

The Materials Cloud 2D database

Davide Campi, Nicolas Mounet, Marco Gibertini, Giovanni Pizzi, Nicola Marzari

Definitions and details

- All the properties are computed at the DFT-PBE level. The only exceptions are binding energies, which were calculated using the DF2-C09 and the rVV10 van-der-Waals functionals. All 3D and 2D structures are treated as non-magnetic using spin-unpolarized DFT. The magnetic order has a negligible effect on the binding energies as discussed in Ref.[1] but caution is needed when looking at the electronic properties of materials with elements that might support a magnetic ground state. The magnetic properties of a subset of materials, easily exfoliable with at most 6 atoms per unit cell, have been computed in Ref.[1] and can be browsed at <https://www.materialscloud.org/discover/mc2d/dashboard/ptable> or downloaded <https://doi.org/10.24435/materialscloud:2017.0008/v1>. For consistency with the rest of the database, these materials are reported in this archive in their non-magnetic state.
- Binding energies are calculated as total energy differences between relaxed 3D parents and as-exfoliated, unrelaxed 2D children. More details can be found in the Methods section of the main paper.
- Each 2D structure has at least one 3D parent structure. In those cases when the monolayers can be exfoliated from more than one parent, for each functional we choose as parent the one with the lowest binding energy, and then we select the functional giving the most favourable 2D classification, with a preference for DF2-C09 when an ambiguity persists. The list of all possible 3D parents of a given monolayer is reported in the dataset.
- In metals, the zero for energy bands is the Fermi energy, while for semiconductors the zero is set midway between the highest occupied state in the valence bands and the lowest unoccupied state in the conduction bands. For simplicity, we call this Fermi energy in the captions. Calculations have been performed with a finite smearing that might slightly influence its position
- Paths and special k-points follow the conventions for 2D systems from Ref. [2] as implemented in AiiDA [3,4].

References:

- [1] N. Mounet, M. Gibertini, P. Schwaller, D. Campi, A. Merkys, A. Marrazzo, T. Sohler, I. E. Castelli, A. Cepellotti, G. Pizzi, N. Marzari, Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds, *Nature Nanotech.*, (2018). DOI:10.1038/s41565-017-0035-5.
- [2] R. Ramírez and M. C. Bohm, Simple geometric generation of special points in Brillouin-zone integrations. Two-dimensional Bravais lattices. *Int. J. Quantum Chem.* 30, 391-411 (1986).
- [3] G. Pizzi, A. Cepellotti, R. Sabatini, N. Marzari, and B. Kozinsky. AiiDA: automated interactive infrastructure and database for computational science. *Computational Materials Science* 111, 218 - 230 (2016).
- [4] S.P. Huber, S. Zoupanos, M. Uhrin, L. Talirz, L. Kahle, R. Häuselmann, D. Gresch, T. Müller, A. V. Yakutovich, C. W. Andersen, F. F. Ramirez, C. S. Adorf, F. Gargiulo, S. Kumbhar, E. Passaro, C. Johnston, A. Merkys, A. Cepellotti, N. Mounet, N. Marzari, B. Kozinsky, and G. Pizzi. AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance. *Scientific Data* 7, 300 (2020).

Potentially exfoliable materials up to 6 atoms per unit cell

Contents

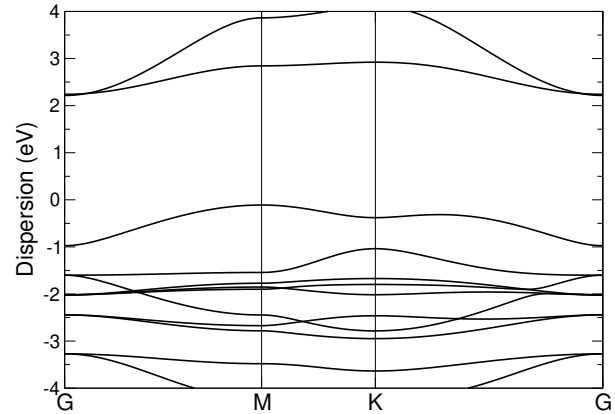
AgNO ₃ (P3m1 (156))	4	CrAuTe ₄ (Pm (6))	72	K ₂ PdSe ₂ (Pmmm (47))	152	MnSe ₂ (P-4m2)	226
AgTe (Pmm2 (25))	6	CrS ₂ (P3m1 (156))	74	K ₂ PtS ₂ (Pmmm (47))	154	Na (P6/mmm (191))	228
AgTe ₂ (P-4m2 (115))	8	CrSe ₂ (P3m1 (156))	76	K ₂ PtSe ₂ (Pmmm (47))	156	NaCuSe (P4/nmm (129))	230
AgTl (Pmmm (47))	10	CrTe ₂ (P-3m1 (164))	78	K ₂ PtTe ₂ (Pmmm (47))	158	NaCuTe (P4/nmm (129))	232
As (P-3m1 (164))	12	CsBr ₂ F (P4/mmm (123))	80	KAuS (Pmma (51))	160	NaF ₂ (P-3m1)	234
As ₂ O ₃ (P6mm)	14	CsBr ₃ (P-6m2)	82	KAuSe (P2/m (10))	162	NaMgAs (P4/nmm (129))	236
AuTe ₂ (P-3m1 (164))	16	CsBr ₃ (P-6m2)	84	KCuTe (Pmmn (59))	164	NaMnTe ₂ (P3m1 (156))	238
Ba ₂ Cd (P4/mmm (123))	18	Cu ₂ Cl ₄ (P2/m)	86	KNO ₃ (P3m1)	166	NaO ₄ (P3)	240
Ba ₂ Hg (P4/mmm (123))	20	Cu ₂ F ₄ (Pbam)	88	KO ₃ Br (P3m1 (156))	168	NaSnP (P3m1 (156))	242
Ba ₂ N (P-3m1 (164))	22	CuS (P4/nmm (129))	90	KO ₃ Cl (P3m1 (156))	170	Ni(OH) ₂ (P-3m1 (164))	244
Ba ₂ Ni ₃ (P-3m1 (164))	24	CuSe (P-6m2 (187))	92	KO ₃ I (P3 (143))	172	Ni ₂ SbTe ₂ (P-6m2 (187))	246
Ba ₂ Pt (P-3m1)	26	CuSe (P4mm (99))	94	KSeO ₂ F (Pm (6))	174	Ni ₃ GeTe ₂ (P-6m2)	248
BaCu (P6/mmm (191))	28	CuTe (P4/nmm (129))	96	KSnAs (P3m1 (156))	176	NiO ₂ H (P3m1)	250
BaMnGe (P4/nmm (129))	30	CuTe ₂ (P-3m1)	98	KTiS ₂ (P3m1 (156))	178	NiSe (P4mm (99))	252
Bi ₂ S ₃ (P-3m1 (164))	32	Fe(OH) ₂ (P-3m1)	100	Li ₂ C ₂ (C2/m)	180	NiTe (P-3m1 (164))	254
Bi ₂ Se ₄ (C2/m)	34	FeAs (P4mm (99))	102	Li ₂ CeAs ₂ (P-3m1 (164))	182	NiTe ₂ (P-3m1 (164))	256
BiO (P4/nmm (129))	36	FeSe ₂ (P4/mmm)	104	Li ₂ CeP ₂ (P-3m1 (164))	184	PbS ₂ (P-3m1)	258
BiTe ₂ (P-3m1 (164))	38	GaSe (P-3m1 (164))	106	Li ₂ CuAs (P-6m2 (187))	186	PdBi ₂ (P4/mmm (123))	260
C (P6/mmm)	40	Ge ₂ Te ₂ (P1)	108	Li ₂ NdAs ₂ (P-3m1 (164))	188	PdTe ₂ (P-3m1 (164))	262
Ca ₂ C ₄ (C2/m)	42	HfGeTe (P4/nmm (129))	112	Li ₂ PdH ₂ (P4/mmm (123))	190	PtTe (P3m1 (156))	264
Ca ₂ Cu (P-1 (2))	44	HfSiSe (P4/nmm (129))	114	Li ₂ PrAs ₂ (P-3m1 (164))	192	PtTe ₂ (P-3m1 (164))	266
Ca ₂ N (P-3m1 (164))	46	Hg ₂ N ₂ Cl ₂ (Pmma)	116	Li ₂ PrP ₂ (P-3m1 (164))	194	Rb ₂ Cu ₂ Te ₂ (Pmmn)	268
CaClF (P4/nmm (129))	48	Hg ₃ Br ₂ (P-3m1 (164))	118	Li ₂ PtH ₂ (Pmmm)	196	RbGeI ₃ (P3m1)	270
CaHCl (P4/nmm (129))	50	Hg ₃ N ₂ (P321)	120	Li ₃ As (P-6m2)	198	ReN ₂ (P3m1)	272
CaMnGe (P4/nmm (129))	52	Hg ₃ S ₂ (C2/m (12))	122	LiCoAs (P4/nmm (129))	200	ReS ₂ (P3m1)	274
CaMnSi (P4/nmm (129))	54	HgO (Pmmm (47))	124	LiFeAs (P4/nmm (129))	202	Rh ₂ As ₂ (P4/nmm)	276
CaOHCl (P3m1)	56	In (P4/mmm (123))	126	LiFeP (P4/nmm (129))	204	RhP (P4mm (99))	278
CdO ₂ (P-3m1)	58	In (P6/mmm (191))	128	LiHfS ₂ (P3m1)	206	RhTe ₂ (P-3m1 (164))	280
CdOHCl (P3m1 (156))	60	In ₂ Te ₃ (P-3m1 (164))	130	LiMnSe ₂ (P3m1 (156))	208	Ru ₂ As ₂ (P4/nmm)	282
CdOHCl (P3m1)	62	InBi (P4/nmm (129))	132	LiMnTe ₂ (P3m1 (156))	210	Sb ₂ Te ₂ (P-3m1)	284
CoAs (P4mm (99))	64	InSe (P3m1 (156))	134	LiNbS ₂ (P3m1)	212	Sb ₂ Te ₂ (P-3m1)	286
CoS (P4/nmm (129))	66	InSe ₂ (P3m1 (156))	136	LiO (P3m1)	214	SbAs (P3m1)	288
CoSe (P4/nmm (129))	68	Ir ₂ As ₂ (P4/nmm)	138	LiO ₂ (P-3m1)	216	Sn (P4/mmm (123))	290
CoTe ₂ (P-3m1 (164))	70	Ir ₂ P ₂ (P4/nmm)	140	LiTiS ₂ O (P3m1)	218	Sn ₂ As (P-3m1 (164))	292
		IrTe ₂ (P-3m1 (164))	142	LiTl (P3m1 (156))	220	Sn ₂ P (P-3m1 (164))	294
		K (P4/mmm (123))	144	Mn ₂ Bi ₂ (Pmma)	222	SnAs (P-3m1 (164))	296
		K (P6/mmm (191))	146	MnCl ₄ (P4/mmm)	224	SnI ₃ (P4mm)	298
		K ₂ Ag ₂ Te ₂ (Pm)	148				
		K ₂ PdS ₂ (Pmmm (47))	150				

