407489
1	PtI_4			Pt I	15173

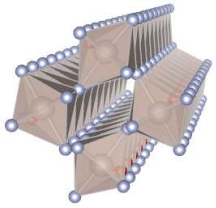
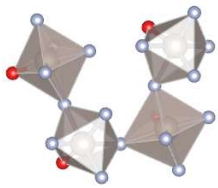
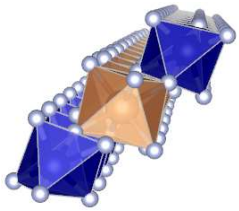
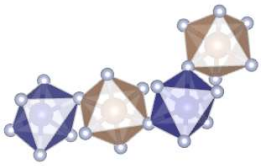
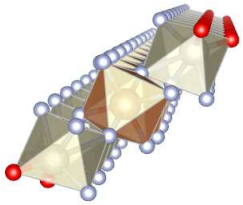
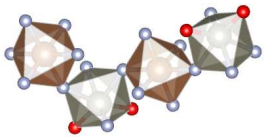
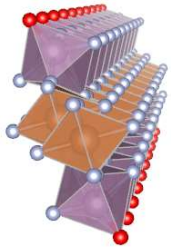
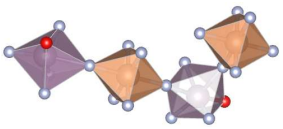
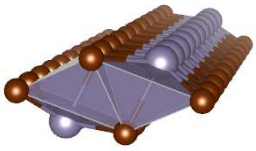
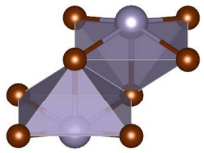
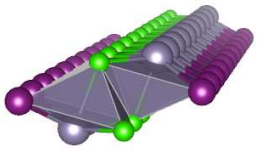
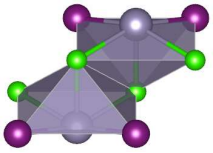
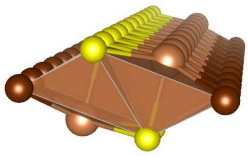
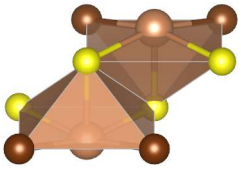
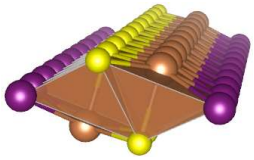
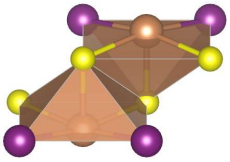
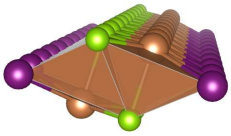
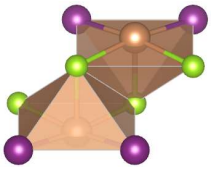
1	$TcBr_4$			Tc Br	260163
1	$ZrCl_4$			Zr Cl	26049
1	$TcCl_4$			Tc Cl	26055
1	TiI_4			Ti I	39820
1	$HfCl_4$			Hf Cl	402054
1	$OsBr_4$			Os Br	61042
1	$MoOCl_3$			Mo O Cl	16150
1	ReO_3F			Re O F	415418

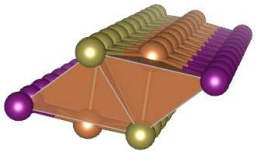
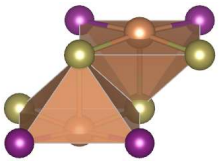
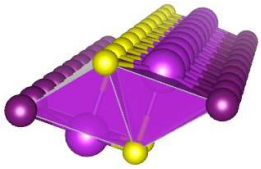
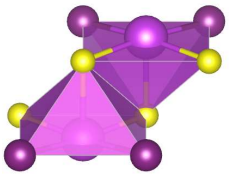
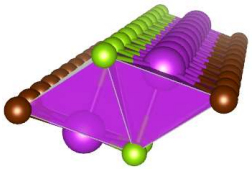
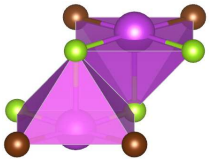
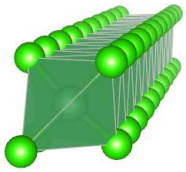
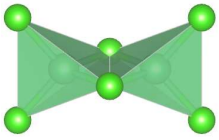
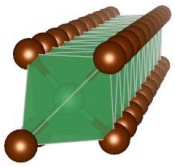
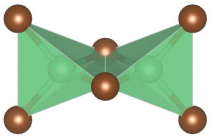
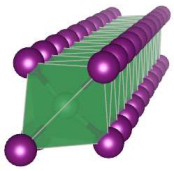
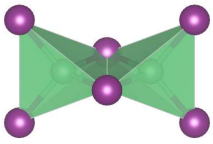
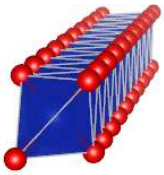
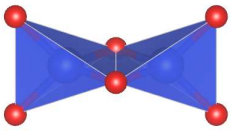
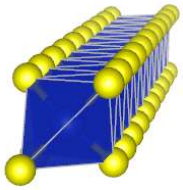
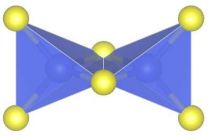
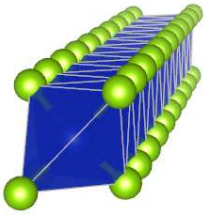
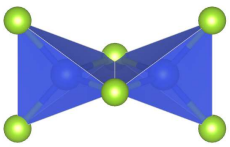
1	HfI_4			Hf I	200826
1	ZrI_4			Zr I	8068
2	NbI_3			Nb I	109145
2	$ZrBr_3$			Zr Br	165302
2	TiI_3			Ti I	173784
2	$RuCl_3$			Ru Cl	22090
2	$ZrCl_3$			Zr Cl	23163
2	ZrI_3			Zr I	23946

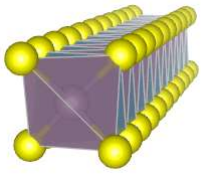
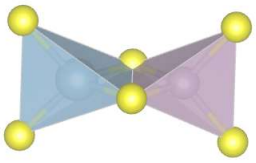
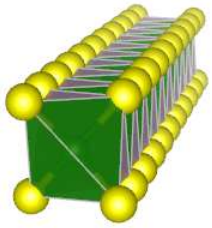
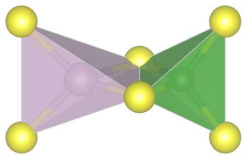
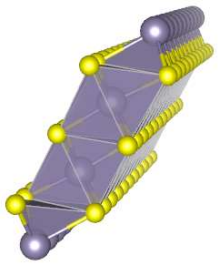
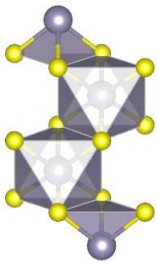
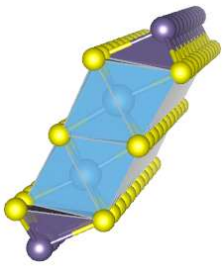
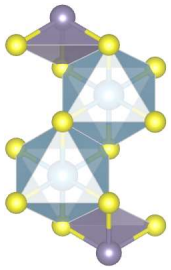
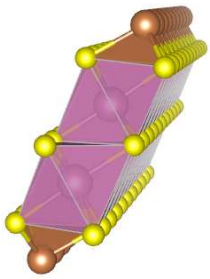
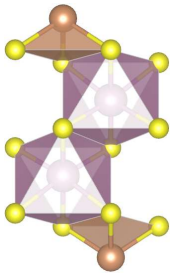
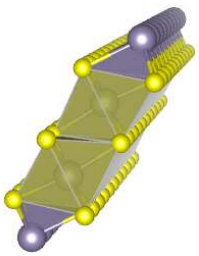
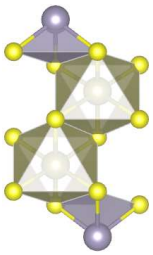
2	HfI_3			Hf I	23947
2	MoI_3			Mo I	242166
2	$TcBr_3$			Tc Br	260162
2	$TiCl_3$			Ti Cl	26069
2	$RuBr_3$			Ru Br	28119
2	$MoBr_3$			Mo Br	413690
2	Cs_3O			Cs O	15695
2	Ti_3O			Ti O	23575

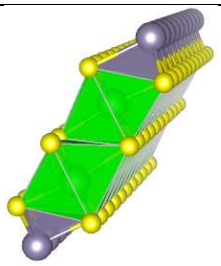
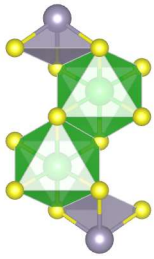
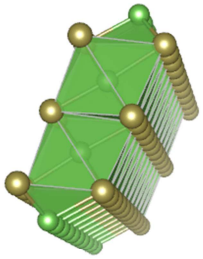
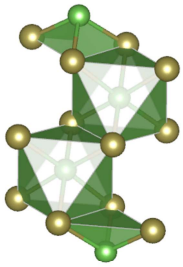
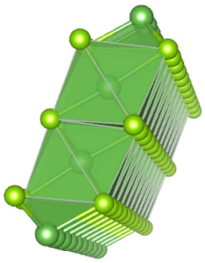
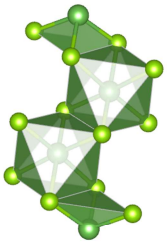
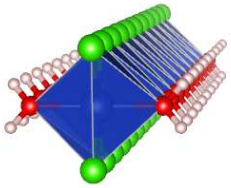
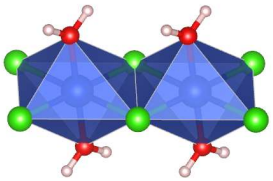
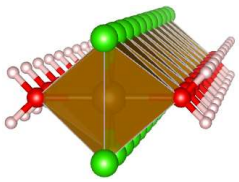
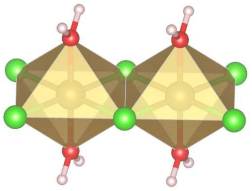
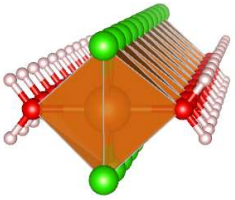
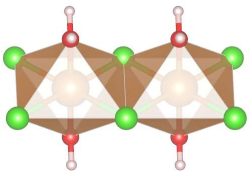
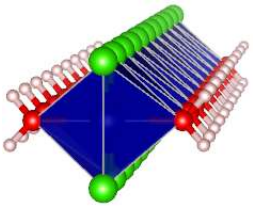
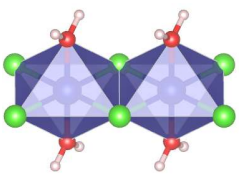
2	Ba_3N			Ba N	77730
2	K_3N			K N	99999
3	BiF_5			Bi F	25023
3	$WOCl_4$			W O Cl	25519
3	$WOBr_4$			W O Br	49547
3	NbI_5			Nb I	25503
3	CrF_5			Cr F	419661

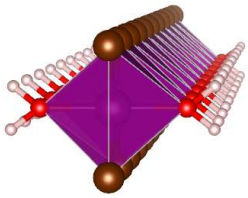
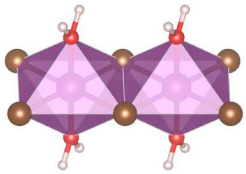
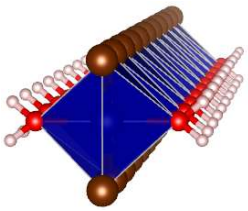
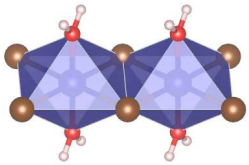
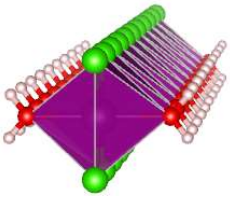
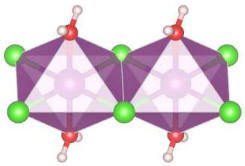
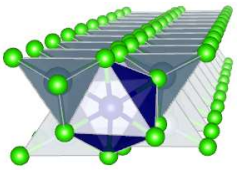
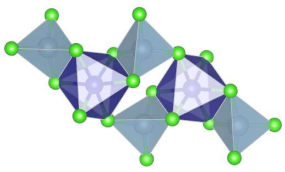
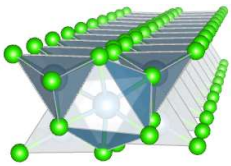
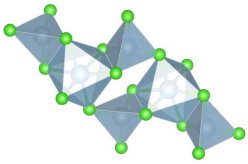
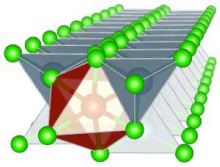
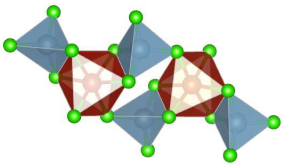
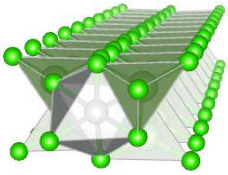
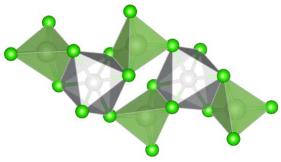
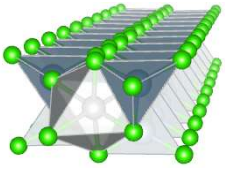
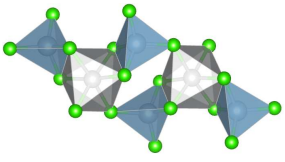
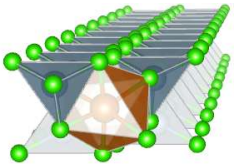
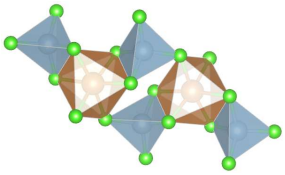
3	VF_5			V F	9887
3	$NbSbF_{10}$			Nb Sb F	16095
3	$MoOF_4$			Mo O F	16867
3	ReO_2F_3			Re O F	415421
3	OsO_3F_2			Os O F	73732
3	$Os_2O_4F_6$			Os O F	240330
3	$OsOF_4$			Os O F	417245

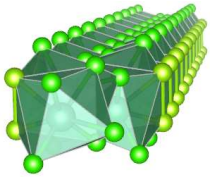
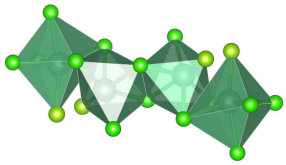
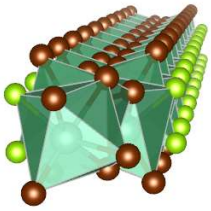
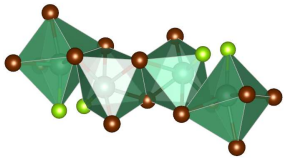
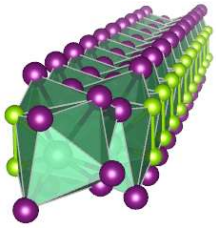
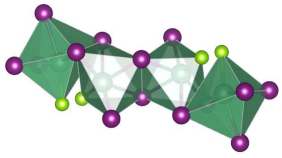
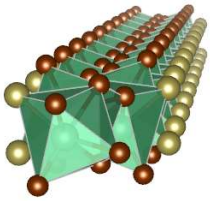
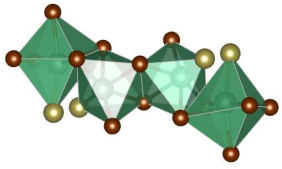
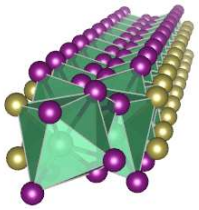
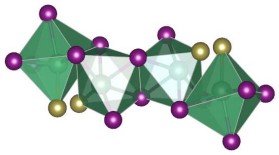
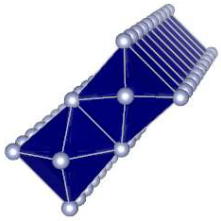
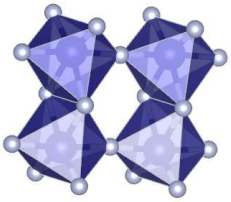
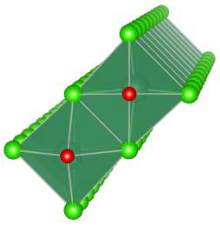
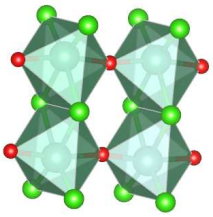
3	$RuOF_4$			Ru O F	417248
3	$CrSbF_{10}$			Cr Sb F	419662
3	$SbReO_2F_8$			Sb Re O F	280248
3	$MoSbOF_9$			Mo Sb O F	201410
4	$SnBr_2$			Sn Br	411177
4	SnICl			Sn I Cl	23262
4	SbSBr			Sb S Br	25571
4	SbSI			Sb S I	25572
4	SbSeI			Sb Se I	31292