SnP (P-3m1 (164))	300	Ta ₂ Se (P4/nmm (129))	314	YbSe ₂ (P-3m1 (164))	330	ZrGeTe (P4/nmm	
SnPbS ₂ (Pm)	302	Tl (P6/mmm (191))	316	ZnF ₂ (P4/mmm)	332	(129))	344
SnS (P1 (1))	304	Tl (P4/mmm (123))	318	ZnN ₃ OH (P3m1)	334	ZrSiSe (P4/nmm	
SnSe (P1 (1))	306	Tl ₂ CS ₃ (P1 (1))	320	ZnO ₂ (P-3m1)	336	(129))	346
Sr ₂ N (P3m1 (156))	308	Tl ₂ S ₂ Cl ₂ (P4/nmm)	322	ZnOHF (P3m1)	338		
SrCu (P6/mmm (191))	310	TlO ₃ I (P3m1)	324	ZnTe ₂ (P-3m1)	340		
SrMnGe (P4/nmm		TlSbSe ₂ (Pmmm (47))	326	ZrGeSe (P4/nmm			
(129))	312	Y ₂ Se ₂ F ₂ (P-3m1)	328	(129))	342		

AgNO₃ (P3m1 (156))

Structural and electronic properties

	Formula	AgNO ₃
	Spacegroup	P3m1 (156)
	Prototype	KNO3
	Parent 3D	AgNO ₃
	Source DB	COD
	DB ID	2105347
DF2-C09	Binding energy [meV/ Å²]	31.28
RVV10	Binding energy [meV/ Å²]	47.51
	Band gap (PBE) [eV]	2.33

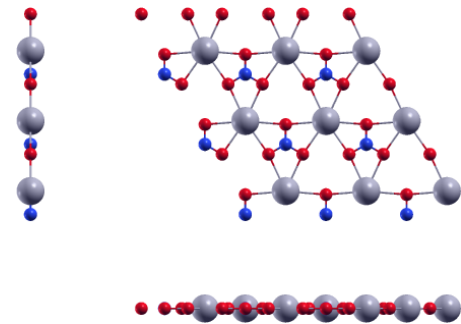


Band structure: Electronic band structure of AgNO₃ (P3m1 (156)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of AgNO₃ (P3m1 (156)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		5.16323801	−0.00000000	0.00000000
a₂		−2.58161901	4.47149528	0.00000000
a₃		0.00000000	0.00000000	20.66416824
		x [Å]	y [Å]	z [Å]
•	N	2.58161901	4.47149528	10.51856986
•	O	1.48605245	3.83896964	10.51859569
•	O	−1.48605245	3.83896964	10.51859569
•	O	0.00000000	1.26505129	10.51859569
•	Ag	2.58161901	1.49049843	10.51926701



Orthographic projections: views of AgNO₃ (P3m1 (156)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	6	0.111	1	1
K	6	0.2574	1	1
Ag ₂	7	0.265	1	1
Ba ₂ Pt	8	0.2647	1	1
CaI ₂	8	1.5949	1	1
Br ₂ Cu	8	1.6671	1	1
Ca ₂ Si	8	0.2712	1	1
PdTe ₂	8	4.8738	1	1
HgI ₂	8	0.1182	1	1
CNRb	8	0.1816	1	1
I ₂ Tm	8	1.5862	1	1
I ₂ Pb	8	0.2673	1	1
DyI ₂	8	0.2488	1	1
Br ₂ Cd	8	4.8541	1	1
Bi ₂ In ₂	9	0.1278	1	1
Cu ₂ Te ₂	9	0.1144	1	1
S ₂ Sn ₂	9	0.1077	1	1
Au ₂ Br ₂	9	0.4443	1	1
Ge ₂ Te ₂	9	0.1118	1	1
N ₃ Na	9	0.1193	1	1
Ge ₂ S ₂	9	0.1093	1	1
Sb ₂ Te ₂	9	0.2693	1	1
La ₂ S ₂	9	0.1109	1	1
SbSe ₂ Tl	9	0.7947	1	1
Ag ₂ I ₂	9	0.1187	1	1
Br ₂ CsF	9	0.1265	1	1
Sn ₂ Te ₂	9	0.123	1	1
O ₂ Sn ₂	9	0.226	1	1
Sm	9	0.0059	1	4
F ₄ Pb	10	0.1147	1	1
GeI ₂ La ₂	10	1.5843	1	1
NaO ₄	10	0.0008	1	1
I ₂ La ₂ Sb	10	0.2579	1	1
Cl ₄ Mn	10	0.1318	1	1
I ₂ La ₂ Te	10	0.2541	1	1
Ba ₂ H ₂ I ₂	11	0.1252	1	1
HfS ₂	11	0.2187	1	2
AlH ₄ Na	11	0.1337	1	1
S ₂ Zr	11	0.2257	1	2
Cu ₂ Na ₂ Te ₂	11	0.1122	1	1
Cl ₄ Cu ₂	11	0.3132	1	1
Br ₂ Cr ₂ S ₂	11	0.1159	1	1
I ₂ Pr ₂ S ₂	11	0.2661	1	1
C ₂ Br ₂ Gd ₂	11	0.1822	1	1
CoTe ₂	11	0.2191	1	2
Dy ₂ I ₂ S ₂	11	0.2479	1	1
Br ₂ Ca ₃ Si	11	0.254	1	1
Cu ₂ Rb ₂ Te ₂	11	0.1276	1	1
Cl ₂ N ₂ Ti ₂	11	0.1146	1	1
Ag ₂ K ₂ Te ₂	11	0.1381	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

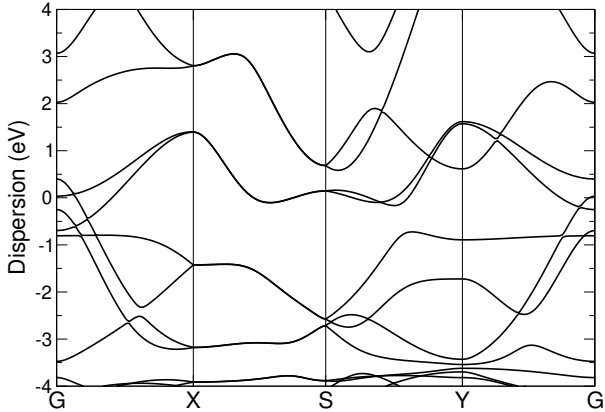
Formula	N° atoms	strain	cell size 1	cell size 2
Bi ₂ SeTe ₂	305	0.0	25	36
CCL ₂ Sc ₂	65	0.0	4	9
PdTe ₂	488	0.0001	49	81
I ₂ S ₂ Tb ₂	629	0.0001	49	64
Br ₂ Tb ₂	429	0.0001	37	61
CuTe ₂	432	0.0001	39	79
Bi ₂ S ₃	490	0.0001	37	61
Br ₂ HLa	180	0.0002	16	25
Ca ₂ N	545	0.0002	49	100
I ₂ Pb	705	0.0002	81	100
Ba ₂ Pt	638	0.0002	73	91
HfS ₂	432	0.0002	39	79
Se ₄ TiZr	863	0.0002	79	78
AsCuLi ₂	180	0.0003	16	25
DyI ₂	437	0.0003	49	64
CoH ₂ O ₂	170	0.0003	9	25
CaI ₂	386	0.0003	43	57
Cl ₂ Zr ₂	56	0.0003	4	9
Br ₂ Ho ₂	429	0.0004	37	61
Br ₂ H ₂ Zr ₂	74	0.0004	4	9
Br ₂ Hf ₂ N ₂	845	0.0004	49	100
I ₂ Pr ₂ Si ₂	230	0.0005	16	25
GeTe ₂	93	0.0005	9	16
Ag ₂	547	0.0005	73	91
C ₂ Br ₂ Gd ₂	613	0.0005	41	68
Ga ₂ Te ₂	180	0.0005	16	25
C	14	0.0006	1	9
Ba ₂ Ni ₃	205	0.0006	16	25
CeLi ₂ P ₂	205	0.0006	16	25
CaH ₂ O ₂	590	0.0006	39	79
CoTe ₂	432	0.0006	39	79
Bi ₂	197	0.0006	25	36
CrSe ₂	317	0.0006	25	64
FeI ₂	93	0.0006	9	16
Br ₂ Er ₂ Se ₂	440	0.0006	40	40
Cu ₂ Te ₂	757	0.0006	65	108
I ₂ Ni	93	0.0007	9	16
ReS ₂	120	0.0007	9	25
LiO	253	0.0007	25	64
PdTe ₂	368	0.0007	37	61
Ga ₂ S ₂	511	0.0007	39	79
As ₂ Ir ₂	877	0.0007	81	118
As ₂	445	0.0007	49	100
Cd ₂ I ₃	425	0.0007	36	49
Br ₂ Mg	93	0.0007	9	16
GeI ₂	155	0.0008	16	25
Te ₄ TiZr	93	0.0008	9	8
AsI ₂ La ₂	425	0.0008	36	49
Cl ₂ N ₂ Zr ₂	669	0.0008	39	79
NaO ₄	10	0.0008	1	1