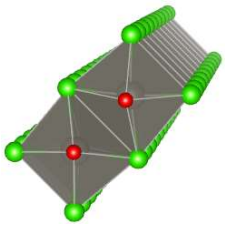
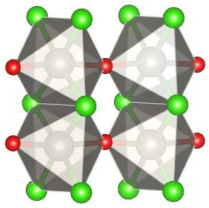
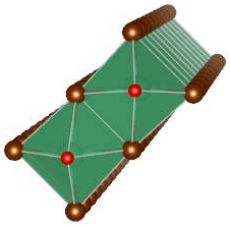
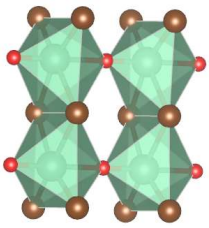
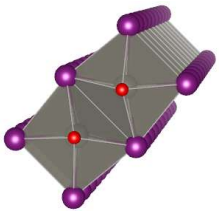
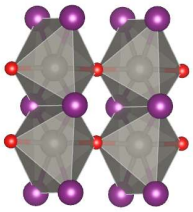
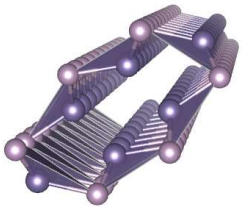
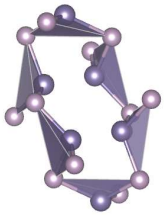
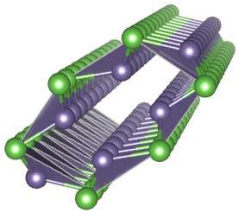
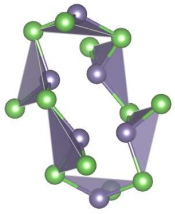
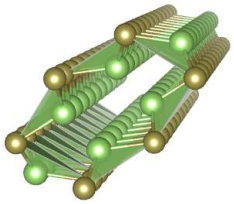
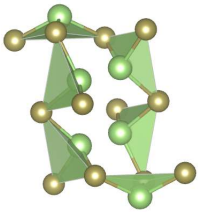
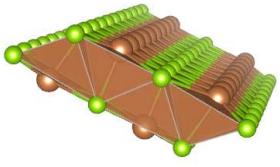
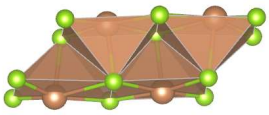
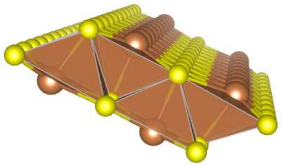
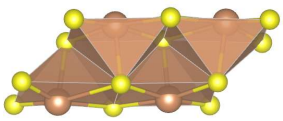
4	SbTeI			Sb Te I	31355
4	BiSI			Bi S I	25575
4	BiSeBr			Bi Se Br	76649
5	$BeCl_2$			Be Cl	31696
5	$BeBr_2$			Be Br	92584
5	BeI_2			Be I	92585
5	SiO_2			Si O	25632
5	SiS_2			Si S	26858
5	$SiSe_2$			Si Se	24592

5	$AlPS_4$			Al P S	15910
5	BPS_4			B P S	24618
6	Sn_2S_3			Sn S	15338
6	$GeTiS_3$			Ge Ti S	263128
6	$SbInS_3$			Sb In S	300207
6	$HfSnS_3$			Hf Sn S	65667

6	$ZrSnS_3$			Zr Sn S	73711
6	As_2Te_3			As Te	18208
6	As_2Se_3			As Se	611373
7	$CuCl_2{\cdot}2H_2O$			Cu Cl H O	15087
7	$FeCl_2{\cdot}2H_2O$			Fe Cl H O	15597
7	$MgCl_2{\cdot}2H_2O$			Mg Cl H O	172992
7	$CoCl_2{\cdot}2H_2O$			Co Cl H O	22082

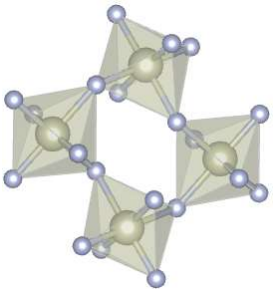
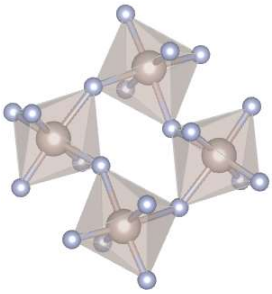
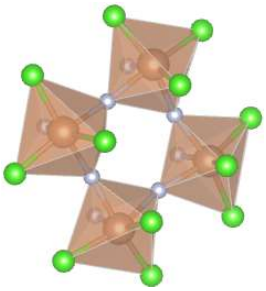
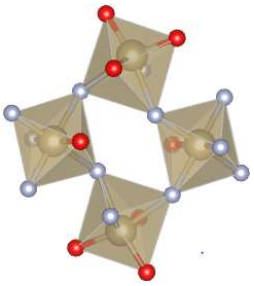
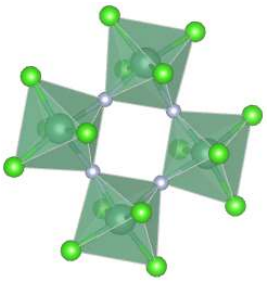
7	$MnBr_2 \cdot 2H_2O$			Mn Br H O	22084
7	$CoBr_2 \cdot 2H_2O$			Co Br H O	22085
7	$MnCl_2 \cdot 2H_2O$			Mn Cl H O	15596
8	$CoAl_2Cl_8$			Co Al Cl	22143
8	$TiAl_2Cl_8$			Ti Al Cl	39565
8	VAl_2Cl_8			V Al Cl	415951
8	$NiGa_2Cl_8$			Ni Ga Cl	417870
8	$NiAl_2Cl_8$			Ni Al Cl	417872
8	$MgAl_2Cl_8$			Mg Al Cl	62046

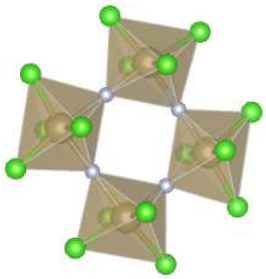
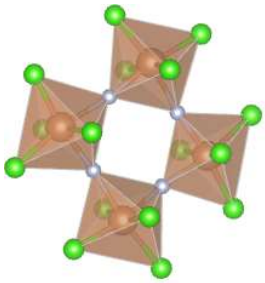
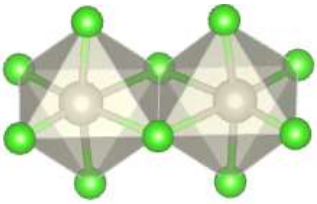
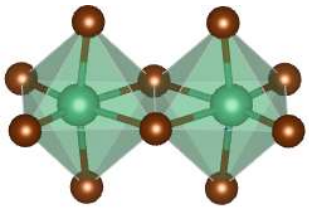
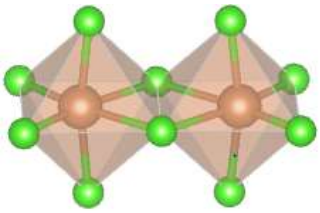
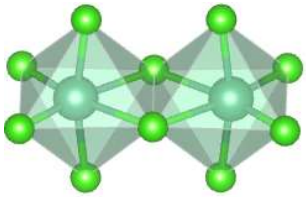
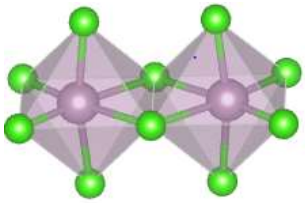
9	$NbSeCl_3$			Nb Se Cl	172519
9	$NbSeBr_3$			Nb Se Br	35375
9	$NbSeI_3$			Nb Se I	410743
9	$NbTeBr_3$			Nb Te Br	35376
9	$NbTeI_3$			Nb Te I	35377
10	CrF_4			Cr F	78778
10	$NbOCl_3$			Nb O Cl	26471

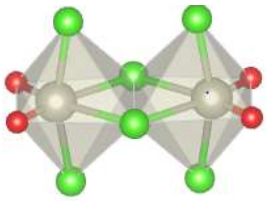
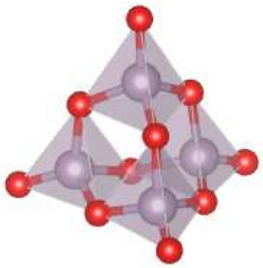
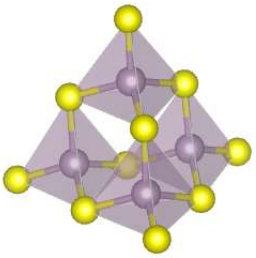
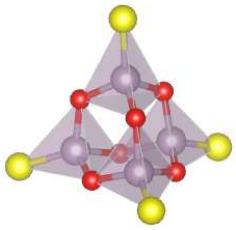
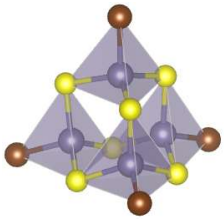
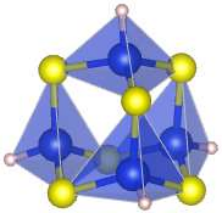
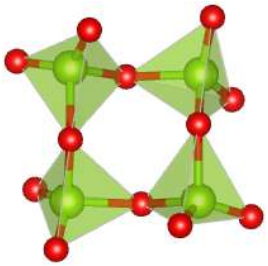
10	$WOCl_3$			W O Cl	416393
10	$NbOBr_3$			Nb O Br	418089
10	$WOBr_3$			W O Br	65183
11	Ge_6P_6			Ge P	427243
11	Ge_6As_6			Ge As	610598
11	Ga_6Te_6			Ga Te	153456
12	Sb_2Se_3			Sb Se	16680
12	Sb_2S_3			Sb S	171850

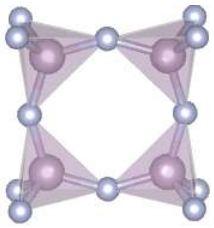
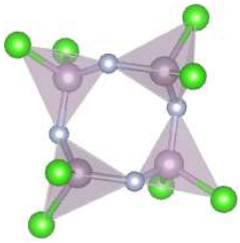
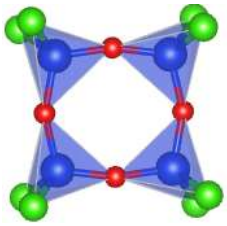
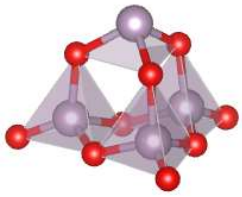
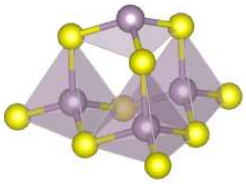
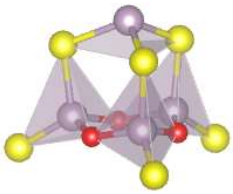
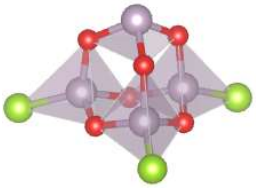
3.2 0D atomic clusters

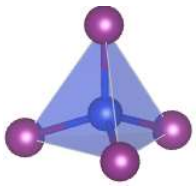
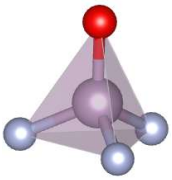
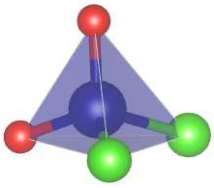
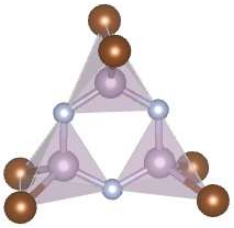
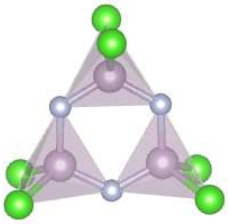
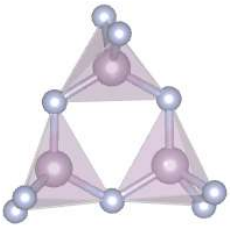
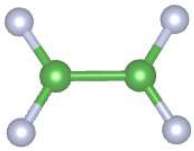
Supplementary Table 5 | The formula, structure, and ICSD number (parent bulk crystal) of the representative 0D materials

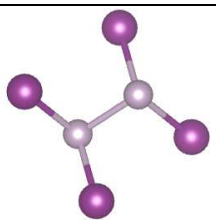
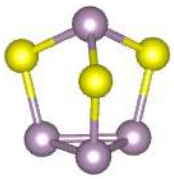
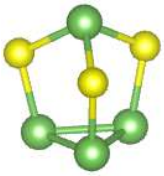
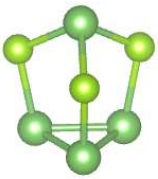
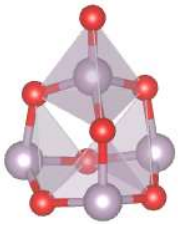
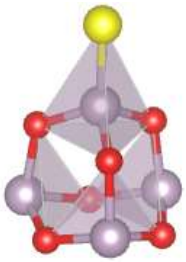
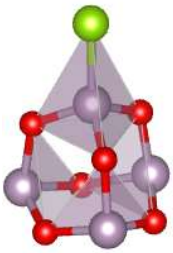
Type	Formula	Structure	Element	ICSD
1	Rh_4F_{20}		Rh F	10173
1	Ru_4F_{20}		Ru F	165397
1	$Sb_4Cl_{12}F_8$		Sb Cl F	200039
1	$Os_4F_{12}O_8$		Os F O	240331
1	$Nb_4Cl_{16}F_4$		Nb Cl F	26155