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

AgTe (Pmm2 (25))

Structural and electronic properties

	Formula	AgTe
	Spacegroup	Pmm2 (25)
	Prototype	AgTe
	Parent 3D	Ag ₃ TlTe ₂
	Source DB	COD
	DB ID	2105385
DF2-C09	Binding energy [meV/ Å²]	72.63
RVV10	Binding energy [meV/ Å²]	69.6
	Band gap (PBE) [eV]	0.0

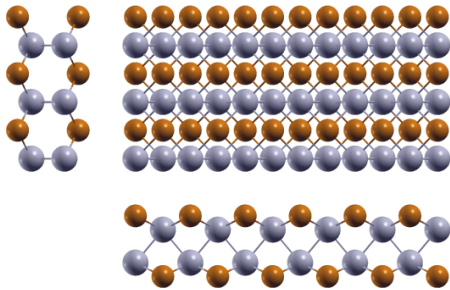


Band structure: Electronic band structure of AgTe (Pmm2 (25)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of AgTe (Pmm2 (25)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.76139913	0.00000000	0.00000000
a₂		0.00000000	3.88385884	0.00000000
a₃		0.00000000	0.00000000	23.45335994
		x [Å]	y [Å]	z [Å]
●	Ag	1.88069956	0.00000000	10.59472450
●	Te	1.88069956	1.94192942	13.80369626
●	Ag	0.00000000	0.00000000	12.85870766
●	Te	0.00000000	1.94192942	9.64959146



Orthographic projections: views of AgTe (Pmm2 (25)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.4078	1	1
K	5	0.1978	1	1
In	5	0.1098	1	1
InSe	6	0.1558	1	1
HgO	6	0.5688	1	1
Bi ₂	6	0.1618	1	1
Ag ₂	6	0.2053	1	1
PbTe	6	0.1576	1	1
Sb ₂	6	0.1409	1	1
I ₂ Mg	7	0.1459	1	1
CdI ₂	7	0.1594	1	1
AgTe ₂	7	0.5432	1	1
Ba ₂ Pt	7	0.205	1	1
Br ₂ Ca	7	0.1607	1	1
CaI ₂	7	0.1857	1	1
HfTe ₂	7	0.1288	1	1
I ₂ Pr	7	0.0132	1	1
Br ₂ La	7	0.1462	1	1
Br ₂ Cu	7	0.1148	1	1
Ca ₂ Si	7	0.2114	1	1
I ₂ Yb	7	0.1826	1	1
BiClTe	7	0.1598	1	1
ReS ₂	7	0.1118	1	1
AuTe ₂	7	0.1345	1	1
BrCdI	7	0.1488	1	1
Cl ₂ Zn	7	0.0151	1	1
PdTe ₂	7	0.1326	1	1
HgI ₂	7	1.2041	1	1
I ₂ Zn	7	0.1381	1	1
BaF ₂	7	0.152	1	1
BiBrTe	7	0.1657	1	1
Bi ₂ Pd	7	0.5975	1	1
GeI ₂	7	0.1442	1	1
Ba ₂ Hg	7	0.3601	1	1
Ba ₂ N	7	0.1299	1	1
AsKSn	7	0.1506	1	1
Te ₂ Zr	7	0.1291	1	1
I ₂ Nd	7	0.014	1	1
I ₂ Tm	7	0.1843	1	1
GeI ₂	7	0.1578	1	1
I ₂ Pb	7	0.2076	1	1
STl ₂	7	0.1529	1	1
BiTe	7	0.1732	1	1
GeS ₂	7	0.2359	1	1
DyI ₂	7	0.1894	1	1
CeI ₂	7	0.0126	1	1
Se ₂ Yb	7	0.1444	1	1
BiTe ₂	7	0.1446	1	1
GdI ₂	7	0.1689	1	1
PtTe ₂	7	0.1342	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

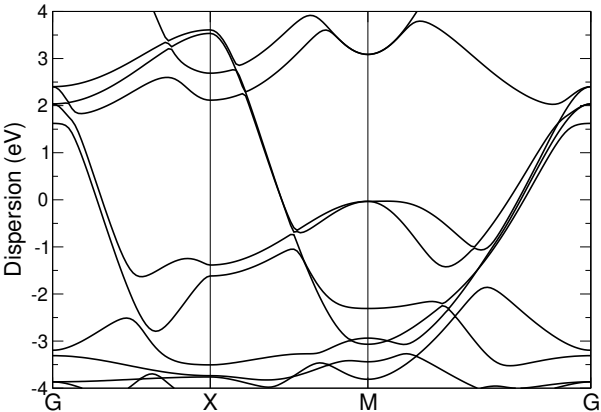
Formula	N° atoms	strain	cell size 1	cell size 2
AgTe ₂	416	0.0004	50	72
Mg ₂	342	0.0004	48	75
Br ₂ Zr ₂	800	0.0005	85	115
O ₄ PTl	348	0.0005	42	30
Bi ₂ S ₃	645	0.0005	70	73
Br ₂ Tb ₂	572	0.0005	70	73
Br ₂ Ho ₂	572	0.0006	70	73
Br ₂ Cr ₂ S ₂	548	0.0007	56	54
Ag ₂ K ₂ Te ₂	588	0.0008	75	48
Te ₂ V	635	0.0008	80	105
Se ₂ Ti	685	0.0008	85	115
PdTe ₂	499	0.0009	70	73
Ba ₂ F ₂ I ₂	348	0.0009	42	30
AgClO ₄	348	0.0009	45	28
Br ₂ Mn	635	0.0009	80	105
Li ₂ P ₂ Pr	576	0.001	64	64
Ga ₂ Ge ₂ Te ₂	640	0.001	64	64
Sb ₂	384	0.001	64	64
C ₂ Li ₂	352	0.001	45	43
Cl ₂ Hf ₂ N ₂	950	0.001	80	105
Er ₂ I ₂ Se ₂	876	0.001	114	70
OTl ₂	635	0.001	80	105
Ba ₂ H ₂ I ₂	588	0.001	72	50
Br ₂ La ₂	512	0.0011	64	64
S ₂ Zn ₂	688	0.0011	82	90
LiO ₂	232	0.0011	28	40
CoH ₂ O ₂	858	0.0012	67	118
C ₂ Br ₂ Y ₂	646	0.0012	61	67
CdClO	635	0.0012	80	105
ReS ₂	794	0.0012	86	150
Dy ₂ I ₂ S ₂	814	0.0012	103	67
La ₂ S ₂	580	0.0012	81	64
C ₂ Br ₂ La ₂	174	0.0013	18	17
As ₂ Mg ₂ Na ₂	698	0.0013	80	63
P ₂ Sn ₂	688	0.0013	82	90
KS ₂ Ti	740	0.0013	80	105
H ₂ I ₂ Sr ₂	708	0.0013	81	64
PtTe ₂	499	0.0014	70	73
In	277	0.0014	49	81
Se ₂ Ta ₄	732	0.0014	63	80
GeI ₃ Rb	348	0.0014	72	12
FeSe ₂	192	0.0014	21	36
LiOS ₂ Ti	276	0.0015	24	36
K	383	0.0015	80	63
Gd ₂ I ₂ S ₂	722	0.0015	92	59
Ho ₂ I ₂ Se ₂	852	0.0015	111	68
SnTe ₂	448	0.0015	64	64
Cl ₂ V	267	0.0015	30	49
NbS ₂	228	0.0015	27	40
Br ₂ O ₂ V ₂	66	0.0015	6	7

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

AgTe₂ (P-4m2 (115))

Structural and electronic properties

Formula	AgTe ₂
Spacegroup	P-4m2 (115)
Prototype	HgI ₂
Parent 3D	AgTlTe ₂
Source DB	COD
DB ID	1509558
DF2-C09 Binding energy [meV/ Å²]	60.02
RVV10 Binding energy [meV/ Å²]	68.66
Band gap (PBE) [eV]	0.0

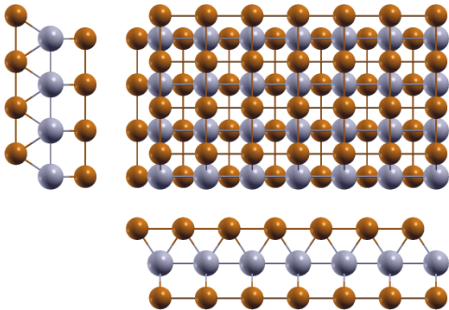


Band structure: Electronic band structure of AgTe₂ (P-4m2 (115)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of AgTe₂ (P-4m2 (115)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.18339933	−0.00000000	0.00000000
a₂	−0.00000000	3.18339933	0.00000000
a₃	0.00000000	0.00000000	24.49672752
	x [Å]	y [Å]	z [Å]
● Te	3.18339933	3.18339933	9.84825332
● Ag	1.59169967	3.18339933	12.24836376
● Te	1.59169967	1.59169967	14.64847420