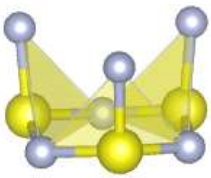
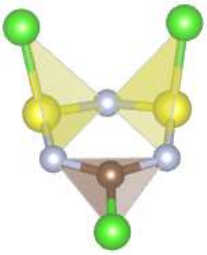
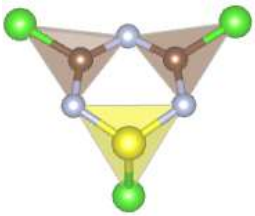
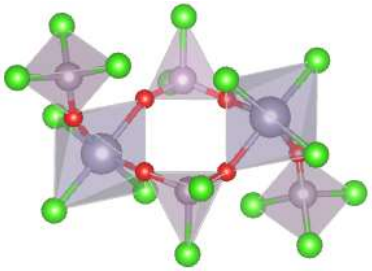
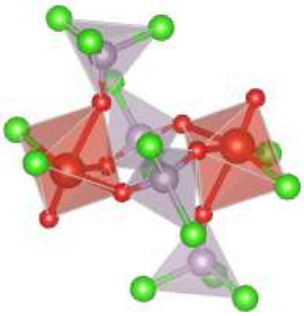
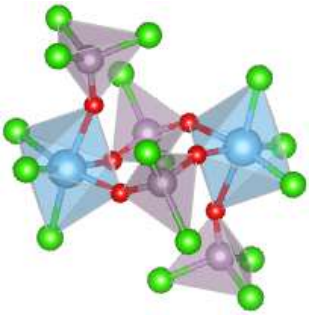
1	$Ta_4Cl_{16}F_4$		Ta Cl F	27413
1	$Sb_4Cl_{16}F_4$		Sb Cl F	30629
2	Re_2Cl_{10}		Re Cl	22139
2	Nb_2Br_{10}		Nb Br	409917
2	Sb_2Cl_{10}		Sb Cl	412110
2	Nb_2Cl_{10}		Nb Cl	66537
2	Mo_2Cl_{10}		Mo Cl	84622

2	$Re_2Cl_6O_4$		Re Cl O	416056
3	P_4O_{10}		P O	16610
3	P_4S_{10}		P S	174009
3	$P_4S_4O_6$		P S O	27058
3	$Ge_4S_6Br_4$		Ge S Br	24370
3	$Si_4S_6H_4$		Si S H	36379
4	Se_4O_{12}		Se O	18180

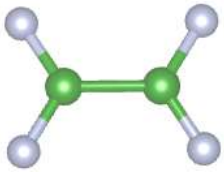
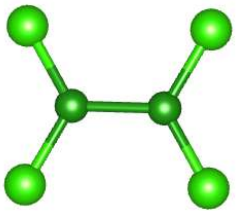
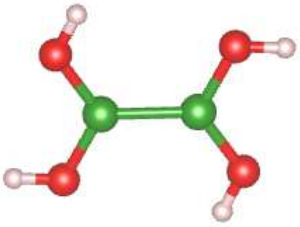
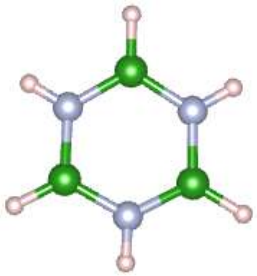
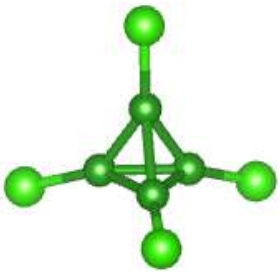
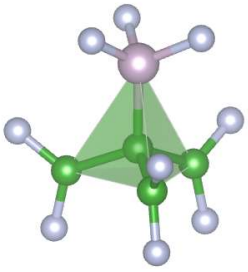
4	$P_4F_8N_4$		P F N	31038
4	$P_4Cl_8N_4$		P Cl N	33711
4	$Si_4Cl_8O_4$		S Cl O	71445
5	P_4O_9		P O	27434
5	P_4S_9		P S	26169
5	$P_4S_6O_3$		P S O	86494
5	$P_4Se_3O_6$		P Se O	404499

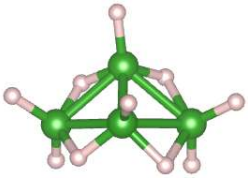
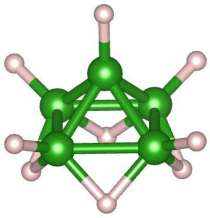
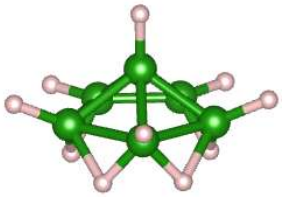
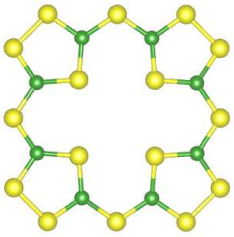
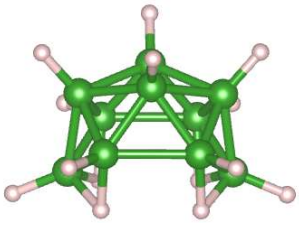
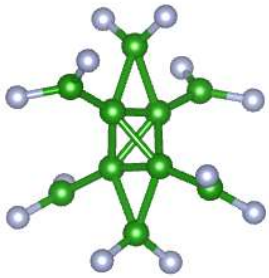
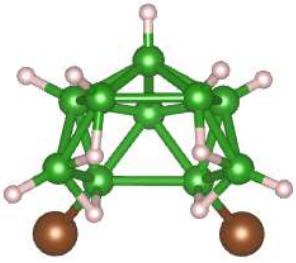
6	SiI_4		Si I	22100
6	PF_3O		P F O	250498
6	$CrCl_2O_2$		Cr Cl O	416750
7	$P_3Br_6N_3$		P Br N	109142
7	$P_3Cl_6N_3$		P Cl N	109272
7	$P_3F_6N_3$		P F N	26649
8	B_2F_4		B F	27867
8	B_2Cl_4		B Cl	14213

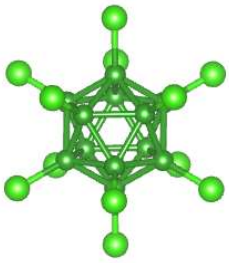
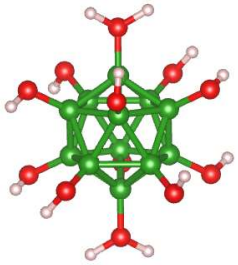
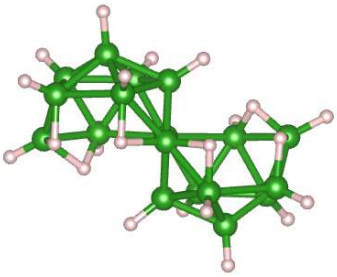
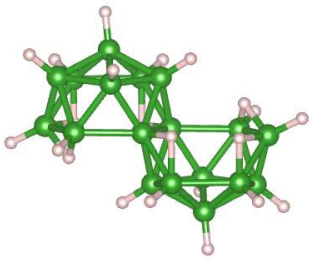
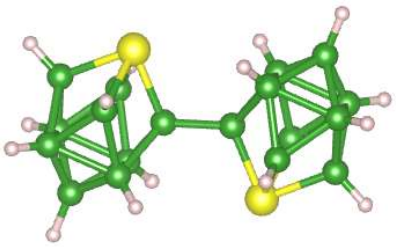
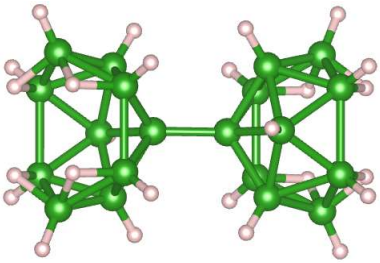
8	P_2I_4		P I	203216
9	P_4S_3		P S	406048
9	As_4S_3		As S	16105
9	As_4Se_3		As Se	611376
10	P_4O_7		P O	16321
10	P_4SO_6		P S O	69977
10	P_4SeO_6		P Se O	78782

11	$S_3F_3N_3$		S F N	21015
11	$S_2CCl_3N_3$		S C Cl N	86482
11	$SC_2Cl_3N_3$		S C Cl N	86483
12	$Sn_2P_4Cl_{16}O_6$		Sn P Cl O	26182
12	$V_2P_4Cl_{14}O_8$		V P Cl O	420125
12	$Ti_2P_4Cl_{16}O_6$		Ti P Cl O	65139

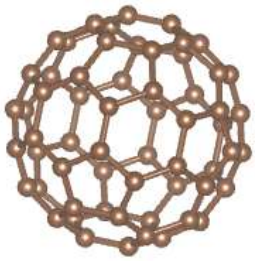
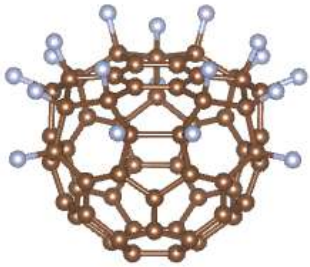
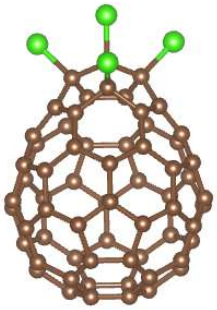
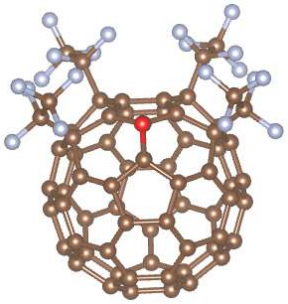
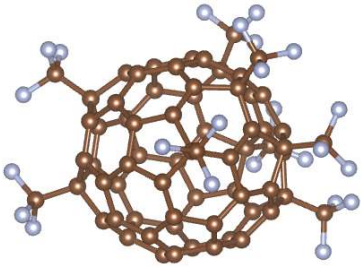
Supplementary Table 6 | The formula, structure, and ICSD number (parent bulk crystal) of 0D boron compounds

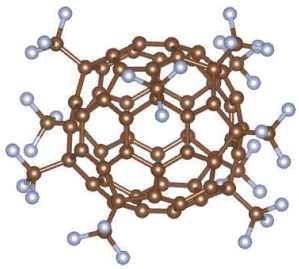
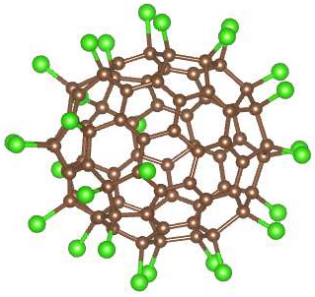
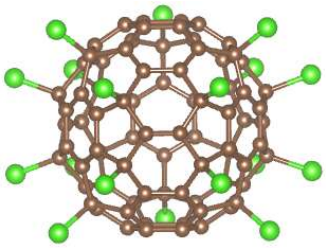
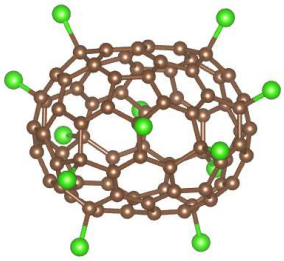
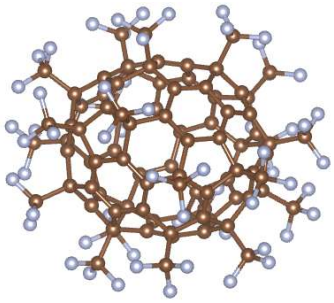
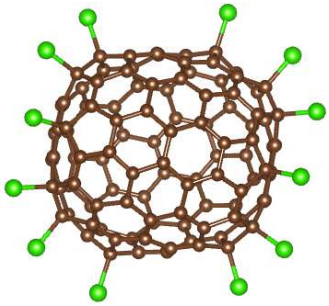
Formula	Structure	Element	ICSD
B_2F_4		B F	27867
B_2Cl_4		B Cl	14213
$B_2O_4H_4$		B O H	170953
$B_3N_3H_6$		B N H	401085
B_4Cl_4		B Cl	27872
B_4PF_9		P B F	15215

B_4H_{10}		B H	31695
B_5H_9		B H	24636
B_6H_{10}		B H	43253
B_8S_{16}		S B	15267
$B_{10}H_{14}$		B H	31566
$B_{10}F_{12}$		B F	412618
$B_{10}Br_2H_{12}$		Br B H	2303

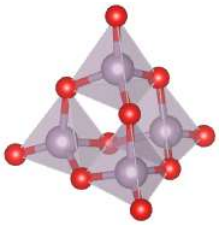
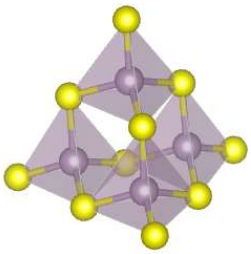
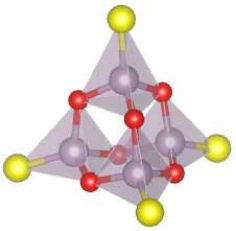
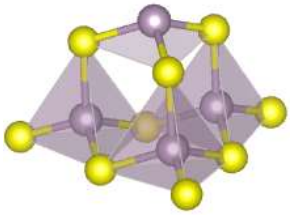
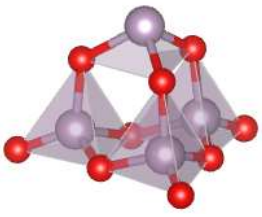
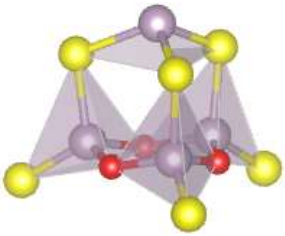
$B_{12}Cl_{12}$		Cl B	421891
$B_{12}O_{12}H_{14}$		B O H	170318
$B_{18}H_{22}$		B H	15802
$B_{18}H_{22}$		B H	15823
$B_{18}S_2H_{16}$		S B H	4003
$B_{20}H_{26}$		B H	279587

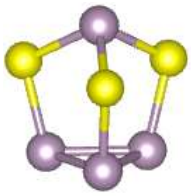
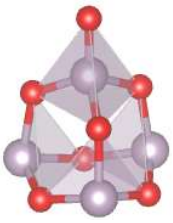
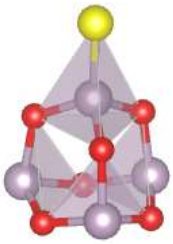
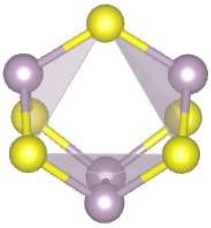
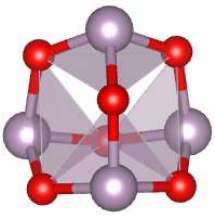
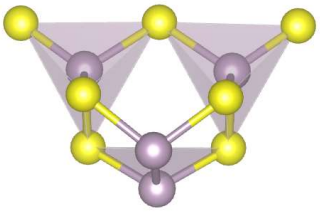
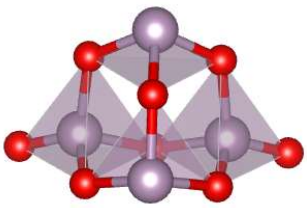
Supplementary Table 7 | The formula, structure, and ICSD number (parent bulk crystal) of fullerene-like carbon compounds

Formula	Structure	Element	ICSD
C_{60}		C	602518
$C_{60}F_{18}$		C F	95694
$C_{64}Cl_4$		C Cl	249692
$C_{68}OF_{20}$		O C F	249217
$C_{68}F_{24}$		C F	249154

$C_{70}F_{30}$		C F	249331
$C_{76}Cl_{28}$		C Cl	182903
$C_{78}Cl_{18}$		C Cl	249729
$C_{80}Cl_{12}$		C Cl	249788
$C_{90}F_{60}$		C F	263786
$C_{108}Cl_{12}$		C Cl	252548

Supplementary Table 8 | The formula, structure, and ICSD number (parent bulk crystal) of 0D phosphorus compounds

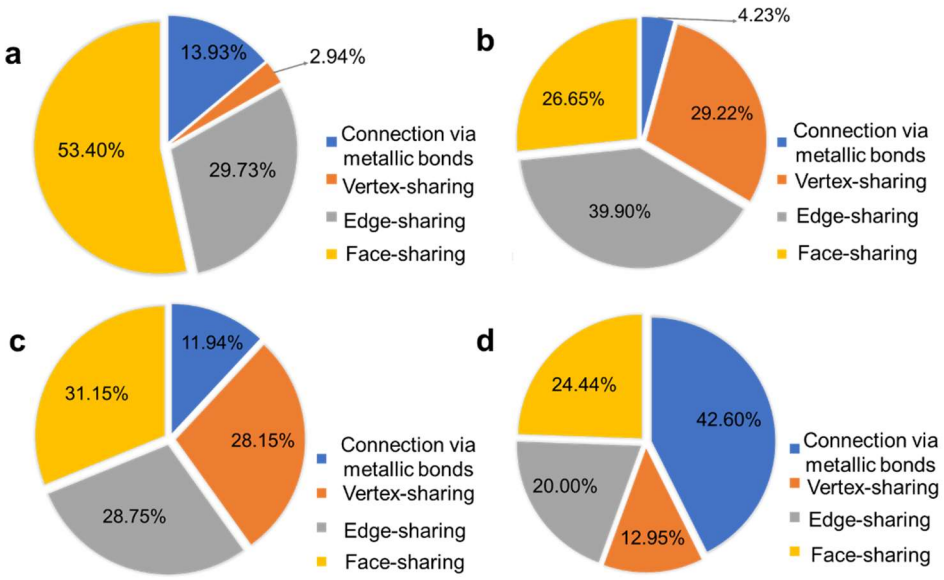
Formula	Structure	Element	ICSD
P_4O_{10}		P O	16610
P_4S_{10}		P S	174009
$P_4S_4O_6$		P S O	27058
P_4S_9		P S	26169
P_4O_9		P O	27434
$P_4S_6O_3$		P S O	86494

P_4S_3		P S	406048
P_4O_7		P O	16321
P_4SO_6		P S O	69977
P_4S_5		P S	1995
P_4O_6		P O	24407
P_4S_7		P S	23842
P_4O_8		P O	406625

4 Cation connectivity

4.1 Cation connection motifs

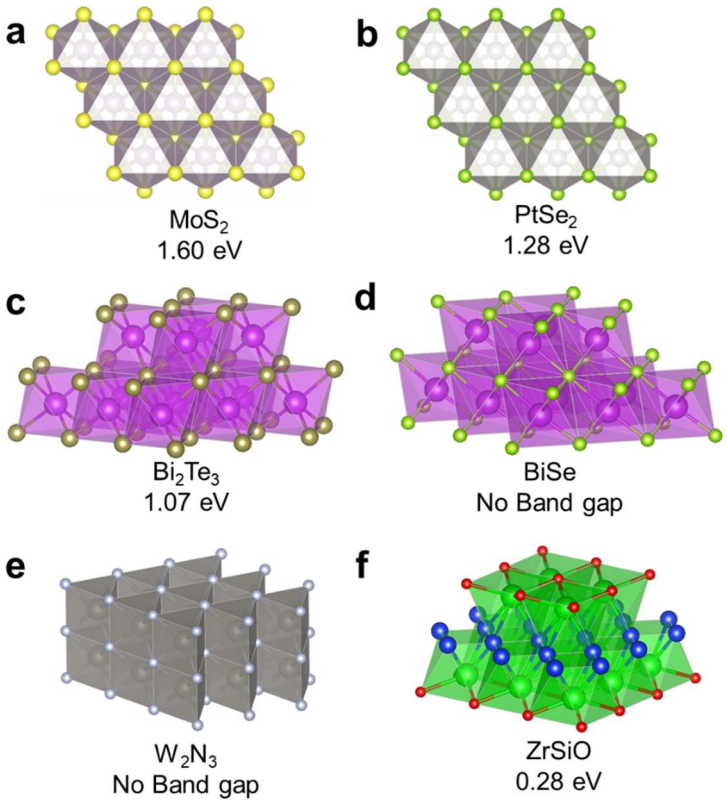
Except for the cases where cations are directly connected through metallic bonding, the connection of cations in a compound can be described by the linkage between neighboring cation-centered coordination polyhedra (CP). As a measure of cation connectivity, the connection motifs of cation-centered CP can be used to highlight the topological proximity between both cations, which does not rely on their interatomic distances. If both cations are linked by three or more anions, we say that both CP are face-sharing. When there are double and single linkages, they are defined as edge-sharing and vertex-sharing, respectively. In Supplementary Fig. 12, we show the ratio of different cation connection motifs for LDMs, as compared with bulk compounds that cannot be partitioned into low-dimensional structural blocks.



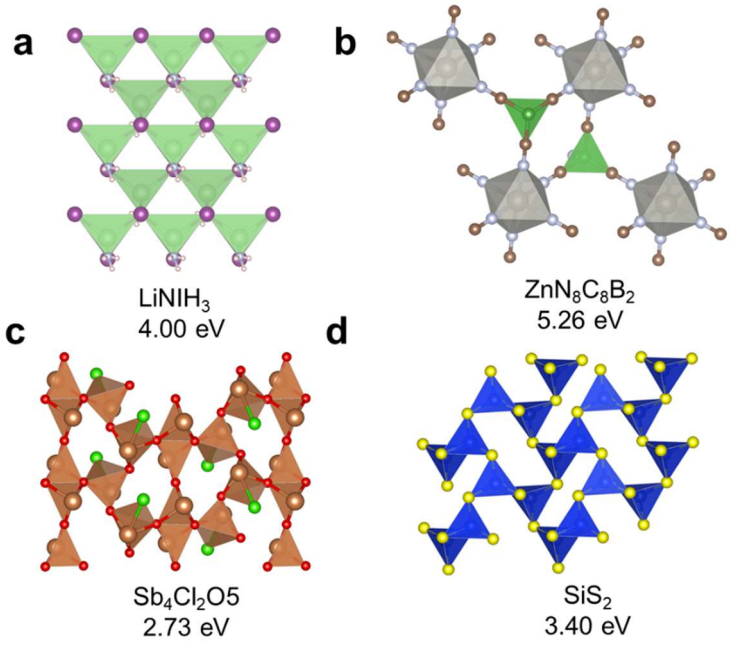
Supplementary Fig. 12 | Statistics on the cation connection motifs. a, Bulk compounds that cannot be partitioned into low-dimensional structural blocks. **b,** 2D atomic layers. **c,** 1D atomic chain. **d,** 0D atomic clusters.

4.2 Cationic percolation network/chain

We propose a 'rule-of-thumb' for estimating the degree of connectivity between neighboring cation-centered CP: face/edge-sharing linkages of CP are defined as intimate connection, and vertex-sharing linkage is regarded as disconnected. While heuristic, this can serve the purpose for gauging the topological connectivity between two cations with the use of the structure graphs of the compounds. In this context, the portfolio of 2D and 1D compounds can be divided into two groups, with and without a percolation network/chain made up of cations and cation-centered CP. Supplementary Fig. 13 depicts several 2D structures that are characterized by such percolation network, while in Supplementary Fig. 14, we present 2D structures without a cationic percolation network. Their electronic band gaps are also provided.

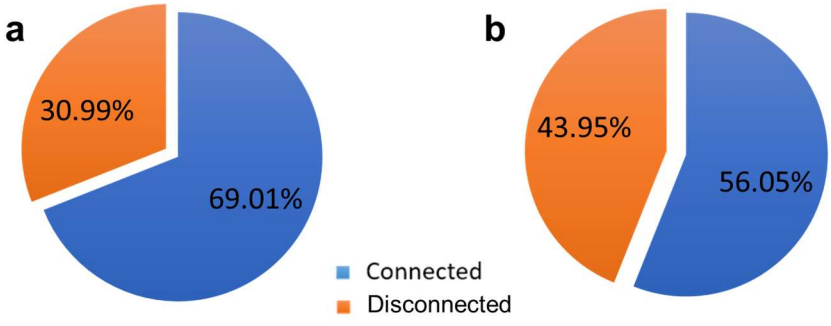


Supplementary Fig. 13 | 2D structures with cationic percolation network, and their electronic band gaps. a, MoS_2. **b,** $PtSe_2$. **c,** Bi_2Te_3. **d,** BiSe. **e,** W_2N_3. **f,** ZrSiO.



Supplementary Fig. 14 | 2D structures without cationic percolation network, and their electronic band gaps. a, $LiNIH_3$. **b,** $ZnN_8C_8B_2$. **c,** $Sb_4Cl_2O_5$. **d,** SiS_2.

It is worth mentioning that for some of the compounds, not all cations are involved in forming the percolation network. Nevertheless, due to the dense packing of the relevant cation sublattice in these compounds, they are still categorized into the group of compounds with cationic percolation network. Supplementary Fig. 15 shows the percentages of compounds with and without the cationic percolation network/chain.



Supplementary Fig. 15 | The percentages of compounds with and without cationic percolation network/chain. a, 2D atomic layers. **b,** 1D atomic chains.

5 All of the predicted low-dimensional materials

In Supplementary Table 9-11, we list all the LDMs in our database. LDMs are classified according to the number of atoms per unit cell. The ICSD numbers of the parent bulk compounds are also given behind the names of these LDMs.

Supplementary Table 9 | The list of 2D compounds.

Number of atoms	2D compounds (ICSD number)
1-6	ClSc (1004), NMoTa (100437), S_2Sn (100610), TeBi (100654), SSn (100672), SeSn (100673), NaAlGe (10147), $TiSe_4Zr$ (104188), OTiBr (10419), S_2Mo (105091), Te_2Pt (105813), SSn (106028), InBi (106325), STe_2Bi_3 (107587), CTb_2 (108187), SeSn (108293), PTa (108656), $TiSe_2$ (108739), I_2Pb (108906), CdI_2 (108915), BrIHg (109010), Se_2Zr (109291), BrZr (1168), NaZnSb (12154), SGe (1256), HO_2Cr (1372), Cl_2Ni (14208), Te_2W (14348), $MoTe_2$ (14349), P (150873), $MoTe_2$ (15431), H_2O_2Ca (15471), OSn (15516), $TiTe_2$ (15543), SiZrTe (15572), ClGaTe (15582), OClTi (155833), OKTl (1570), ClHg (157979), BrHg (157980), Te_3Bi_2 (158366), Ni_2SbTe_2 (158485), Cl_2V (15901), NGa (159250), SIn (15931), $NiTe_2$ (159382), OClFe (16013), O_2Co (160556), O_2NiAg_2 (160574), OTl_2 (16220), Se_2Nb (16304), CNb_2 (163747), O_2Pt (164289), NCrNb (16496), H_2O_2Cd (165224), Se_3Bi_2 (165226), SCu_2 (166578), Se_2Mo (167357), SGa (167394), BAlMo (16777), F_4Sn (16794), F_4Pb (16795), BN (168892), NRe_2 (169886), H_2O_2Ni (169978), H_2O_2Mg (169979), GeSe (17006), Se_3In_2 (17008), $MgCl_2$ (17063), OScBr (170774), NNaSn (172471), CRe_2 (180376), FeTe (180602), Se_2Ta (18130), Se_2Ta (18133), I_2Hg (181575), SeIn (185172), NTa_2 (185289), Sb_2Te_3 (185945), N_3W_2 (186207), H_4LiB (186262), Te_2Ir (189371), AgI (1899), NClZr (190379), NBrZr (190380), NZrI (190381), NClHf (190382), NBrHf (190383), NIHf (190384), BW (191911), C (193439), OClBi (195115), Se_2Hf (195308), As_2Te_3 (196147), S_2W (196773), $ZrTe_2$ (196804), Se_2W (196992), CdHf (197212), $CoTe_2$ (197241), Sm_2Bi (197920), S_2Zr (197981), NiI_2 (197996), $PdTe_2$ (198013), OClV (1981), S_2Ti (198127), Se_2Pt (198445), S_2Ta (198476), S_2Hf (198540), GaSe (2002), HNi_2 (200593), Cl_2Zr (20144), OBrSm (202064), I_2La (202452), NCaGa (2027), HClEr (203143), OAg_2 (20368), SeBi (20458), $SeSb_2Te_2$ (2085), $NiBr_2$ (22106),

I_2Hg (22242), CY_2 (22283), BS (230149), BrIn (23126), GeI_2 (23176), Cl_2Ti (23177), Cl_2Hg (23277), ClTb (23351), BrLa (23354), S_2KSn (23448), S_2RbSn (23449), OTi_2 (23574), H_2O_2Mn (23591), FHg (23719), CS_2Ta_2 (23790), SFe (238590), CrI_2 (23892), $CrBr_2$ (23903), F_4Nb (23949), OClIn (24058), OBrIn (24059), TeI_2La_2 (240698), OILu (240948), OFBi (24096), OCl_2V (24380), $OVBr_2$ (24381), ClLa (24410), OBrBi (24609), OIBi (24610), OILa (24613), IAu (24619), VBr_2 (246906), VI_2 (246907), SZr (24754), S_2Ta (24756), ZrI_2 (24807), OBrLu (249338), S_2Nb (250594), S_2Nb (250595), NBrHf (250913), $CrSe_2$ (251718), BAlW (251809), $BGdPt_3$ (253999), $BTbPt_3$ (254002), $BDyPt_3$ (254006), S_2Mo (254956), HCaBr (25542), HCaI (25545), HSrI (25546), HClCa (25601), H_2O_2Co (257275), OSiZr (25731), SiTeHf (25737), Br_2Cd (25782), Te_2Hf_3 (259226), CrI_2 (2596), P_2CaIn_2 (260562), P_2SrIn_2 (260563), $TiBr_2$ (26078), Cl_2Zn (26152), NClTi (261525), GeSnDy (261753), BrTeBi (264198), $BrTeBi_2$ (264199), $RhTe_2$ (26618), Cl_2Cu (26667), Cl_2Hg (26722), Si_2Zr (26758), O_3La_2 (26864), O_3Ce_2 (26865), OVBr (27010), OCrBr (27092), NZrI (27392), NBrZr (27393), NTiI (27394), NTiBr (27395), HLiO (27543), OIEu (27666), GeI_2 (27674), Cl_2Fe (27810), OAlCl (27812), OCs_2 (27919), FIPb (279599), CSc_2 (280743), SLa (280989), MgI_2 (281551), FAg_2 (28280), OClCr (28318), $BCePt_3$ (290490), CuBr (30091), Br_2Hg (30290), CuI (30363), ClY (30708), MnI_2 (33673), Cl_2Mn (33752), H_2O_2Mg (34401), InI (38129), CCl_2Gd_2 (400348), SCoSb (40044), $TiZrTe_4$ (40496), ClRhTe (405714), LiI_4Au (406967), NaPSn (409010), CTa_2 (409555), $FeBr_2$ (409571), HClSc (40981), NBa_2 (409851), NCa_2 (410312), NSr_2 (410315), OBrGd (41071), TePt (41370), S_2Pt (41375), GeI_2La_2 (414170), HSi (41478), OPd (41617), HTa_2 (41774), NaMgSb (41797), PBr_2La_2 (418009), PI_2La_2 (418010), Cl_2Pd (421221), P_2CaGa_2 (422525), $CaGa_2As_2$ (422526), BCDy (42477), $CuAgTe_2$ (42482), S_2Ge (425582), CuTe (42591), BCY (42626), $AsSe_2$ (428192), BNiNb (43005), SHf_2 (43203), $TeIBi_3$ (432224), GaTe (43328), $SeTe_2Bi_2$ (43512), Se_2Sn (43594), Cl_2Co (44398), Se_3In_2 (4478), ZnI_2 (48016), CV_2 (5005), CaI_2 (52280), Se_2Sb_2Te (52295), $CoBr_2$ (52364), $MgBr_2$ (52366), CoI_2 (52368), FeI_2 (52369), CaMnGe (52758), MnGeSr (53707), CrI_2 (5433), Se_2TeBi_2 (54838), $PdBi_2$ (56280), InBi (58790), HTiFe (602022), Se_3In_2 (602266), $MnBr_2$ (60250), Te_2Hf (603713), S_3Ti (604398), OClY (60585), TiAg (605930), NaMnSb (60734), OClYb (6077), SBrLu (6082), Se_2Sb_2Te (60963), As_2SrSn_2 (611428), BCGd (612618), BCHo (612623), HV_2 (61423), BNiTa (615023), BPt_2 (615207), CW_2 (619097), HClLu (62226), CCl_2Lu_2 (62227), PCoSm (624632), MgCuGe (627730), Cu_2Te (629340), PFeSm (633100),