Orthographic projections: views of AgTe₂ (P-4m2 (115)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	4	0.003	1	1
Tl	4	0.1299	1	1
Na	4	0.1572	1	1
Sm	4	0.1105	1	1
HgO	5	0.0093	1	1
AsSb	5	0.7666	1	1
GeTe	5	0.7901	1	1
As ₂	5	0.1657	1	1
CaCl	5	0.4005	1	1
Cl ₂ Zn	6	0.1645	1	1
CdCl ₂	6	0.7859	1	1
Cl ₂ Mn	6	0.1342	1	1
MoTe ₂	6	0.1595	1	1
PSn ₂	6	0.1759	1	1
MoSe ₂	6	0.1294	1	1
ReSe ₂	6	0.1452	1	1
S ₂ Ta	6	0.1358	1	1
Br ₂ Zn	6	0.1892	1	1
HfS ₂	6	0.1687	1	1
InSe ₂	6	0.7874	1	1
AsSn ₂	6	0.1805	1	1
GeTe ₂	6	0.782	1	1
SiTe ₂	6	0.1946	1	1
Te ₂ V	6	0.1616	1	1
I ₂ Mn	6	0.7864	1	1
CuTe ₂	6	0.1683	1	1
S ₂ Zr	6	0.175	1	1
NSr ₂	6	0.7728	1	1
Br ₂ Co	6	0.1652	1	1
Ca ₂ N	6	0.1663	1	1
LiO ₂	6	0.1219	1	1
Cl ₂ Zn	6	1.1612	1	1
FeI ₂	6	0.7778	1	1
I ₂ Ni	6	0.7827	1	1
S ₂ Ti	6	0.1399	1	1
Mg ₃	6	0.0087	1	1
Te ₂ Ti	6	0.1896	1	1
NbS ₂	6	0.1355	1	1
CrI ₂	6	0.7761	1	1
Te ₂ Zn	6	0.1593	1	1
RhTe ₂	6	0.184	1	1
N ₂ W	6	0.1086	1	1
Br ₂ Mn	6	0.1632	1	1
Cl ₂ Ni	6	0.146	1	1
Cl ₂ Co	6	0.1396	1	1
CrTe ₂	6	0.1518	1	1
PtS ₂	6	0.1582	1	1
NbS ₂	6	0.1322	1	1
CoTe ₂	6	0.1691	1	1
Br ₂ V	6	0.1445	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

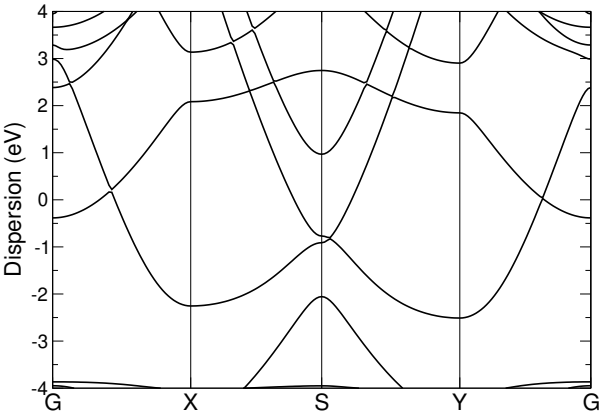
Formula	N° atoms	strain	cell size 1	cell size 2
As ₂ Co ₂	388	0.0	64	49
Ca ₂ Ge ₂ Mn ₂	429	0.0	61	41
Fe ₂ SeTe	499	0.0	85	61
Cu ₂ I ₂	439	0.0001	81	49
Cu ₂ F ₄	129	0.0001	25	9
Co ₂ S ₂	887	0.0001	145	113
As ₂ Ir ₂	139	0.0002	25	16
Cu ₂ K ₂ Te ₂	645	0.0002	109	53
O ₂ Pb ₂	578	0.0002	106	65
Cl ₂ Zn	255	0.0002	49	36
Br ₂ Er ₂ O ₂	258	0.0003	36	25
Br ₂ H ₂ Sr ₂	537	0.0003	81	49
Br ₂ H ₂ Yb ₂	621	0.0003	85	61
Bi ₂ Br ₂ O ₂	942	0.0003	136	89
I ₂ La ₂ O ₂	945	0.0003	145	85
As ₂ Fe ₂ Li ₂	621	0.0004	85	61
C ₄ Ca ₂	540	0.0004	82	49
Fe ₂ S ₂	499	0.0004	81	64
F ₂ I ₂ Sm ₂	708	0.0004	106	65
Ge ₂ Se ₂ Zr ₂	495	0.0004	65	50
Ag ₂ Te ₂	416	0.0004	72	50
Ca ₂ Cl ₂	395	0.0004	65	50
O ₄ PSn	594	0.0004	100	49
Ag ₂ K ₂ Te ₂	51	0.0004	9	4
Ba ₂ F ₂ I ₂	891	0.0005	149	74
Eu ₂ F ₂ I ₂	708	0.0005	106	65
Br ₂ La ₂ O ₂	708	0.0006	106	65
I ₂ O ₂ Y ₂	942	0.0006	136	89
O ₄ PTl	891	0.0006	149	74
Br ₂ HLa	678	0.0006	118	81
Ag ₂ K ₂ Se ₂	297	0.0006	49	25
As ₂ Cd ₂ K ₂	594	0.0007	100	49
Ca ₂ Cl ₂	388	0.0007	64	49
Ge ₂ Se ₂ Zr ₂	486	0.0007	64	49
Br ₂ Lu ₂ O ₂	621	0.0007	85	61
CeLi ₂ P ₂	759	0.0007	118	81
Er ₂ I ₂ O ₂	942	0.0007	136	89
I ₂ N ₂ Zr ₂	603	0.0007	87	57
Ca ₂ Cl ₂ H ₂	363	0.0008	49	36
Fe ₂ Se ₂	679	0.0008	113	85
Br ₂ Nd ₂ O ₂	942	0.0008	136	89
Br ₂ Eu ₂ F ₂	942	0.0008	136	89
CaCl	661	0.0008	145	113
AsCuLi ₂	678	0.0008	118	81
Br ₂ F ₂ Sr ₂	639	0.0008	97	58
Ca ₂ H ₂ I ₂	171	0.0009	25	16
Ge ₂ S ₂	447	0.0009	81	51
Fe ₂ Li ₂ P ₂	849	0.0009	113	85
MnSe ₂	774	0.0009	145	113
Br ₂ Dy ₂ S ₂	261	0.0009	45	21

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

AgTl (Pmmm (47))

Structural and electronic properties



Formula	AgTl
Spacegroup	Pmmm (47)
Prototype	FeSe
Parent 3D	Ag ₃ TlTe ₂
Source DB	COD
DB ID	2105385
DF2-C09 Binding energy [meV/ Å²]	72.63
RVV10 Binding energy [meV/ Å²]	69.6
Band gap (PBE) [eV]	0.0

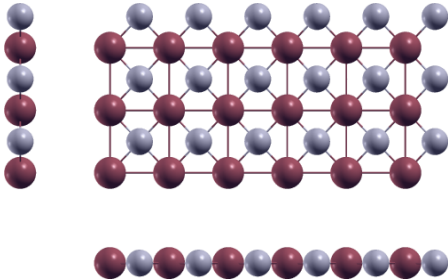


Band structure: Electronic band structure of AgTl (Pmmm (47)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of AgTl (Pmmm (47)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.94480159	0.00000000	0.00000000
a₂	0.00000000	4.15751577	0.00000000
a₃	0.00000000	0.00000000	20.00000000
	x [Å]	y [Å]	z [Å]
 Tl	0.00000000	0.00000000	10.00000000
 Ag	1.97240079	2.07875789	10.00000000



Orthographic projections: views of AgTl (Pmmm (47)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	3	0.1649	1	1
InSe	4	0.1323	1	1
Bi ₂	4	0.1368	1	1
Ag ₂	4	0.1711	1	1
PbTe	4	0.1337	1	1
CaCl	4	0.2208	1	1
I ₂ Mg	5	0.1253	1	1
CdI ₂	5	0.135	1	1
Nd	5	0.1781	1	3
Ba ₂ Pt	5	0.1708	1	1
Br ₂ Ca	5	0.1359	1	1
CaI ₂	5	0.1553	1	1
I ₂ Pr	5	0.0198	1	1
Br ₂ La	5	0.1255	1	1
Br ₂ Cu	5	0.105	1	1
Ca ₂ Si	5	0.1761	1	1
BiClTe	5	0.1353	1	1
BrCdI	5	0.1273	1	1
Cl ₂ Zn	5	0.2385	1	1
HgI ₂	5	0.3656	1	1
BaF ₂	5	0.1296	1	1
GeI ₂	5	0.1241	1	1
Ba ₂ Hg	5	0.0208	1	1
AsKSn	5	0.1286	1	1
PbTe ₂	5	0.1267	1	1
I ₂ Nd	5	0.0191	1	1
Cl ₂ Cu	5	0.1009	1	1
I ₂ Tm	5	0.1541	1	1
GeI ₂	5	0.1338	1	1
I ₂ Pb	5	0.1729	1	1
STl ₂	5	0.1302	1	1
MnSe ₂	5	0.2207	1	1
CeI ₂	5	0.0204	1	1
Se ₂ Yb	5	0.1243	1	1
BiTe ₂	5	0.1244	1	1
CNNa	5	0.0842	1	1
F ₂ Ni	5	0.2334	1	1
I ₂ La	5	0.016	1	1
F ₂ Zn	5	0.0228	1	1
Ba ₂ Cd	5	0.0232	1	1
I ₂ Pr	5	0.1353	1	1
Bi ₂ Te ₂	6	0.192	1	1
Bi ₂ In ₂	6	1.162	1	1
Cu ₂ I ₂	6	0.0137	1	1
Cl ₂ OOs	6	0.2352	1	1
LiMnTe ₂	6	0.1341	1	1
Ir ₂ P ₂	6	0.0193	1	1
Bi ₂ Mn ₂	6	0.1836	1	1
Ag ₂ Br ₂	6	0.0157	1	1
AgNO ₂	6	0.1102	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