	FeSe (633480), PGa (635031), PSrSn (63594), $ScGe_2$ (637830), GeTe (638005), Ge_2W (638120), In_2Te_3 (640609), S_2KTi (641335), Se_2Nb (645379), Se_2Pd (648835), Se_2Re (650091), SSn (651020), S_2V (651361), VSe_2 (652158), $SiTe_2$ (652385), Te_2W (653170), KAsSn (65413), Br_2La (65481), CS_2Nb_2 (656705), $SeTa_2$ (657372), S_3Nb_2 (66358), Cl_3Cu_2 (66645), MgMnGe (66952), MgMnGe (66953), CaMnSn (66958), MnGeBa (66964), Mg_2SiPt (68513), SCrBr (69659), TeIBi (74501), S_2Cr (75420), PNb (76027), NiTe (76730), SeLa (77829), I_2Yb (77907), S_2TiRb (77990), O_2Ni (78698), SIDy (79107), ClTeBi (79362), $NaAs_2Sn_2$ (82366), OCl_2Ru (83883), OCl_2Os (83884), Cl_2Cd (86440), ClZr (868), SBrLu (87131), PMnCs (89598), O_2Zr (93028)
6-12	Na_2AgSb (10010), O_3As_2 (100434), InTeI (100703), BrInTe (100705), S_4FeGa_2 (100706), O_3SbTl (10142), $O_2Ca_2CuBr_2$ (1028), Sn_3Gd (104135), O_2As (10436), Cl_2Se_2Nb (10483), $MgAl_2S_4$ (107308), $O_2CuBr_2Sr_2$ (1178), $AlPd_5I_2$ (14164), P_3Sn_4 (15014), Te_5Hf (15051), Cl_3Fe (151400), O_3Mo (151750), S_3As_2 (15239), H_8MgAl_2 (152537), F_4SnPb (152949), $TeIBi_2$ (153858), OPb (15402), OPb (15403), HO_2Fe (1544), $Fe_2Se_5In_2$ (155025), S_4ZnIn_2 (15636), CNOAg (157548), O_3Sr_2Tl (157837), O_3Ca_2Co (160557), FTl (16113), CN_2Cu (161460), S_4ZnIn_2 (16200), $Ge_3Te_6Bi_2$ (16207), PdSnTe (162404), $PFeSe_3$ (16246), FeSe (165957), TeIAu (1661), F_4SnBa (166207), H_3NBrAg (169137), YI_3 (170773), S_2CuSb (171051), FSe_2SrSb (171430), $O_4Ni_2Ag_3$ (172878), Se_3Pt_2Hg (185808), B_4Ta_3 (191904), BRe_3 (191913), P_2Se_6AgBi (195334), P_2ScSe_6Ag (195336), P_2CuSe_6Bi (195341), $PtBi_2$ (195775), $PtBi_2$ (197309), $H_2O_6P_2Zr$ (201970), P_2S_6AgIn (202185), Se_2Br_2Nb (202821), O_3TeHg_2 (203064), Se_3Bi_4 (20319), Se_4Bi_3 (20386), O_3FPSn (2039), I_3Bi (20676), Cl_3Ru (20717), $S_4GaCdIn$ (20785), CNNaS (22273), PSPd (2331), O_4AsSb (23316), $CuSe_2Sb$ (238476), $GeAs_2$ (23872), Cl_3Tb (23938), OTiBr (240499), $GeTe_4Hf$ (241122), CuBi (243921), $H_2O_6P_2Ce$ (244036), Li_4BGe_2 (244236), $S_4GaCdIn$ (2465), O_3CuGe (246664), $H_3LiC_2O_5$ (246786), O_3SePd (249504), Sb_2Te_4Pb (250250), SeBi (251717), $CrGeTe_3$ (252343), OS_2LaBi (252466), C_2Ca (252716), C_2Ca (252737), Be_4B (25535), Se_3Zr (25621), PS_3Hg (2564), Cl_8Nb_3 (257110), Se_3Pd_2Hg (259367), As_2Se_3 (2600), H_2O_2ClLu (260838), H_2O_2ClLu (260841), Se_2Re (26256), O_2Te (26844), SLa (280987), I_2Hg (281133), O_2Cl_2W (28510), SeBrAu (2897), Cl_3Ti (29035), SiS_2 (291212), O_2Te (30222), $Se_5Pb_2Bi_2$ (30372), $GeTe_4Bi_2$ (30394), Te_3Bi_4 (30526), I_3La (31596), O_4PAs (31879), O_3BrHg (31925), $S_5Fe_2Ga_2$ (32551), NO_3IHg (32580), O_8Cl_2Co (33288), O_8Cl_2Ni (33289), $PTiCu_2$ (35419), $ONbI_2$ (36255), O_3AsSb (37187), $TiBr_3$ (39242), Cl_6FeZr (39666), Cl_6FeHf (39817), CYI (400298), Cl_3Dy (40064), Mn_3As (40437), $NaSn_5$ (408045), $O_2NaBr_6W_2$ (408934),

	$PdTeI_2$ (409062), $CuSe_2Br$ (410004), CN_2Pb (410915), $FeBr_3$ (410924), O_3SeHg_2 (412302), $MgPSe_3$ (413165), $SeTe_2La$ (413171), Cl_4GaHg (413579), OBr_2Nb (416669), $MgAl_2Se_4$ (41926), $Mg_2Al_2Se_5$ (41928), OScI (419335), As_3Sn_4 (419884), S_3Ti (42072), S_3Zr (42073), S_3Hf (42074), Se_3Hf (42075), $ZrTe_3$ (42076), NO_2Hg (422481), S_2Br_2Nb (424413), $S_5Zn_2In_2$ (42443), S_4Fe_3 (42537), $MnTe_4Bi_2$ (425966), $S_5Zn_2In_2$ (42666), S_4ZnIn_2 (42668), $Te_5Pb_2Bi_2$ (42708), N_3Cu (428038), $Ge_2Sb_2Te_5$ (42876), NO_3K (428909), SiP_2 (43098), In_3Te_4 (44655), S_4Fe_3 (44885), CBrGd (47225), $S_5Fe_2Ga_2$ (49912), O_8MnRe_2 (51014), O_8CoRe_2 (51015), O_8NiRe_2 (51016), O_8ZnRe_2 (51017), $CaBr_3In$ (54138), $PMnSe_3$ (54140), H_3LiNI (55064), $O_2CuSr_2I_2$ (55710), SbI_3 (56572), $AlCl_4Cd$ (59173), S_4NiGa_2 (59230), LiO_2Cl (59936), $ZrTe_5$ (602282), OSn (60619), I_2Pt (60760), Al_2S_4Fe (607619), Al_2S_4Zn (609280), NO_2Hg (61064), $SiAs_2$ (611405), B_3FeGd_2 (613928), B_4Nb_3 (614896), BTc_3 (615555), Te_4PbBi_2 (616936), PSe_3Cd (620234), $CoGe_2Gd$ (623352), S_3GaIn (62340), $CoGe_2La$ (623462), $SiCrTe_3$ (62379), SCoSb (624859), S_4CrGa_2 (626052), O_4PSb (62977), Te_3Dy (630328), $S_5Fe_2Ga_2$ (631804), P_2S_6ScAg (63273), $P_2Fe_2Se_5$ (633094), $S_5Mn_2Ga_2$ (634664), S_4MnGa_2 (634670), COClCu (63490), Te_3Gd (636467), S_3Hf (638846), Te_3Hf (638958), PS_3Hg (639130), $MnSe_4In_2$ (639980), $ClCuTe_2$ (641), Te_3La (642014), Te_3Lu (642621), $P_2S_5Sn_2$ (648055), S_2Re (650077), Te_2Re (650162), Te_3Tb (652952), YTe_3 (653175), $ZrTe_5$ (653212), $NbTe_4Os$ (656450), $NbTe_4Ir$ (656451), $RuTe_4Ta$ (656452), $RhTe_4Ta$ (656453), Te_4TaOs (656454), F_4BrRb (65713), S_4ZnIn_2 (65725), $SnSb_2Te_4$ (657316), Te_4TaIr (657362), Ni_2Te_2Ta (66346), $SiInTe_3$ (66356), $CuBrTe_2$ (67252), $CuTe_2I$ (67253), PS_4Sc (67559), $ClCuSe_2$ (68292), H_2O_2Cu (68459), $S_6Zn_3In_2$ (68645), SPb (68701), SY (69042), $O_4Ca_3Cu_2Br_2$ (69182), Sb_2Te (69557), $ONa_2Ti_2Sb_2$ (69648), P_2Se_6AgIn (71968), P_2CuSe_6In (71969), P_2GaSe_6Ag (71971), S_4Cu_2W (72529), SeLa (73092), SePb (74334), Cl_3Sc (74517), SSbIr (74630), $AlSiTe_3$ (75001), C_2Cr_3 (76798), PSePd (77772), CBrY (78871), Cl_7Nb_3Te (79213), SSn (79374), OI_2Ta (80109), PS_3Cd (80875), SBr_7Nb_3 (81078), S_2Tc (81816), GeSePt (822), Ni_2Te_3Ta (82605), SeI_7Ta_3 (82791), TeI_7Ta_3 (82792), Te_5Hf (85509), $Ni_2SeTeTa$ (86174), B_4Rh_5 (86395), C_4N_6Zn (86672), Nb_3TeI_7 (86723), O_3SiCu (89669), O_2Co (89837), H_2NClHg (92480), O_3CoSr_2 (99894)
12-18	Br_3Bi (100293), Br_3Bi (100294), $C_2N_2S_2Hg$ (10304), Br_3Ir (14212), $H_5O_{10}As_3$ (14327), $NbTe_2$ (14389), $H_5Li_2NO_6F_2P_2$ (1439), Te_2Ta (14390), O_4SHg_2 (15005), $O_3Cu_2Sr_2$ (150912), S_4As_2Pb (15464), O_5V_2 (156051), Cl_3Y (15684), $B_3C_{10}N_3$ (161278), $P_2S_8Pd_3$ (16296), $O_6MnMoTe$ (163978), $O_6ZnMoTe$ (163981), O_5P_2 (16611), NOF_5KOs (166586), O_2ClAg (16717),

O_2NaAs (16762), $H_4O_9Mg_3Si_2$ (17046), O_4Cl_2Ca (171020), O_4Cl_2Sr (171021), $C_2O_6F_6S_2Rb$ (171662), $C_2O_6F_6S_2Cu$ (172335), $O_7F_2V_2Te_2$ (173748), O_4Sn_3 (174299), $O_6MgMoTe$ (184714), Si_3Mn_5 (185917), $O_6MoCdTe$ (188038), LiC_{12} (193440), C_3AlY_3 (194877), S_2SbCs (200798), H_2O_4W (201806), O_4ZnAs_2 (202249), $H_4O_9Mg_3Si_2$ (202358), $H_4O_9Mg_3Si_2$ (202359), Cl_3Cr (22080), Cl_3Au (22146), O_6CuI_2 (2232), H_4O_2NaI (23134), Cl_3Ir (23171), $S_2Sn_2SbI_3$ (23344), Se_3In_4 (23465), S_3Nb (2380), $H_6O_6MgCl_2Cu_3$ (240663), H_2NO_5Gd (243494), H_2NO_5La (243495), H_2NO_5Y (243496), $O_3Sn_2Cs_2$ (24392), $O_6CoMoTe$ (247052), F_5K_2Sb (24742), O_4SHg_2 (248726), O_5PMo (24894), $C_2N_2S_2Co$ (250692), $H_6Li_2O_6Pt$ (251041), CrI_3 (251654), $H_3O_3ClCuZn$ (252429), LiO_2Bi (25385), F_5Sn_2IBa (254413), Cl_3Rh (25764), $H_2O_5V_2$ (260368), O_4AsHg_3 (2604), Br_3Gd (2610), Cl_9Mo_4 (26108), Cl_3Mo (26109), Na_2SrSn_4 (261117), LiO_2Sb (262075), Cl_3Tc (262639), $LiSi_2Ge_4La_2$ (262950), O_5VMo (27315), $S_7CdSb_5I_4$ (27733), LiO_2F_4Re (280011), $O_4F_7KRe_2$ (280012), $SeMoSb_2$ (280615), N_6Cu (28171), Br_3Rh (28245), $O_6MnMoTe$ (291413), $C_2N_2S_2Ni$ (31320), O_6SAs_2 (32581), $OIHg_2$ (33275), $CrSe_5Nb$ (35044), $ClSe_4Re_3$ (35623), $H_4O_8Na_2MgS_2$ (35767), $NaCl_6Nb$ (36518), $NaCl_6Ta$ (36519), $H_2O_4Sn_2Ba$ (37115), H_2LiNO_3 (37180), VTe_2 (38369), $HOClCu$ (38384), $F_{12}CaAu_2$ (39315), $AlCl_3$ (39566), $H_4C_2N_4Cl_2Hg$ (405834), H_2O_4CoSe (408099), $CoSe_5Nb_2$ (41026), O_4PHg_3 (410760), $In_7La_3Au_4$ (411183), $F_{12}MnSb_2$ (411522), O_6I_2Hg (413033), $AlBr_6Bi$ (414262), $O_3Cl_2Co_2Te$ (415798), $O_3CoBr_2Sb_2$ (418858), $LiO_{11}InI_4$ (422056), $O_2F_8V_2Pb$ (424541), HO_5AsTe (425501), O_5PV (425536), O_5PV (425552), $Al_2S_3Cl_8Ag_2Bi_2$ (428725), $Al_2S_3Cl_8Cu_2Bi_2$ (428727), P_2CuSe (430942), Se_3Ta (43213), $B_2Al_2Fe_3$ (433027), In_2Te_5 (501), $C_6N_6FeSn_2$ (51494), H_3BO_3 (52290), Mn_5Ge_2 (53683), H_2O_4SeCd (59347), HO_4ClHg (59874), NMo (60168), S_5NiTa_2 (61147), $NiSe_5Ta_2$ (61148), O_6SI_2 (6220), S_4Cr_2Co (622499), $F_{12}AgTa_2$ (62543), Te_5La_2 (642015), $F_{12}AgSb_2$ (65186), Br_3In (65198), $NbPdTe_5$ (68103), $O_8CaCu_2Sr_2Bi_2$ (68188), O_4Cl_2Pb (68484), $H_3O_3ClCu_2$ (70101), $NiTe_2Ta$ (71063), $CoNbTe_2$ (71196), Te_5TaPt (71292), $FeNbTe_2$ (71520), $NiNbTe_2$ (71841), O_8NaBa_4Au (73189), $NiNbTe_5$ (73316), $CoSe_5Ta_2$ (73319), $SeAu$ (73668), $CoTe_2Ta$ (73738), H_2O_4SMn (74810), H_2O_4VAg (75941), $H_4O_9Mg_3Si_2$ (76919), $H_3C_2O_3K$ (77115), O_3I (78903), H_2O_4ZnSe (78916), Al_2Te_5 (78941), $F_{12}AgBi_2$ (79879), O_4SrBi_2 (80668), $SiNb_2Te_4$ (81416), $GeNb_2Te_4$ (81417), $N_2Ge_2Ba_3$ (81819), $H_2CNOSClBa$ (82878), $HOClCu$ (91088), $H_6O_6Na_2Sn$ (92464), F_6CaSn_2 (92907), F_6BrAu (93481), $O_3FeBrSr_2$ (93509), $O_9Ge_3Sb_2$ (95735), $H_4O_2Cl_2Ca$ (960),

	$HO_4FNaPSn$ (96768), $HOFCu$ (98698), $SClCuHg$ (98872), CO_3F_3SHg (98942)
18-30	Cu_3Pd (103086), S_2Cl_2Nb (10484), F_2Sn (10485), SZn (107137), LiO_3FS (1384), Al_2Cl_8Cu (14107), $P_3S_{16}Zn_5$ (1434), S_3Ta (15251), H_5CO_4PFe (153033), $SiAs$ (153457), H_3CN_4ONa (15874), $P_3S_{12}Fe_4$ (16252), $H_2O_9NaVI_2$ (166893), $H_4C_6N_8O_4Cu$ (168724), Ge_4Se_9 (170758), $H_4O_4P_2Cd$ (171022), FSe_2SbBa (171429), $H_5B_4O_{13}Bi_2$ (172480), H_5CNO_3PClZn (173537), $O_3ClSeIn$ (174539), O_3AgI (188065), $H_9C_3O_{12}NaS_3Au$ (188831), OS_2Sb_2 (189831), O_4VTe (19021), $O_4Fe_3Br_4Sb_2$ (190854), $O_5Mn_2Sb_3I_3$ (190856), S_2Ge (1947), $H_4O_8CuI_2$ (200326), F_4NaSb (200573), Cl_8CuGa_2 (201414), $H_3NO_6Cu_2$ (201478), O_8SeTe_3 (201784), $P_3S_{12}Zn_4$ (201933), P_2S_6VAg (202045), O_6NaAs_4Br (202369), $ClInTe$ (21031), O_2Na_2Pb (21058), $OFSb$ (21099), $O_5Cl_2Sb_4$ (2233), SiP (23724), Cl_5FeW (237305), $H_2O_7Ti_3$ (237518), O_3CaTe (238569), $AsPd_5$ (239291), $H_{16}LiB_4Y$ (239762), Li_2O_4S (239962), $O_5Br_2Sb_4$ (24030), $O_6Cl_2Cu_3Se_2$ (240496), H_4MgGa (240696), H_6NO_4FNaP (240974), $H_8BO_{10}SGd$ (244355), $HB_3O_7Sn_2$ (244732), $H_{10}B_2N_2Ca$ (246139), IBi_4 (246145), $O_7BrLaPb_6$ (249390), O_3FTc (249509), O_2F_2Cr (249513), H_2LiO_2P (250176), $H_4O_{14}P_4KFe$ (250262), $NaBr_{20}Tc_9$ (251005), $AlCl_4Se_2BrBi_2$ (251017), HO_6Se_2Bi (251033), H_8N_4NaAl (2539), H_8N_4NaGa (2540), PSe_3Hg (2565), O_3FInTe (260009), $H_4CO_5Cu_2$ (260600), PS_4Ga (2613), $SeNb_2$ (26183), $P_{11}S_9Cu_3Br_4$ (261887), B_2Ni_3Zn (261932), O_7STe_2 (265), H_3O_3Al (26830), PPd_6 (26898), $O_3ClInTe$ (279576), H_4O_5FPCa (2802), $H_4O_4P_2Cu$ (280917), $H_4O_4P_2Cu$ (280921), $H_3O_6KSe_2$ (2838), Se_3Nb (30002), $H_3NO_6Cu_2$ (31353), HO_6PAs_2 (32614), H_3O_2Na (33909), SBr_2Mo_2 (35356), P_2S_6CrAg (36456), Li_2O_3Te (38416), HBO_2 (39129), $H_2O_5F_2SSn_2$ (39455), Al_2Te_3 (406353), $H_4LiO_2Cl_3Cu$ (40746), Mo_6AgTe_6 (40793), $O_2Cl_7Mo_2Tl$ (408775), $C_3N_3Se_3Cs$ (4101), Te_3Ta_2 (41047), $Si_2RhI_{12}Bi_{14}$ (410739), $Si_2I_{12}IrBi_{14}$ (410740), $H_4O_6P_2Sr$ (410936), H_4O_8NaPS (411163), S_3GeSn (411241), PS_4Lu (412857), Se_5BrIn_5 (414218), O_3FPHg_2 (414292), $O_6Cu_3Br_2Te_2$ (414443), $B_2C_8N_8Zn$ (415547), O_3SePd (415955), $NiSe_7Ta_2$ (41619), O_8NaI_3 (418336), $O_{15}Cl_4Ca_2Co_4Te_5$ (418681), $O_3BrInTe$ (420301), $Cl_{10}FeW_2$ (422521), $Cl_{10}CoW_2$ (422522), $O_5Cl_2As_2In_2$ (422701), $H_4N_2O_8Ni$ (423975), $H_4N_2O_8Mg$ (423976), $O_9V_3As_2$ (424067), $GeSe_2$ (425644), H_4O_6NaCl (425697), $LiAlP_2S_6$ (425979), $B_2O_9S_2$ (426544), H_8LiN_4Ga (427080), H_8LiN_4Ga (427081), $O_7SiMn_4Br_2Te$ (427407), $O_7SiCl_2Mn_4Te$ (427408), SZn (42799), LiF_7Sb_2 (428176), $O_{14}S_2CuSb_6$ (428356), H_4O_5FPMn (428896), $SiSe_2$ (431202), $H_4O_4P_2Ca$ (44413), PS_3Co (4813), $P_3S_{12}Co_4$ (4814), KBr_3In (50510), $H_2O_8P_2Ti$ (51099), SBr_7Ta_3 (51101),

	$Na_2Al_2Sb_3$ (52628), O_3TeIBi (56218), Al_2Cl_8Sr (56732), Al_2Cl_8Ba (56735), PS_4Cr (56835), $H_4O_5S_2Cd$ (59239), STl_2 (59735), $H_4O_4P_2Sr$ (59932), $H_4O_4P_2Pb$ (59933), $H_4O_4P_2Ba$ (59934), $O_{22}Mo_4Hf_3$ (59998), $P_3S_{12}Ni_4$ (602341), Se_7Ta_2Pt (61353), $P_3S_{12}Mn_4$ (61391), $P_3S_{12}Cd_4$ (61393), PS_3Cd (620232), Al_2Cl_8Cd (62037), $P_3S_{12}Co_4$ (624616), $H_{12}O_{12}FP_2Co_2$ (62512), $P_3Cr_4Se_{12}$ (626521), $H_4O_{14}AlP_4K$ (63033), PSe_3Hg (639132), $MgPS_3$ (642729), S_3Nb (645316), $P_3Ni_4Se_{12}$ (646145), $P_3S_{12}Pd_4$ (647926), $P_3S_{12}Sn_4$ (648056), $P_3S_{12}V_4$ (648076), S_3Sc_2 (650834), S_3Ta (651099), Se_3Ta (651959), $H_4O_4P_2Zn$ (66911), $O_6CuSr_2Bi_2$ (67426), $P_3V_2Se_{12}Ag_2$ (68143), O_9SZr_3 (68335), $S_3Ni_6Bi_4$ (70053), Co_2Te_2Ta (71197), $SiNb_3Te_6$ (71681), $GeNb_3Te_6$ (72208), H_4BO_4Na (72913), H_8N_4NaAl (73163), H_8N_4NaGa (73164), $P_3S_{12}Cr_2Cu_2$ (74024), $SiTe_6Ta_3$ (75617), Se_3Nb (76578), $TeHf_2$ (83965), F_9KTe_2 (84364), $N_4O_8K_2Ca$ (85505), O_9VRe_2 (92317), $H_4N_2O_8Zn$ (9286), S_2Br_2SbLa (93666)
30-50	H_2LiBO_4 (100854), $Cl_{23}Sc_{17}$ (1018), $F_{12}Ge_5$ (10295), $BFe_{14}Tb_2$ (106300), $H_6O_7P_2Cd$ (1382), F_7KSb_2 (14118), I_7Ta_3 (14211), $H_2CO_4F_3NaS$ (151031), $H_8C_4O_4Sn$ (151276), H_5CO_4Na (151358), $H_{14}N_4O_{19}Cl_4Ca_4$ (1532), $O_{12}ZrI_4$ (15405), NaP_2S_6Sb (155269), $H_6C_2O_7Ca$ (159351), $O_3CoZnBr_2Te$ (162428), O_8ZrMo_2 (164732), H_4CN_2SClAg (167547), H_4CNO_2Na (16765), $H_{14}B_2N_2Ca$ (169344), $F_{10}Cl_3K_3Sn_5$ (170697), $C_2O_6F_6S_2Ba$ (172338), $O_3Cl_2Zn_2Se$ (172981), H_6C_2CuSeI (174213), $H_6C_2ClCuSe$ (174215), $AlCl_4BrTe_2Bi_2$ (174525), H_2O_4SrTe (182022), $LiC_4O_{12}F_{11}S_4Au$ (187382), $H_4O_{21}Mg_6Si_7$ (188062), H_8BN_2Na (189248), H_6LiBN (189250), $O_9Fe_3Sb_5I_3$ (190851), $O_9Mn_3Sb_5I_3$ (190855), Sb_2Te_3 (193589), As_5Te_7 (196148), $H_6O_8ZnSe_2$ (200525), F_7RbSb_2 (200574), MoI_2 (201280), $O_{11}Al_2Si_4$ (201706), H_4CNO_2Na (2244), H_4O_2NaCl (2313), $H_{16}O_{21}Cl_3Sr_2$ (237722), $P_{15}Ag$ (239083), NaP_{15} (239084), $O_3Zn_2Br_2Te$ (241121), $H_4O_{16}Cl_3Mn_4Sb_8$ (242084), HO_5VTe (243760), H_9B_6NNa (243977), H_6BO_9SLa (244350), $I_{11}W_5$ (244435), $OClSb$ (24751), O_6Sn_3W (249534), O_7Cu_2SeMo (249957), $H_3B_5O_{10}Ca$ (250069), $H_8C_4N_8Cl_2Cu$ (250269), $H_4O_9Al_2Si_2$ (250459), $H_{12}LiC_4Al$ (250721), $H_{15}B_3NY$ (251865), F_5ClSn_2Ba (254412), $H_3C_2S_2Ag$ (255949), Cl_2Mo (26110), $H_8C_2O_6P_2Ca$ (261905), $O_{11}Se_2SrMo_2$ (262629), $O_{11}Se_2Mo_2Pb$ (262630), H_3O_5CaAs (2714), $H_6O_7P_2Ca$ (280575), $O_3Cl_2Zn_2Te$ (281324), Cl_7Nb_3 (28535), $H_6C_4N_8Cu$ (290326), $C_4OY_9I_8$ (300279), $O_{11}Al_2Si_4$ (30119), $H_4O_9Al_2Si_2$ (30996), $H_4C_2N_2S_2ClCu$ (31340), N_4S_4CuBr (33515), H_4O_2NaBr (34465), H_8BO_6Na (34652), $CrTe_3$ (35266), F_7KAs_2 (36332), H_3NO_5Cd (36557), P_2S_8Nb (37326), $O_{12}Cl_7Cu_4Zn_4Te_4$ (391095), I_3Bi_{14} (39257), Cl_7Se_2Rh (39583), Br_7Ta_3 (402031), $H_4O_{12}S_3Sr$ (404139), Br_2W (405808), Br_2Mo (409228), P_4CuSe_4I (410913), NF_5ClKW (411443),

	H_3O_4PCa (411737), H_3O_4PSr (411738), $SMoSb_2$ (412092), $H_8O_7Na_3Bi$ (412583), $CCl_{16}W_6$ (413027), $O_{13}Te_5Dy_2$ (413664), $O_{13}Te_5Lu_2$ (413669), $S_9V_4Br_4$ (415351), $B_2C_8N_8Cu$ (415546), $Na_3Cl_{13}W_3$ (415717), $O_3Co_2Br_2Te$ (415797), $O_{16}Al_3P_4$ (416135), AsI_5Hg_4 (416238), $O_{12}Co_5Br_2Te_4$ (416967), $O_{12}Cl_2Co_5Te_4$ (416968), $O_{22}Cl_7Co_{10}Te_8$ (417179), $H_8O_{12}S_2Ce$ (417357), $O_{13}Sc_2Te_5$ (417712), $O_8Cl_2Co_2SrTe_3$ (418682), $O_8Cl_2Ni_2SrTe_3$ (418683), O_6FSTc (418710), $O_{13}Y_2Te_5$ (418855), $Sc_{13}Br_{16}Os_3$ (421535), $F_{18}Sb_3Tl$ (421924), $O_{13}S_2Re_2$ (421956), $PCl_{11}W_4$ (422269), $P_4ClCuSe_3$ (422535), $O_{24}As_{10}Br_5In_8$ (422702), $H_2N_2O_7Zn$ (423979), $C_2N_2O_3F_9Na_2S_2Sb_5$ (424972), H_4LiCN_3 (425947), $H_2O_{14}S_4Pd$ (426138), $H_9C_2N_2O_2Ag$ (426384), H_2O_4FPSr (429339), $Cl_2I_4W_3$ (429579), Se_5SnIr_2 (430682), $O_2F_5Sb_3$ (431210), $O_8Cl_2Cu_2CdTe_3$ (431270), $H_4O_9Al_2Si_2$ (431456), $P_4S_{20}Ti_3Cu_4$ (433152), $O_{12}Cl_2CaCo_4Te_4$ (434245), $BFe_{14}Er_2$ (44217), $BFe_{14}Y_2$ (44248), $BFe_{14}Y_2$ (44304), H_3NF_4Zr (50233), $Se_{24}Ta_{13}$ (51572), $Se_{23}Ta_{13}$ (52430), $CFe_{14}Lu_2$ (57046), $S_3Nb_{12}I_{28}$ (59254), $BCo_{14}Y_2$ (600333), $BCo_{14}Tb_2$ (600335), $BFe_{14}Ho_2$ (600352), $BFe_{14}Y_2$ (601203), $BFe_{14}Y_2$ (602899), $BFe_{14}Lu_2$ (603908), $BFe_{14}Tb_2$ (603928), $BFe_{14}Dy_2$ (60519), $BCo_{14}Tb_2$ (613337), $BFe_{14}Dy_2$ (613605), $BFe_{14}Dy_2$ (613610), $BFe_{14}Lu_2$ (613995), $BFe_{14}Y_2$ (614277), $CFe_{14}Dy_2$ (617585), $CFe_{14}Lu_2$ (617761), $CFe_{14}Tb_2$ (617851), $C_2Sc_6I_{11}$ (62042), $H_4O_9Al_2Si_2$ (63315), $O_3Cl_2Zn_2Se$ (67606), $C_3OY_7I_6$ (67889), $CFe_{14}Lu_2$ (68073), $CFe_{14}Lu_2$ (68786), H_4O_3PClCo (69561), $H_{18}B_2O_{20}Mg_3P_2$ (69609), H_9O_5ClSr (71446), P_2GaSe_6Ag (71970), $O_4SiI_2La_2$ (72653), H_4O_3PClNi (74050), $H_6N_2O_6V_2Cu$ (74337), $H_6C_2O_7Ca$ (77096), $LiC_2NO_4F_6S_2$ (78506), $H_2N_2O_7Cu$ (78739), $H_6CN_2O_{10}CaRe_2$ (79119), $H_4O_9Al_2Si_2$ (80081), $P_2S_{11}Ti_2Ag_2$ (84606), $H_4O_9Al_2Si_2$ (87771), $O_{12}Cl_2Ni_5Te_4$ (96911), $O_{12}Ni_5Br_2Te_4$ (96912), $H_4O_9Al_2Si_2$ (98132)
>50	$H_8O_{12}FAl_2P_2K$ (100036), $H_{57}Li_4B_4C_{20}N_4O_{12}$ (109580), $H_4B_5O_{10}Na$ (1386), H_6O_6SMn (14029), $H_7O_{17}Cr_4Cu_2$ (14078), $S_{18}As_9Pb_5$ (15461), H_7O_7MgP (158937), $H_{18}C_6N_2O_9S_4Pb$ (163099), $H_{19}C_2O_{22}P_4Cl_4Cd_4$ (165583), $H_2F_{20}As_3La$ (165625), F_9Sn_3Sb (166583), $H_8C_2N_4S_2ClAg$ (167542), $H_{13}B_2N_3Mg$ (168510), $P_3S_9In_2$ (1700), $H_4B_5O_{10}K$ (170595), $H_{10}B_{12}O_{24}Ni$ (171506), H_4N_8Co (173371), $C_4O_{12}F_{12}S_4RbAu$ (187384), N_3O_9Tb (192252), N_3O_9Y (192259), N_3O_9Dy (192262), H_7O_7PMn (193725), H_9LiBN_3 (238484), Pd_8Cd_{27} (240774), $H_8C_5O_2F_3S_2Ag$ (249361), $O_7ClLaPb_6$ (249389), $H_{10}C_{31}N_{20}Co_2$ (250694), $H_6C_3NS_2IPb$ (251755), $H_{10}B_{12}O_{24}Zn$ (252582), $H_{14}C_8O_{13}Pb_6$ (261064), $H_{13}B_2N_3Ca$ (262498), Br_5W_2 (262722), $H_{16}O_{22}KV_5Co$ (281298), $H_{17}C_{11}N_8O_2S_4Cd_2$ (290272), $C_2NO_4F_6NaS_2$ (291412), $PS_{10}Nb_2$ (33233), $N_4O_2F_6S_6AsAg$ (33501),