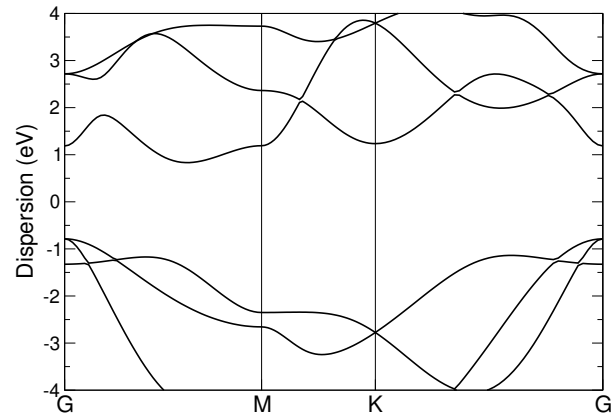
Formula	N° atoms	strain	cell size 1	cell size 2
BrCdI	320	0.0004	61	66
SSb ₂ Te ₂	452	0.0005	61	66
Br ₂ Cu	56	0.0006	10	12
MnNaTe ₂	386	0.0008	61	66
Sb ₂ Te ₃	369	0.0009	52	53
KS ₂ Ti	236	0.001	30	44
Br ₂ Mn	192	0.001	30	44
Br ₂ CsF	356	0.001	70	54
Fe ₂ O ₄	458	0.001	40	63
Cl ₂ N ₂ Zr ₂	78	0.001	9	10
Br ₂ OV	708	0.0011	98	128
AsKSn	607	0.0011	116	125
H ₂ Li ₂ O ₂	536	0.0011	55	71
I ₂ La ₂	386	0.0011	61	66
Hf ₂ Se ₂ Si ₂	932	0.0012	94	124
Ba ₂ H ₂ I ₂	472	0.0012	71	55
Bi ₂ STe ₂	748	0.0012	104	108
Bi ₂ SeTe ₂	369	0.0012	52	53
CdI ₂	532	0.0012	104	108
Cu ₄ Te ₂	422	0.0012	52	53
Br ₂ La ₂ P	748	0.0013	104	108
PbTe ₂	320	0.0013	61	66
LiMnTe ₂	640	0.0013	104	108
LiO ₂	335	0.0013	49	79
Br ₂ H ₂ Zr ₂	722	0.0013	64	99
Se ₂ Si ₂ Zr ₂	528	0.0013	54	70
Cl ₂ Zn	192	0.0014	30	44
Fe ₂ S ₂	434	0.0014	61	78
CdI ₂	532	0.0014	104	108
GeI ₂	532	0.0015	104	108
NbS ₂	294	0.0015	42	70
C ₂ Cl ₂ Y ₂	606	0.0016	63	80
Br ₂ H ₂ Zr ₂	812	0.0016	70	112
H ₂ Li ₂ O ₂	528	0.0016	54	70
As ₂ CeLi ₂	748	0.0016	104	108
AgNO ₂	426	0.0016	71	71
PbTe	424	0.0016	104	108
BiClTe	532	0.0016	104	108
As ₂ Fe ₂	684	0.0016	94	124
AsKSn	320	0.0016	61	66
Cl ₂ NSe ₂	434	0.0017	42	70
I ₂ Pr	532	0.0017	104	108
S ₂ Ta	294	0.0017	42	70
Bi ₂	210	0.0017	52	53
CrO ₂	532	0.0017	56	140
LiNbS ₂	364	0.0017	42	70
Ba ₂ H ₂ I ₂	464	0.0017	70	54
C ₄ Ca ₂	846	0.0017	108	105
Se ₂ Ta	316	0.0018	47	74
NbSe ₂	316	0.0018	47	74

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

As (P-3m1 (164))

Structural and electronic properties

	Formula	As
	Spacegroup	P-3m1 (164)
	Prototype	As
	Parent 3D	As ₂
	Source DB	COD
	DB ID	9008574
DF2-C09	Binding energy [meV/ Å²]	41.17
RVV10	Binding energy [meV/ Å²]	37.0
	Band gap (PBE) [eV]	1.62

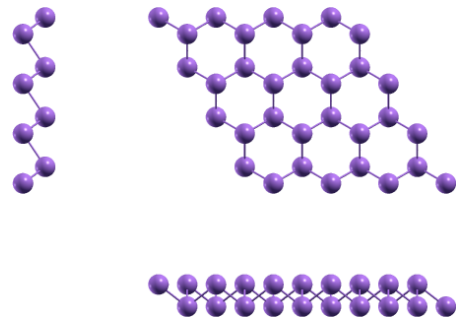


Band structure: Electronic band structure of As (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of As (P-3m1 (164)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.60867693	0.00000000	0.00000000
a₂	-1.80433846	3.12520589	0.00000000
a₃	0.00000000	0.00000000	21.31149308
	x [Å]	y [Å]	z [Å]
● As	1.80433846	1.04173530	11.35187477
● As	-0.00000000	2.08347059	9.95961831



Orthographic projections: views of As (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	3	0.3106	1	1
Tl	3	0.1209	1	1
Sn	3	0.4224	1	1
Na	3	0.0078	1	1
In	3	0.4323	1	1
In	3	0.2498	1	1
HgO	4	0.1284	1	1
LiO	4	0.2642	1	1
P ₂	4	0.2753	1	1
Mg ₂	4	0.1132	1	1
Sb ₂	4	2.8396	1	1
Cl ₂ Zn	5	0.001	1	1
I ₂ Mg	5	2.9125	1	1
S ₂ V	5	0.2541	1	1
MoS ₂	5	0.2551	1	1
MoTe ₂	5	0.0056	1	1
AgTe ₂	5	0.1226	1	1
PSn ₂	5	0.0091	1	1
HfS ₂	5	0.0027	1	1
HfTe ₂	5	0.4497	1	1
Te ₂ V	5	0.0037	1	1
CuTe ₂	5	0.0024	1	1
S ₂ Zr	5	0.0083	1	1
Br ₂ La	5	2.9169	1	1
Br ₂ Co	5	0.0004	1	1
ReS ₂	5	1.5571	1	1
Ca ₂ N	5	0.0005	1	1
Cl ₂ Ti	5	0.2756	1	1
AuTe ₂	5	0.469	1	1
PdTe ₂	5	0.4628	1	1
Mg ₃	5	0.1178	1	1
I ₂ Zn	5	0.4807	1	1
Te ₂ Zn	5	0.0058	1	1
S ₂ W	5	0.2551	1	1
Bi ₂ Pd	5	0.1355	1	1
GeI ₂	5	0.4994	1	1
Br ₂ Mn	5	0.0022	1	1
PtS ₂	5	0.0068	1	1
CoTe ₂	5	0.0031	1	1
CdClO	5	0.0042	1	1
Ba ₂ N	5	0.4534	1	1
AsKSn	5	2.9785	1	1
Te ₂ Zr	5	0.4509	1	1
Te ₂ W	5	0.0055	1	1
Cl ₂ Cu	5	0.5798	1	1
S ₂ Sn	5	0.0085	1	1
SnTe ₂	5	0.4934	1	1
Cl ₂ V	5	0.2607	1	1
I ₂ Pb	5	13.6346	1	1
STl ₂	5	3.0104	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

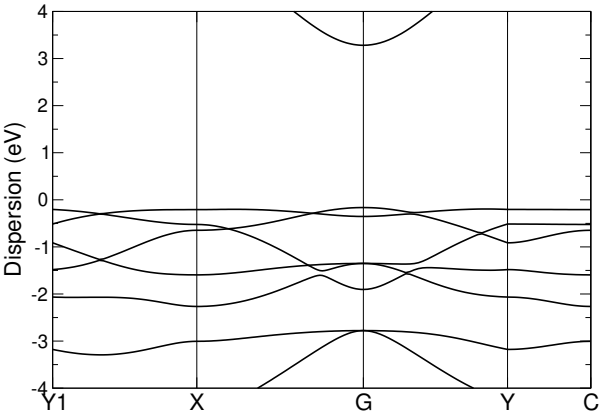
Formula	N° atoms	strain	cell size 1	cell size 2
BiBrTe	147	0.0	36	25
LiO	328	0.0001	73	91
BaF ₂	206	0.0001	49	36
Nd	34	0.0001	9	16
FHOZn	452	0.0001	64	81
MoS ₂	333	0.0001	57	73
Li ₂ Tl ₂	198	0.0001	49	25
NaO ₄	445	0.0001	100	49
CCL ₂ Lu ₂	7	0.0001	1	1
I ₂ Mg	243	0.0001	57	43
Ga ₂ I ₂ Y ₂	314	0.0002	49	36
CeLi ₂ P ₂	373	0.0002	64	49
Cl ₄ Mn	178	0.0002	39	20
Br ₂ La	243	0.0002	57	43
CrSe ₂	371	0.0002	64	81
I ₂ O ₂ Yb ₂	418	0.0002	65	48
S ₂ W	333	0.0002	57	73
Br ₂ Cd	443	0.0003	100	81
Bi ₂ Se ₃	329	0.0003	57	43
Dy ₂ I ₂ S ₂	146	0.0003	25	16
I ₂ Pr	274	0.0003	65	48
I ₂ Pr ₂ S ₂	344	0.0003	61	37
NS ₂ Ta	194	0.0003	25	36
MoS ₂	333	0.0003	57	73
Br ₂ Fe	5	0.0004	1	1
Ce ₂ I ₂ Si ₂	372	0.0004	57	43
CoH ₂ O ₂	317	0.0004	36	49
DyI ₂	98	0.0004	25	16
In	162	0.0004	49	64
Ag ₂	196	0.0004	61	37
PtTe ₂	401	0.0004	91	73
Br ₂ Co	5	0.0004	1	1
Br ₂ PY ₂	605	0.0004	100	81
Gd ₂ I ₂	286	0.0005	57	43
Cl ₂ La ₂	418	0.0005	81	64
BH ₄ Li	422	0.0005	64	49
I ₂ Pb	309	0.0005	81	49
Ca ₂ N	5	0.0005	1	1
F ₂ Lu ₂ Se ₂	488	0.0005	73	57
Br ₂ Ho ₂	474	0.0005	91	73
Ir ₂ P ₂	322	0.0006	65	48
Br ₂ HLa	324	0.0006	64	49
Br ₂ Er ₂ Se ₂	666	0.0006	135	66
I ₂ O ₂ Pr ₂	722	0.0006	118	81
PdTe ₂	443	0.0007	100	81
Ba ₂ Pt	233	0.0007	61	37
Br ₂ O ₂ Sm ₂	418	0.0007	65	48
Sb ₂ Se ₂ Te	329	0.0007	57	43
In ₂ Se ₂	418	0.0007	81	64
AgNO ₃	445	0.0007	100	49