	$H_4O_5Na_2Sn_2$ (35421), H_9O_5K (36598), $H_{16}O_{22}MgKV_5$ (39216), $H_9O_{13}Al_2P_2K$ (407354), $B_4C_8Y_{16}I_{19}$ (408701), $H_{12}N_2O_{10}S_2Ca$ (410199), $P_8Cu_2Se_3I_2$ (411332), $Ga_4As_4Br_{16}Hg_{11}$ (411676), $LiCl_{19}Nb_6$ (411688), $H_{10}O_{17}S_3Sc_2$ (413609), $P_8Cu_2Se_3Br_2$ (413695), $O_3CuBrSb_2$ (415539), $O_3ClCuSb_2$ (415540), $H_{18}O_{23}Na_3V_5$ (421746), H_6O_7SMn (423300), $O_{21}S_6GePb$ (423710), $Al_2P_3S_9$ (428186), $H_4B_5O_{10}Na$ (431106), $H_{10}O_{14}S_2Co_5$ (432191), $H_{10}O_{14}S_2Co_5$ (432192), H_3O_5PZn (60934), H_7O_7PMn (65686), H_3O_4PCo (68563), $O_9F_3S_3Au$ (69984), $H_8B_6O_{14}Ca$ (7748), $H_4O_6SiMn_2$ (80118), H_6O_6SFe (8239), $O_{22}Fe_4As_{10}Pb$ (82486), $C_7O_2Y_{16}I_{14}$ (85450), $H_{23}O_{12}F_{15}Zr_2Cd_4$ (86514), $C_{60}K$ (86639), C (96620)

In Supplementary Table 10 and 11, compounds with exfoliation energy lower than the threshold of 52.60 meV/Å^2 are shown in red.

Supplementary Table 10 | The list of 1D compounds.

Number of atoms	1D compounds (ICSD number)
1-6	Te_2I (107), TeI (108), Cl_4Os (1165), O_2Cu (150886), N_2O_2CoI (15286), Cl_2Sn (15452), $AlPS_4$ (15910), CNAu (165173), F_2Ge (18030), OFSb (19019), BrAu (200286), ClSnI (23262), O_2Se (24022), $GeZrTe_4$ (240906), $SiSe_2$ (24592), BPS_4 (24618), F_5Bi (25023), OCl_4W (25519), SBrSb (25571), SSbI (25572), SIBi (25575), O_2Si (25632), SiS_2 (26858), Br_2Pd (27443), Cl_2Pd (30209), SeSbI (31292), SbTeI (31355), $BeCl_2$ (31696), SeIn (32714), Cl_2Hg (36171), NS (4025), Br_2Sn (411177), AsSeI (200799), Cl_2Pt (44512), OBr_4W (49547), $AlPS_4$ (56821), FClSn (647), SeBrBi (76649), S_3Ti (81124), $SiCl_2$ (85526), CNAu (85782), CNAg (85783), $BeBr_2$ (92584), BeI_2 (92585), ONb (95729)
6-12	Cl_4Nb (1010), Cl_4Re (10293), NCl_3VI (10470), Cl_2Te_3 (105), NbI_3 (109145), O_3Cr (109366), Br_3Sb (14217), O_2V (1501), $H_4O_2Cl_2Cu$ (15087), I_4Pt (15173), S_3Sn_2 (15338), GaTe (153456), O_2Si (155252), $H_4O_2Cl_2Mn$ (15596), $H_4O_2Cl_2Fe$ (15597), BrBi (1560), OCs_3 (15695), $F_{10}NbSb$ (16095), OCl_3Mo (16150), Cl_4W (165263), Br_3Zr (165302), Se_3Sb_2 (16680), OF_4Mo (16867), S_3Sb_2 (171850), $H_4O_2MgCl_2$ (172992), H_2OMgCl_2 (172993), TiI_3 (173784), $NiBi_3$ (180771), O_4SCo (18176), As_2Te_3 (18208), $CoBi_3$ (193272), SSn_2I_2 (207), $H_4O_2Cl_2Co$ (22082), $H_4O_2MnBr_2$ (22084), $H_4O_2CoBr_2$ (22085), Cl_3Ru (22090), Cl_3Zr (23163), H_2OCl_2Mn (237381), H_2OCl_2Co (237382), NbI_4 (23916), ZrI_3 (23946), I_3Hf (23947), Br_4Nb (239640), O_2F_3Os (240330), MoI_3 (242166), N_6Cu (24340), O_3S (24723), Cl_6GaSb (24786), $H_2O_3Cl_2Mo$ (25031), NbI_5 (25503), Br_3Tc (260162), Br_4Tc (260163), Cl_4Zr (26049), Cl_4Tc (26055), Cl_3Ti (26069), S_3TiGe (263128), OCl_3Nb (26471), O_3Sb_2 (27595), S_2Cl_3Mo (28062), O_2FI (280804), Br_3Ru (28119), NCl_4V (28128), O_4PFe (290337), S_3InSb (300207), $H_4O_2Cl_2Co$ (34651), $H_4O_2Cl_2Fe$ (38012), $NaCl_3Hg$ (38302), $NiBi_3$ (391336), Al_2TiBr_8 (39243), TiI_4 (39820), Cl_4Hf (402054), Cl_4Ta (402406), Cl_2NbI_2 (407489), S_3GePd (408505), Br_3Mo (413690), O_2F_3Re (415421), NCl_8W_2 (415768), OCl_3W (416393), Al_2Cl_8Cr (416836), OBr_3Nb (418089), F_5Cr (419661), Br_4W (423461), PGe (427243), SCl_3Re (429458), C_2N_3Cu (432067), $SeIn_2$ (44646), $RhBi_3$ (58853), Br_4Os (61042), GeAs (610598), $NbTe_4$ (61113),

	As_2Se_3 (611373), O_2I (63651), In_2Te (640618), Se_4Nb (645375), Se_3Sb_2 (651519), OI_3W (65183), S_3SnHf (65667), Te_4ITa (67533), Cl_2I_2Ta (69688), S_3ZrSn (73711), O_3F_2Os (73732), PSe (74878), NBa_3 (77730), F_4Cr (78778), S_3Sb_2 (85302), F_4Te (85452), Se_3Sb_2 (85676), H_3LiO_2 (9138), $NbTe_4$ (93095), OF_2Sn_2 (948), NF_2P (9684), F_5V (9887), NK_3 (99999)
12-18	O_5Se_2 (10471), $H_6C_4O_2S_4Cd$ (110011), H_3LiCO_3 (151229), $H_8N_4Cl_2Zn$ (15875), N_3Cl_3Ti (15996), $H_4C_2O_6Fe$ (161344), La_4SbBr_3 (170144), O_5VSb_2 (2292), Ti_3O (23575), $H_4C_2O_6Mn$ (240902), $F_{13}KSb_4$ (24740), $H_8N_4Cl_2Mn$ (25784), $O_8P_2Cr_3$ (261640), H_3CCl_3Te (281531), $N_3S_2Cl_2V$ (30742), As_5Te_7I (31877), C_3N_3As (35330), $SiTe_4Ta_4$ (40207), $O_{11}S_2I_2$ (405696), O_3FRe (415418), P_4S_3CuI (418076), $S_3ClCuAs_4$ (419754), P_4S_3CuBr (421076), P_4CuSe_3I (422534), P_2S_7 (423061), HO_5AsTe (425500), SiS_4Sn_2 (429072), $H_5BO_6Cu_2$ (54883), C_2O_4Sn (54909), $H_4C_2O_6Zn$ (56466), $H_4C_2O_6Co$ (59927), $N_3S_2VBr_2$ (61088), $CrTe_4Ta_4$ (659267), $FeTe_4Ta_4$ (659268), $NiTe_4Ta_4$ (659270), $SiNb_4Te_4$ (659271), $FeNb_4Te_4$ (659272), $TiGeTe_6$ (73014), F_4Ti (78737), $OTi_4Te_9I_4$ (82142), $O_3F_2Te_2$ (82162), OF_2Te (88415)
18-30	$Cl_7Se_5Nb_3$ (10066), SeInI (100704), $H_{12}N_2O_6CuSn$ (103), $H_8C_4N_6S_4Fe$ (10452), NCl_3Mo (15117), $H_8C_6N_6O_2Cu$ (156682), $H_{12}C_3N_6S_3Br_2Ag_2$ (167545), S_4V (16797), $H_8C_2N_4O_8S_2CdRe_2$ (170223), $H_{16}B_6Cr$ (170564), $H_8C_4N_6S_4Cd$ (170723), H_8N_4ZnTe (170880), $C_4O_4F_6Ru$ (171337), Cl_3SeNb (172519), $H_6N_2Cl_2Cu$ (180189), $O_2F_{10}Te_2Hg$ (194226), H_6O_5NaCl (1954), I_4Hf (200826), OF_9MoSb (201410), $H_4C_3O_2ClCu$ (20522), Al_2Cl_8Co (22143), $H_{10}N_4O_8S_2Cd$ (240376), $H_{10}N_4O_8S_2Fe$ (240720), $H_4C_2N_4Cl_2Zn$ (240736), $H_6CN_2O_2NaCl$ (241250), $H_6CN_2O_2NaCl$ (241251), $H_8C_4O_{12}NaFe$ (244234), H_6O_6SMn (249139), $H_{10}N_4O_8S_2Mn$ (249335), I_3Re (25114), $H_{10}C_2O_8S_2Hg$ (251311), $H_{10}C_3OSn$ (252900), $H_6CN_2O_3Cu$ (2779), $H_{10}N_4O_8S_2Cr$ (279585), O_2F_8SbRe (280248), $H_3C_3O_6Sc$ (281595), $SeBr_3Nb$ (35375), Br_3NbTe (35376), $NbTeI_3$ (35377), $H_6O_{16}MgS_4$ (39276), Al_2Cl_8Ti (39565), $H_6O_{16}S_4Zn$ (404089), $H_6O_{16}S_4Cd$ (40438), H_9C_3IPb (405865), HO_8S_2I (407853), $H_6O_{16}S_4Mn$ (408754), $SeNbI_3$ (410743), $H_4O_8ZnI_2$ (410881), H_5O_7CuI (411345), $O_4F_{12}S_2CoSb_2$ (411789), CCl_8W_2 (412384), NCl_8Mo_2 (412397), Al_2Cl_8V (415951), OF_4Os (417245), OF_4Ru (417248), Cl_8NiGa_2 (417870), Al_2Cl_8Ni (417872), $AlInI_4$ (418802), $F_{10}CrSb$ (419662), N_2O_8Mo (421223), $H_8N_{10}Zn$ (421952), Cl_3RhTe_6 (422367), Br_3RhTe_6 (423669), Te_6I_3Ir (423670), $RhTe_6I_3$ (423671), Cl_3Te_6Ir (423672), Br_3Te_6Ir (423673), O_7TiI_2 (424632), H_4LiCNO_2S (425060), Te_8I_5Ir (425201), $H_6N_2ZnSe_4$ (425783), $H_2F_{14}As_2Hg$ (429284), PSnI (430054),