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

As₂O₃ (P6mm)

Structural and electronic properties

	Formula	As ₂ O ₃
	Spacegroup	P6mm
	Prototype	As ₂ O ₃
	Parent 3D	As ₄ INO ₆
	Source DB	MPDS
	DB ID	S1614726
DF2-C09	Binding energy [meV/ Å²]	54.41
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	3.45

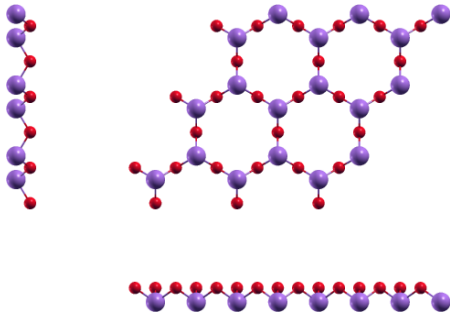


Band structure: Electronic band structure of As₂O₃ (P6mm) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of As₂O₃ (P6mm) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		2.71455531	4.70174771	0.00000000
a₂		-2.71455531	4.70174771	0.00000000
a₃		0.00000000	0.00000000	13.95777656
		x [Å]	y [Å]	z [Å]
●	As	-2.71455531	-1.56724924	0.56326372
●	As	-2.71455531	1.56724924	0.56326372
●	O	-1.35727765	2.35087386	-0.37550915
●	O	-2.71455531	0.00000000	-0.37550915
●	O	-4.07183296	2.35087386	-0.37550915



Orthographic projections: views of As₂O₃ (P6mm) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Ag ₂	7	1.5293	1	1
Ba ₂ Pt	8	1.5275	1	1
HgI ₂	8	0.4304	1	1
CNRb	8	0.0919	1	1
DyI ₂	8	1.4473	1	1
CNNa	8	0.1143	1	1
Bi ₂ Te ₂	9	0.2557	1	1
Bi ₂ In ₂	9	0.1147	1	1
Nd	9	0.0013	1	4
AsSb	9	0.223	1	2
N ₃ Na	9	0.4571	1	1
As ₄	9	0.1127	1	1
P ₄	9	0.1173	1	1
Sb ₂ Te ₂	9	1.5506	1	1
Ag ₂ I ₂	9	0.4328	1	1
Br ₂ CsF	9	0.1139	1	1
Sn ₂ Te ₂	9	0.1118	1	1
K ₂ PtTe ₂	10	6.9334	1	1
Cl ₄ Mn	10	0.1173	1	1
Ba ₂ H ₂ I ₂	11	0.1131	1	1
AlH ₄ Na	11	0.1186	1	1
NSr ₂	11	0.2251	1	2
PbS ₂	11	0.2196	1	2
I ₂ Pr ₂ S ₂	11	1.5345	1	1
Cu ₂ Rb ₂ Te ₂	11	0.1146	1	1
F ₂ Se ₂ Y ₂	11	0.2628	1	1
Ag ₂ K ₂ Te ₂	11	0.1215	1	1
Ag ₂ K ₂ Se ₂	11	0.4269	1	1
O ₄ PSn	11	0.1112	1	1
Br ₂ Hf ₂ N ₂	11	0.1124	1	1
CoI ₂	11	0.2235	1	2
Br ₂ O ₂ Ti ₂	11	0.1163	1	1
I ₂ Ti	11	0.224	1	2
As ₂ Cd ₂ K ₂	11	0.1111	1	1
In	11	0.1632	2	1
AgClO ₄	11	0.1259	1	1
Ce ₂ I ₂ S ₂	11	1.5599	1	1
Se ₂ Sn	11	0.2248	1	2
Cu ₂ K ₂ Te ₂	11	0.112	1	1
C ₂ Br ₂ La ₂	11	0.1833	1	1
Cl ₂ S ₂ Tl ₂	11	0.135	1	1
S ₂ V	13	0.1635	2	1
MoS ₂	13	0.1635	2	1
Cl ₂ Zn	13	0.1548	2	1
S ₂ W	13	0.1635	2	1
Ba ₂ Hg	13	0.1593	2	1
Ga ₂ Se ₂	13	0.2189	1	2
C ₂ Li ₂	13	0.2155	1	2
Au ₂ I ₂	13	0.4384	1	2
Br ₂ Y ₂	13	0.2193	1	2

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

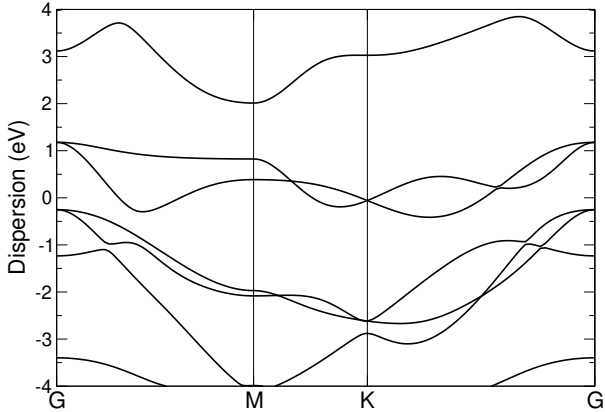
Formula	N° atoms	strain	cell size 1	cell size 2
I ₂ Ni	272	0.0	25	49
ReS ₂	227	0.0	16	49
In ₂ Te ₃	490	0.0001	37	61
Cl ₂ O ₂ Y ₂	669	0.0001	39	79
Sb ₂ SeTe ₂	490	0.0001	37	61
Bi ₂ Te ₂	577	0.0002	57	73
GeTe ₂	272	0.0002	25	49
Br ₂ Hf ₂ N ₂	74	0.0003	4	9
Cl ₂ N ₂ Zr ₂	74	0.0003	4	9
Se ₂ Zr	545	0.0003	49	100
STl ₂	488	0.0004	49	81
Cu ₂ Sr ₂	180	0.0004	16	25
Ga ₂ Se ₂	511	0.0004	39	79
I ₂ O ₂ Tm ₂	973	0.0004	65	108
I ₂ Zn	93	0.0004	9	16
I ₄ Sr ₂	437	0.0004	49	32
Cl ₂ Er ₂ O ₂	845	0.0005	49	100
Sb ₂ Te ₂	376	0.0005	36	49
Bi ₂ Se ₂ Te	490	0.0005	37	61
N ₂ W	368	0.0005	25	81
Cl ₂ O ₂ Ti ₂	300	0.0005	18	35
I ₂ La ₂ P	205	0.0005	16	25
CaH ₂ O ₂	65	0.0005	4	9
I ₂ S ₂ Tb ₂	341	0.0006	25	36
I ₂ V	545	0.0006	49	100
Ni ₂ Te ₂	321	0.0006	25	49
Br ₂ Er ₂ S ₂	327	0.0007	27	32
Br ₂ Ho ₂ S ₂	327	0.0007	27	32
I ₂ N ₂ Zr ₂	596	0.0007	40	66
In ₂ Se ₂	109	0.0007	9	16
I ₂ Nd	649	0.0007	65	108
Ba ₂ Hg	759	0.0007	81	118
SiTe ₂	545	0.0007	49	100
Br ₂ O ₂ Sm ₂	973	0.0007	65	108
Br ₃ Cs	189	0.0008	25	16
Br ₂ Y ₂	511	0.0008	39	79
CdCl ₂	272	0.0008	25	49
Cl ₂ Ho ₂ O ₂	669	0.0008	39	79
Gd ₂ I ₂ S ₂	553	0.0009	47	53
Ca ₂ N	47	0.0009	4	9
Hg ₃ N ₂	490	0.0009	61	37
I ₂ Pb	327	0.0009	36	49
Ir ₂ P ₂	757	0.0009	65	108
I ₂ Mn	272	0.0009	25	49
CuTe ₂	47	0.001	4	9
GeI ₂ Y ₂	490	0.001	37	61
DyI ₂	233	0.001	25	36
PbS ₂	432	0.001	39	79
CoH ₂ O ₂	325	0.001	16	49
STl ₂	368	0.001	37	61

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

AuTe₂ (P-3m1 (164))

Structural and electronic properties

	Formula	AuTe ₂
	Spacegroup	P-3m1 (164)
	Prototype	CdI ₂
	Parent 3D	AuTe ₂
	Source DB	COD
	DB ID	9011287
DF2-C09	Binding energy [meV/ Å²]	74.33
RVV10	Binding energy [meV/ Å²]	75.1
	Band gap (PBE) [eV]	0.0

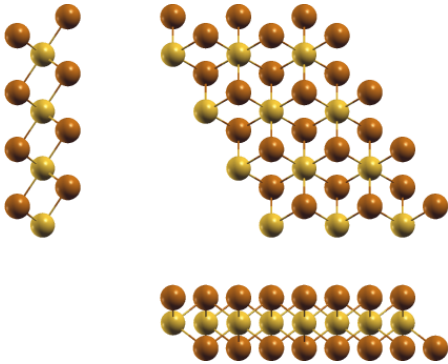


Band structure: Electronic band structure of AuTe₂ (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of AuTe₂ (P-3m1 (164)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.03611575	0.00000000	0.00000000
a₂	-2.01805787	3.49537877	0.00000000
a₃	0.00000000	0.00000000	22.97419521
	x [Å]	y [Å]	z [Å]
● Te	0.00000000	2.33025251	9.93391218
● Te	2.01805787	1.16512626	13.04028302
● Au	0.00000000	0.00000000	11.48709760



Orthographic projections: views of AuTe₂ (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	4	0.4855	1	1
Na	4	1.6351	1	1
Gd	4	0.2351	1	1
Ag ₂	5	0.5	1	1
As ₂	5	0.2632	1	1
Sb ₂	5	0.008	1	1
CaCl	5	0.1258	1	1
Cl ₂ Zn	6	0.2617	1	1
MoTe ₂	6	0.2553	1	1
Ba ₂ Pt	6	0.4993	1	1
ReSe ₂	6	1.5438	1	1
HfS ₂	6	0.2671	1	1
CaI ₂	6	0.462	1	1
HfTe ₂	6	0.0076	1	1
Te ₂ V	6	0.2579	1	1
CuTe ₂	6	0.2665	1	1
S ₂ Zr	6	0.275	1	1
I ₂ Yb	6	0.4557	1	1
Br ₂ Co	6	0.2626	1	1
Ca ₂ N	6	0.2639	1	1
Cl ₂ Zn	6	0.1363	1	1
PdTe ₂	6	0.0024	1	1
I ₂ Zn	6	0.0046	1	1
Te ₂ Zn	6	0.255	1	1
Bi ₂ Pd	6	0.425	1	1
Br ₂ Mn	6	0.26	1	1
Cl ₂ Ni	6	1.5503	1	1
CrTe ₂	6	1.5949	1	1
PtS ₂	6	0.2536	1	1
CoTe ₂	6	0.2675	1	1
Br ₂ V	6	1.538	1	1
ClN ₂ Zr	6	1.523	1	1
CdClO	6	0.2572	1	1
Ba ₂ N	6	0.0061	1	1
Se ₂ Ti	6	0.2501	1	1
Br ₂ Ti	6	1.5906	1	1
Te ₂ Zr	6	0.0071	1	1
Te ₂ W	6	0.2555	1	1
I ₂ Tm	6	0.4591	1	1
S ₂ Sn	6	0.2754	1	1
SnTe ₂	6	0.0096	1	1
I ₂ Pb	6	2.9116	1	1
OTl ₂	6	0.2575	1	1
NbSe ₂	6	1.5533	1	1
Br ₂ Fe	6	0.2626	1	1
GeS ₂	6	0.1188	1	1
MnSe ₂	6	0.1258	1	1
DyI ₂	6	0.4691	1	1
Br ₂ Ni	6	0.2699	1	1
Se ₂ Ta	6	1.554	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

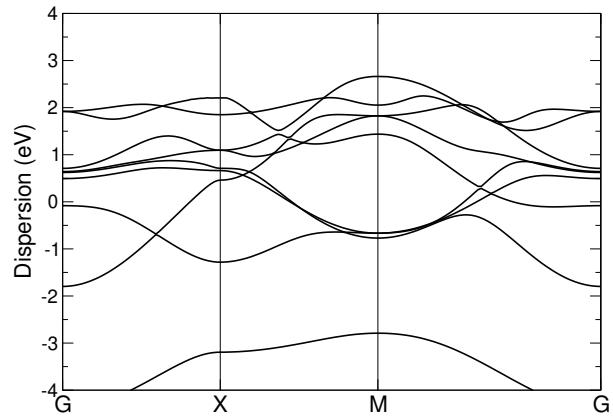
Formula	N° atoms	strain	cell size 1	cell size 2
FeH ₂ O ₂	107	0.0	9	16
Te ₂ W	390	0.0	57	73
CoTe ₂	543	0.0	81	100
Br ₂ Cr	300	0.0001	43	57
Br ₂ H ₂ Zr ₂	471	0.0001	43	57
Ga ₂ S ₂	643	0.0001	81	100
Br ₂ Ca ₃ Si	627	0.0001	81	64
MoTe ₂	390	0.0001	57	73
NiO ₂	447	0.0002	49	100
Dy ₂ I ₂ S ₂	711	0.0002	91	73
I ₂ Pb	300	0.0002	57	43
FeSe ₂	519	0.0002	65	108
Cl ₂ N ₂ Sc ₂	255	0.0002	25	36
Br ₂ Zr ₂	403	0.0002	49	64
Cl ₂ Mn	183	0.0002	25	36
Br ₂ Ti	300	0.0002	43	57
Cl ₂ Sc ₂	357	0.0003	43	57
Br ₂ Hf ₂ N ₂	666	0.0003	76	73
Ca ₂ N	492	0.0003	73	91
Te ₂ Zn	390	0.0003	57	73
Gd ₂ I ₂ S ₂	627	0.0003	81	64
Br ₂ Hf ₂ N ₂	765	0.0003	73	91
CaI ₂	543	0.0003	100	81
CrTe ₂	300	0.0003	43	57
HfS ₂	543	0.0004	81	100
IO ₃ Tl	120	0.0004	25	9
PtTe ₂	6	0.0004	1	1
LiO	98	0.0004	16	25
ReSe ₂	255	0.0004	36	49
CdH ₂ O ₂	536	0.0004	57	73
Cl ₂ Ni	255	0.0005	36	49
I ₂ Nd ₂ S ₂	486	0.0005	64	49
I ₂ S ₂ Sm ₂	561	0.0005	73	57
Br ₂ Mn	435	0.0005	64	81
Br ₂ Er ₂	7	0.0006	1	1
Li ₂ Tl ₂	139	0.0006	25	16
HfLiS ₂	463	0.0006	57	73
Se ₂ Ti	339	0.0006	49	64
Br ₂ Ca ₃ Si	279	0.0007	45	24
CoO ₂	447	0.0007	49	100
CuTe ₂	543	0.0007	81	100
Cl ₂ H ₂ Sc ₂	471	0.0008	43	57
F ₂ Se ₂ Y ₂	258	0.0008	36	25
As ₂	401	0.0008	73	91
I ₂ Tm	543	0.0008	100	81
CrSe ₂	123	0.0008	16	25
Cl ₂ N ₂ Zr ₂	765	0.0009	73	91
K	276	0.0009	73	57
DyI ₂	492	0.0009	91	73
NbSe ₂	255	0.0009	36	49

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Ba₂Cd (P4/mmm (123))

Structural and electronic properties

Formula	Ba ₂ Cd
Spacegroup	P4/mmm (123)
Prototype	Zr ₂ Cu
Parent 3D	Ba ₂ Cd
Source DB	ICSD
DB ID	30083
DF2-C09 Binding energy [meV/ Å²]	43.95
RVV10 Binding energy [meV/ Å²]	44.51
Band gap (PBE) [eV]	0.0

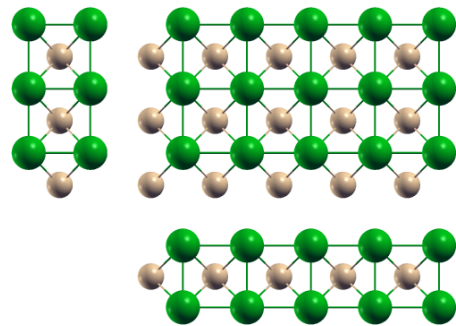


Band structure: Electronic band structure of Ba₂Cd (P4/mmm (123)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ba₂Cd (P4/mmm (123)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.20627768	0.00000000	0.00000000
a₂	0.00000000	4.20627768	0.00000000
a₃	0.00000000	0.00000000	24.04347379
	x [Å]	y [Å]	z [Å]
● Ba	2.10313884	2.10313884	14.04504735
● Ba	2.10313884	2.10313884	9.99842644
● Cd	0.00000000	0.00000000	12.02173690



Orthographic projections: views of Ba₂Cd (P4/mmm (123)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	4	0.146	1	1
AgTl	5	0.0204	1	1
Ag ₂	5	0.1512	1	1
CaCl	5	0.564	1	1
Ba ₂ Pt	6	0.1509	1	1
ReSe ₂	6	0.1104	1	1
CaI ₂	6	0.1381	1	1
Ca ₂ Si	6	0.1554	1	1
I ₂ Yb	6	0.136	1	1
Cl ₂ Zn	6	0.209	1	1
Ba ₂ Hg	6	0.0026	1	1
Cl ₂ Ni	6	0.1102	1	1
CrTe ₂	6	0.1089	1	1
Br ₂ V	6	0.1106	1	1
ClNZr	6	0.1111	1	1
Ba ₂ N	6	0.1084	1	1
Br ₂ Ti	6	0.1091	1	1
AsSe ₂	6	0.1099	1	1
I ₂ Tm	6	0.1371	1	1
I ₂ Pb	6	0.1527	1	1
BiTe	6	0.1301	1	1
BrNZr	6	0.1096	1	1
NbSe ₂	6	0.1101	1	1
MnSe ₂	6	0.5638	1	1
Br ₂ Cr	6	0.109	1	1
DyI ₂	6	0.1404	1	1
Se ₂ Ta	6	0.1101	1	1
NbSe ₂	6	0.1098	1	1
CNNa	6	0.3409	1	1
F ₂ Ni	6	0.595	1	1
Se ₂ Ta	6	0.1092	1	1
Bi ₂ Te ₂	7	0.1691	1	1
Cl ₂ OOs	7	0.6037	1	1
AgCuTe ₂	7	0.1832	1	1
O ₂ Sn ₂	7	0.2157	1	1
Au ₂ Br ₂	7	0.0092	1	1
Bi ₂	7	0.9752	1	2
AlLiTe ₂	7	0.1293	1	1
Ge ₂ Te ₂	7	0.0193	1	1
Fe ₂ Se ₂	7	0.5933	1	1
Cl ₂ ORu	7	0.5888	1	1
N ₃ Na	7	0.0391	1	1
Cu ₂ Te ₂	7	0.2118	1	1
Ge ₂ S ₂	7	0.2322	1	1
As ₄	7	0.0576	1	1
Cl ₂ Zr ₂	7	0.1108	1	1
Au ₂ I ₂	7	0.0273	1	1
Na	7	0.854	1	4
Sb ₂ Te ₂	7	0.1541	1	1
Co ₂ S ₂	7	0.5659	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