	$H_5N_2Cl_3Cu$ (49736), $H_4O_8Br_2Cd$ (54091), $H_{12}O_9S_2Ca$ (59815), $F_{11}Ta_2Hg_2$ (60923), $MgAl_2Cl_8$ (62046), Se_9Nb_2 (62538), OCl_8Mo_2 (65309), $NbTe_4I$ (67532), $H_8O_{16}ZnAs_4$ (68664), Se_3Nb (71498), H_6O_5NaBr (74654), $H_7C_2O_3ClSeSn$ (782622), SBi (79515), $H_8O_4Cl_2Ca$ (8061), ZrI_4 (8068)
30-50	H_8BeB_2 (10315), $O_6MgP_4Cl_{10}$ (15015), $H_9C_3PS_3ClAu$ (156684), $H_{12}C_4NSe_5Ag$ (159458), $H_8C_2N_4S_2BrAg$ (167543), $H_{24}C_9N_6S_3AgI$ (167544), $H_6O_6P_3Fe$ (171138), PS_4Sb (172038), $H_9C_3NO_2Cl_2Cu$ (172192), $H_{14}C_4NSi_2K$ (180206), $H_4LiBC_2O_6F_2$ (185385), $H_8O_{12}CaMn_2$ (187753), $H_{12}O_{12}P_6CaSn$ (188683), $H_{25}C_8O_{10}NaMo_2$ (192735), $C_6O_6F_9Sc$ (196174), F_4Sb (200035), $Se_{10}Br_3Nb_3$ (201731), $H_8O_{12}Cl_2Ca$ (237719), $Cl_3Se_{10}Nb_3$ (240715), $H_8C_4O_8Co$ (244465), $H_8C_2N_4O_5Ca$ (246784), $H_{10}C_2N_2ZnSe_4$ (248322), $H_{12}C_4O_2NaS_2Br$ (249333), $H_4CN_2O_4Mo$ (249697), $H_{10}C_6NS_2IPb$ (251754), $H_{18}B_3N_2Y$ (251866), $PS_7ClCuAs_7$ (262251), PS_7CuAs_7Br (262252), $C_3N_3K_2Ni$ (28032), H_4CNO_2NaS (30920), O_3PCl_5Mo (32649), P (391323), F_4Cr (412032), $N_2Cl_{11}Mo_3$ (412398), $H_4O_9CaSe_2$ (413482), $H_{10}O_5Cl_6SrSn_2$ (415711), $H_{10}O_5Br_6SrSn_2$ (415712), $H_6NO_{10}SNd$ (416245), $Sc_{12}Br_{16}Ir_3$ (421533), $F_{18}InSb_3$ (421923), $O_{14}S_4Zr$ (424062), C_4O_4CoCu (47183), $O_2S_{16}Cl_4Sn$ (61699), N_4Si_3 (67241), $H_6C_2N_2O_3S_2Sr$ (67479), $H_7B_3O_9Ca$ (75922), $H_6C_2N_4O_4Zn$ (9202)
>50	$H_9C_3O_4V$ (163034), $H_{19}C_7Si_2Br_2In$ (163067), $H_{16}C_4N_2O_{10}NaS_4Ag$ (163108), $H_8LiC_2NO_5S_2$ (163109), $H_{62}C_{25}O_6Si_7K$ (168989), $H_{16}C_3NO_{12}MgP_3$ (171671), $H_{16}C_3NO_{12}P_3Zn$ (172319), $H_{11}C_3OAlSi$ (172440), $H_{27}LiC_9O_3Si_4$ (173212), $H_{16}C_3NO_{12}P_3Cu$ (195948), $H_{16}N_9Al_2Ca$ (23464), $H_{16}C_3NO_{12}P_3Co$ (244060), $H_{16}C_3NO_{12}MgP_3$ (244061), $H_{16}C_3NO_{12}P_3Zn$ (244062), $H_{16}C_3NO_{12}P_3Mn$ (244063), $H_{16}C_3NO_{12}P_3Cd$ (244064), $H_9C_7O_4F_4S_2Ag$ (249365), $H_{12}C_4O_8P_2Mn$ (249436), $H_{16}C_7O_3F_3SiS_3Ag$ (249786), $H_{21}C_9N_{15}O_3Co_2$ (253962), $H_{12}C_4O_{15}S_4V_2$ (262179), $H_{10}C_3NAl$ (380172), $H_8C_2N_2O_4S_2Ca$ (409560), C (412242), $Cl_{10}PtBi_6$ (418334), $Br_{10}PtBi_6$ (418335), $H_{20}C_4N_4MnTe_2$ (426735), $F_{22}CdTa_4$ (431293), $F_{22}Ta_4Hg$ (431295), C (94500)

Supplementary Table11 | The list of 0D compounds.

Number of atoms	0D compounds (ICSD number)
1-6	BCl_2 (14213), PI_2 (203216), SiI_4 (22100), OF_3P (250498), $SiBr_4$ (260324), BF_2 (27867), CF_4 (2848), SnI_4 (31093), $TiBr_4$ (39241), $GeBr_4$ (409856), O_2Cl_2Cr (416750), GeI_4 (67895)
6-12	TeI (109), $NPBr_2$ (109142), $NPCl_2$ (109272), $P_4Se_3I_2$ (14281), SAs (15238), N_2O_2FeI (15285), NFS (15422), Al_2Cl_8Pd (15595), S_3As_4 (16105), AsSe (16106), S_5As_4 (16107), P_4Se_5 (16140), $N_5F_2PS_3$ (16275), O_7P_4 (16321), $BP_4S_3Br_3$ (165186), C_4F_6Hg (165635), P_4S_5 (16681), O_3As_2 (16850), O_3Sb_2 (16851), $C_2O_4F_4S$ (170271), H_2BO_2 (170953), H_2NF_5Te (171449), P_4S_5 (1995), HNF_4P_2 (201195), NFS (21015), Cl_5Re (22139), P_4S_7 (23842), O_3P_2 (24407), SAs (24661), Cl_3I (24714), C_2F_8Te (260189), $P_4S_3I_2$ (26219), $P_4S_3I_2$ (26485), NF_2P (26649), BCl (27872), $P_2S_7As_2$ (30706), H_2BN (401085), $C_2O_3F_6$ (401780), P_4S_3 (406048), O_2P (406625), Br_5Nb (409917), $BPBr_6$ (411194), OCl_3As (411196), Cl_5Sb (412110), N_9Sb (413359), O_2Cl_3Re (416056), $C_2NF_5SCl_2$ (417110), H_2NOCl_4Re (419182), OF_7SeNb (4410), C_3S_8 (53591), As_4Se_3 (611376), S_2Cl_6Pt (66013), $O_5F_2S_2$ (66514), Cl_5Nb (66537), O_6P_4S (69977), $NPBr_2$ (76764), P_2S_3 (78765), O_6P_4Se (78782), N_2S_2Cl (81232), $CN_3P_2Cl_5$ (81345), Cl_5Mo (84622), $CN_3S_2Cl_3$ (86482), $C_2N_3SCl_3$ (86483), $H_2O_3F_4Te_2$ (9653)
12-18	CO_2Cl_4Sb (109900), B_4F_9P (15215), O_5P_2 (16610), C_4O_2Se (172229), $H_9C_3OPCl_3Ga$ (173260), $H_9C_4F_3Si$ (173736), P_2S_5 (174009), O_3Se (18180), C_3O_3SFe (184603), $H_9C_3AlPCl_3$ (192497), $C_4F_{10}GeBr_2$ (196448), H_9NSi_3 (201428), $C_3N_3AlCl_6$ (240772), $S_3Ge_2Br_2$ (24370), H_9B_5 (24636), H_4BN (248876), $H_6C_2AlCl_3Te$ (250561), $H_6C_2AlBr_3Te$ (250562), CN_4O_8 (253934), P_4S_9 (26169), $O_3P_2S_2$ (27058), O_9P_4 (27434), C_2N (30814), NF_2P (31038), H_5B_2 (31695), H_3CPS_3 (320555), $NPCl_2$ (33711), $NSCl_5W$ (36292), $H_2Si_2S_3$ (36379), $O_6P_4Se_3$ (404499), Br_6PdTe_2 (405773), $BN_2OF_7S_2$ (414492), $F_{12}P_4Pt$ (418726), $P_4S_4Cl_5Ta$ (419157), $H_6N_4O_4Pd$ (420291), $N_3O_{10}V$ (420596), H_2Si (425931), H_5B_3 (43253), NSi_2Cl_5 (65953), $OSiCl_2$ (71445), H_9Si_3P (72676), $O_3P_4S_6$ (86494), H_9B_5 (88519), Cl_2Pt (98668)
18-30	F_5Rh (10173), Cl_3W (109512), BS_2 (15267), $C_{10}O_{10}Mn_2Hg$ (16124), SCl_4TeRe (165333), $Cl_4SeTeRe$ (165334), Cl_4Te_2Re (165335), F_5Ru (165397), $CN_4P_3Cl_7$ (170282), $S_9Br_8Ta_4$ (171236), F_2Cl_3Sb (200039), $C_6O_6SOs_2$ (201486), $C_4NO_5F_2SMn$ (2280), H_6B_5Br (2303), O_2F_3Os (240331), $H_{16}B_4Zr$ (250640), FCl_4Nb (26155), $O_3P_2Cl_8Sn$ (26182), $H_8N_2O_{10}Ni$ (26322), FCl_4Ta (27413), $OPCl_7Ti$ (27520), H_9BC_2P (281782), FCl_4Sb (30629), H_7B_5 (31566), SClPd (33989), Cl_4Mo (35139), $H_{16}B_4Hf$ (35379), $H_{16}BeB_6$ (36173), H_7B_5 (36282), NF_5Cl_4TeW (37149),

	$C_5O_5SCo_2$ (4014), $H_5C_3O_5F_3SCl_6Sb_2$ (408769), B_5F_6 (412618), O_9S_2ClRe (419178), $O_4P_2Cl_7V$ (420125), BCl (421891), Cl_7Te_7Ir (422863), Br_8RuTe_6 (423674), Cl_7RhTe_7 (425194), Br_7Te_7Ir (425195), $RuTe_7I_6$ (425196), $C_6O_6Fe_3Ge_2I_{10}$ (431991), $NPCl_7Ta$ (51258), $Be_4N_6O_{19}$ (59272), $C_5O_4F_2Mn$ (61132), $N_4S_4Cl_4Ti$ (62306), $O_{16}Cl_4Hf$ (62485), $O_3P_2Cl_8Ti$ (65139), $C_6O_6Ru_2Bi$ (65278), $OS_8Ti_4Br_6$ (68552), Br_7W_3 (74855), $NbTe_4I_6$ (78371), Br_4Te_2Re (78924), H_7B_5 (9152), $N_7P_6Cl_9$ (9449)
30-50	$O_4F_{22}Te_5$ (1275), $C_6O_9P_2Ni_2$ (14337), $H_8N_2O_{10}Ca$ (156303), $H_{11}B_9$ (15802), $H_{11}B_9$ (15823), $H_{15}C_5NSi_2$ (163114), $H_9C_3O_3Cl_3As_3Rh$ (163648), $H_9C_3O_3As_3Br_3Rh$ (163649), $H_{31}C_{10}NSi_6$ (166948), $H_7B_6O_6$ (170318), $H_9C_3OAlSiCl_2$ (170678), $H_{12}C_4OCl_2Sn_2$ (173733), $H_{10}C_{10}O_6SiFe_2Se_2$ (187378), O_2PCl_6Nb (200403), $H_{13}B_{10}$ (201205), $H_3BC_{12}O_{12}Fe_4$ (201318), $F_{29}Sb_7$ (203183), $O_6F_{30}Te_7$ (2173), $H_{12}C_4Cl_4NbTe_2$ (241963), $H_7C_2O_7PCu$ (243353), H_7O_8AlS (244754), $C_{11}O_3F_{24}P_4S_2Ni_2$ (26290), $H_{13}B_{10}$ (279587), $O_6F_{30}MoTe_6$ (33777), $NOPCl_6Mo$ (37107), H_8B_9S (4003), $H_4C_{20}O_{20}Re_5$ (54143), $C_{15}O_{15}Te_2W_3$ (60425), H_4N_2Ni (69723), C_3O_3SeRu (92913), $H_{13}B_{10}$ (9781)
>50	$O_{18}Cl_8Sn_3$ (14036), $H_{21}C_7Si_2ZnAs$ (150977), $H_{46}C_{16}NO_2Si_4PBa$ (151002), $H_{16}C_5N_2O_3F_4Zr$ (153358), $H_{24}C_8Si_2GaAs$ (163056), $H_{41}C_{15}OSi_4In$ (163065), $H_{32}Li_2C_{12}O_2Pt$ (163652), $H_{36}C_{13}Si_4$ (170687), $H_{13}BC_3NPCuI$ (173497), $C_{19}Cl_7$ (182903), $H_{36}C_{12}P_4Cl_2W$ (185488), $H_{18}B_2C_4NAl$ (238330), $H_{36}C_{12}N_6O_7Si_2$ (240233), $H_{22}C_7O_7ClMo_2$ (241972), $C_{17}F_6$ (249154), $H_{36}C_{12}O_5P_4Cl_4Mo_2$ (249208), $C_{68}OF_{20}$ (249217), C_7F_3 (249331), $C_{16}Cl$ (249692), $C_{13}Cl_3$ (249729), $C_{20}Cl_3$ (249788), C_9Cl (252548), HC_4O_4Re (280278), $H_{27}C_9N_2Si_3PBr$ (320225), C (602518), $BCO_5F_{20}AgTe_4$ (71175), $C_{10}F_3$ (95694)

References

1 Bonchev, D. & Rouvray, D. H. *Chemical Graph Theory: Introduction and Fundamentals* (Abacus Press, 1991).

2 Isayev, O. et al. Universal fragment descriptors for predicting properties of inorganic crystals. *Nat. Commun.* **8**, 15679 (2017).

3 Xie, T. & Grossman, J. C. Crystal graph convolutional neural networks for an accurate and interpretable prediction of material properties. *Phys. Rev. Lett.* **120**, 145301 (2018).

4 Weng, M. et al. Identify crystal structures by a new paradigm based on graph theory for building materials big data. *Sci. China-Chem.* **62**, 982-986 (2019).

5 Pauling, L. *The Nature of the Chemical Bond and the Structure of Molecules and Crystals: An Introduction to Modern Structural Chemistry* (Cornell University Press, 1960).

6 Slater, J. C. Atomic radii in crystals. *J. Chem. Phys.* **41**, 3199-3204 (1964).

7 Shannon, R. D. Revised effective ionic radii and systematic studies of interatomic distances in halides and chalcogenides. *Acta Crystallogr. Sect. A* **32**, 751-767 (1976).

8 Mounet, N. et al. Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds. *Nat. Nanotechnol.* **13**, 246-252 (2018).

9 Jia, W. et al. The analysis of a plane wave pseudopotential density functional theory code on a GPU machine. *Comput. Phys. Commun.* **184**, 9-18 (2013).

10 Jia, W. et al. Fast plane wave density functional theory molecular dynamics calculations on multi-GPU machines. *J. Comput. Phys.* **251**, 102-115 (2013).

11 Perdew, J. P., Burke, K. & Ernzerhof, M. Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.* **77**, 3865-3868 (1996).

12 Monkhorst, H. J. & Pack, J. D. Special Points for Brillouin-Zone Integrations. *Phys. Rev. B* **13**, 5188-5192 (1976).

13 Grimme, S. Semiempirical GGA-type density functional constructed with a long-range dispersion correction. *J. Comput. Chem.* **27**, 1787-1799 (2006).

14 Kresse, G. & Furthmuller, J. Efficient iterative schemes for *ab initio* total-energy calculations using a plane-wave basis set. *Phys. Rev. B* **54**, 11169-11186 (1996).

15 Kresse, G. & Furthmüller, J. Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. *Comput. Mater. Sci.* **6**, 15-50 (1996).

16 Kresse, G. & Joubert, D. From Ultrasoft Pseudopotentials to the Projector Augmented-Wave Method. *Phys. Rev. B* **59**, 1758-1775 (1999).

17 Dronskowski, R. & Bloechl, P. E. Crystal orbital Hamilton populations (COHP): energy-resolved visualization of chemical bonding in solids based on density-functional calculations. *J. Phys. Chem.* **97**, 8617-8624 (1993).

18 Deringer, V. L., Tchougreeff, A. L. & Dronskowski, R. Crystal orbital Hamilton population (COHP) analysis as projected from plane-wave basis sets. *J. Phys. Chem. A* **115**, 5461-5466 (2011).

19 Maintz, S., Deringer, V. L., Tchougreeff, A. L. & Dronskowski, R. Analytic projection from plane-wave and PAW wavefunctions and application to chemical-bonding analysis in solids. *J.*

Comput. Chem. **34**, 2557-2567 (2013).

20 Maintz, S., Deringer, V. L., Tchougreeff, A. L. & Dronskowski, R. LOBSTER: A tool to extract chemical bonding from plane-wave based DFT. *J. Comput. Chem.* **37**, 1030-1035 (2016).

21 Jung, J. H., Park, C. H. & Ihm, J. A rigorous method of calculating exfoliation energies from first principles. *Nano Lett.* **18**, 2759-2765 (2018).

22 Silvi, B. & Savin, A. Classification of chemical bonds based on topological analysis of electron localization functions. *Nature* **371**, 683-686 (1994).

23 Becke, A. D. & Edgecombe, K. E. A simple measure of electron localization in atomic and molecular systems. *J. Chem. Phys.* **92**, 5397-5403 (1990).

24 Savin, A. et al. Electron localization in solid-state structures of the elements: the diamond structure. *Angew. Chem. Int. Edit.* **31**, 187-188 (1992).