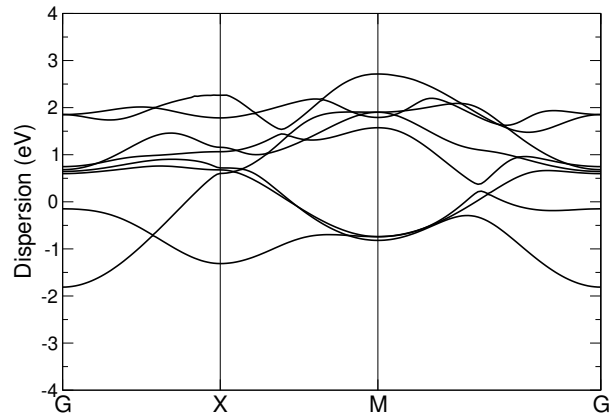
Formula	N° atoms	strain	cell size 1	cell size 2
Si ₂ Te ₂ Zr ₂	531	0.0	49	64
F ₂ Ni	339	0.0	49	64
Co ₂ S ₂	304	0.0	36	49
Co ₂ Se ₂	707	0.0001	85	113
F ₂ I ₂ Pb ₂	9	0.0001	1	1
Cl ₂ Zn	774	0.0002	113	145
N ₃ W ₂	812	0.0002	54	130
CdCl ₂	339	0.0002	48	65
Ge ₂ Hf ₂ Te ₂	678	0.0002	64	81
Ni ₂ Te ₂	404	0.0002	48	65
I ₂ Mn	339	0.0002	48	65
H ₂ Na ₂ Pd	255	0.0003	25	36
Cl ₂ Er ₂ H ₂	534	0.0003	48	65
I ₂ S ₂ Tl ₂	531	0.0003	49	64
As ₂ Co ₂ Li ₂	678	0.0004	64	81
H ₂ Li ₂ O ₂	693	0.0004	61	85
InSe ₂	339	0.0005	48	65
Cl ₂ OV	378	0.0005	42	63
GeS ₂	183	0.0005	25	36
Fe ₂ Se ₂	403	0.0005	49	64
Cu ₂ Se ₂	410	0.0005	50	65
AgClO ₄	849	0.0006	113	85
Cu ₂ Se ₂	403	0.0006	49	64
Ga ₂ Se ₂	715	0.0006	81	118
Hf ₂ Si ₂ Te ₂	933	0.0007	85	113
CaCl	206	0.0007	36	49
Au ₂ Se ₂	144	0.0007	24	18
H ₂ Si ₂	404	0.0008	48	65
LiO	138	0.0008	20	39
I ₂ Ni	339	0.0008	48	65
MnSe ₂	255	0.0008	36	49
Cu ₂ Te ₂	516	0.0008	64	81
AlH ₄ Na	636	0.0009	82	65
Mg ₄	91	0.0009	9	16
GeTe ₂	339	0.001	48	65
Ca ₂ Cl ₂ F ₂	843	0.001	81	100
Cl ₂ S ₂ Tl ₂	621	0.001	85	61
HgO	368	0.001	58	97
Ag ₂ F ₄	225	0.001	35	20
Te ₂ V	615	0.001	79	126
Cl ₂ Hf ₂ N ₂	993	0.001	79	126
OTl ₂	615	0.001	79	126
Cl ₂ Y ₂	715	0.0011	81	118
Br ₂ O ₂ Yb ₂	852	0.0011	82	101
I ₂ N ₂ Zr ₂	951	0.0011	81	118
Te ₄ W ₂	117	0.0011	15	12
CdClO	615	0.0011	79	126
GeTe	274	0.0011	48	65
Cr ₂ O ₄	789	0.0012	61	101
AgBrO ₂	632	0.0012	80	98

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Ba₂Hg (P4/mmm (123))

Structural and electronic properties

Formula	Ba ₂ Hg
Spacegroup	P4/mmm (123)
Prototype	Zr ₂ Cu
Parent 3D	Ba ₂ Hg
Source DB	ICSD
DB ID	30084
DF2-C09 Binding energy [meV/ Å²]	43.45
RVV10 Binding energy [meV/ Å²]	44.35
Band gap (PBE) [eV]	0.0

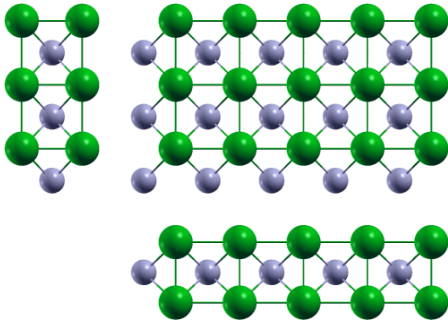


Band structure: Electronic band structure of Ba₂Hg (P4/mmm (123)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ba₂Hg (P4/mmm (123)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.18298171	0.00000000	0.00000000
a₂	0.00000000	4.18298171	0.00000000
a₃	0.00000000	0.00000000	23.97301935
	x [Å]	y [Å]	z [Å]
● Ba	2.09149085	2.09149085	10.00944545
● Ba	2.09149085	2.09149085	13.96357391
● Hg	0.00000000	4.18298171	11.98650968



Orthographic projections: views of Ba₂Hg (P4/mmm (123)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	4	0.1485	1	1
AgTl	5	0.0186	1	1
Ag ₂	5	0.1538	1	1
Ba ₂ Pt	6	0.1535	1	1
ReSe ₂	6	0.1098	1	1
CaI ₂	6	0.1402	1	1
HfTe ₂	6	0.1087	1	1
Br ₂ Cu	6	0.3443	1	1
Ca ₂ Si	6	0.1581	1	1
I ₂ Yb	6	0.1381	1	1
Cl ₂ Zn	6	0.2119	1	1
S ₂ Ti	6	0.1112	1	1
Cl ₂ Ni	6	0.1097	1	1
Cl ₂ Co	6	0.1113	1	1
Br ₂ V	6	0.11	1	1
ClNZr	6	0.1105	1	1
Cl ₂ Fe	6	0.1115	1	1
Ba ₂ N	6	0.1091	1	1
Te ₂ Zr	6	0.1088	1	1
AsSe ₂	6	0.1093	1	1
I ₂ Tm	6	0.1393	1	1
I ₂ Pb	6	0.1553	1	1
BiTe	6	0.132	1	1
BrNZr	6	0.1091	1	1
NbSe ₂	6	0.1096	1	1
DyI ₂	6	0.1427	1	1
Cl ₂ Zr	6	0.1114	1	1
Se ₂ Ta	6	0.1095	1	1
NbSe ₂	6	0.1093	1	1
GdI ₂	6	0.1294	1	1
F ₂ Ni	6	0.2075	1	1
Se ₂ Ta	6	0.1087	1	1
Ba ₂ Cd	6	0.0026	1	1
NaPSn	6	0.1085	1	1
Bi ₂ Te ₂	7	0.1721	1	1
Li ₂ Tl ₂	7	0.7668	1	1
Bi ₂ In ₂	7	0.3794	1	1
Cl ₂ OOs	7	0.2095	1	1
Bi ₂ Mn ₂	7	0.1627	1	1
AgCuTe ₂	7	0.1855	1	1
O ₂ Sn ₂	7	0.2187	1	1
Au ₂ Br ₂	7	0.0113	1	1
Bi ₂	7	0.9878	1	2
AlLiTe ₂	7	0.1312	1	1
Ge ₂ Te ₂	7	0.0214	1	1
Fe ₂ Se ₂	7	0.207	1	1
Cl ₂ ORu	7	0.5967	1	1
As ₂ Co ₂	7	0.5864	1	1
N ₃ Na	7	0.3658	1	1
Cu ₂ Te ₂	7	0.2148	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

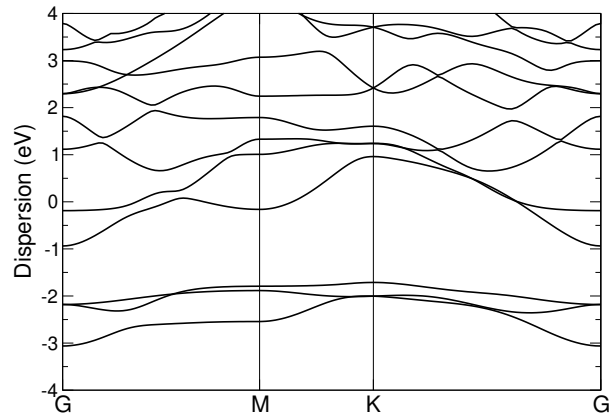
Formula	N° atoms	strain	cell size 1	cell size 2
Ge ₂ Te ₂ Zr ₂	843	0.0001	81	100
Fe ₂ S ₂	304	0.0001	36	49
Ag ₂ K ₂ Te ₂	495	0.0001	65	50
Br ₂ Lu ₂ O ₂	843	0.0001	81	100
Cl ₂ H ₂ Zr ₂	498	0.0002	36	65
Br ₂ Ca ₃ Si	9	0.0002	1	1
CrI ₂	339	0.0002	48	65
Fe ₂ Li ₂ P ₂	531	0.0005	49	64
Br ₂ Mg	339	0.0005	48	65
Cr ₂ O ₄	627	0.0005	49	80
FeI ₂	339	0.0006	48	65
FeSe ₂	486	0.0006	53	109
CdClHO	715	0.0006	81	118
CrSe ₂	177	0.0006	20	39
Ge ₂ Se ₂ Zr ₂	933	0.0006	85	113
Ca ₂ Cl ₂	707	0.0006	85	113
Cl ₂ V	177	0.0007	20	39
K ₂ PtS ₂	185	0.0007	35	16
As ₂ O ₃	759	0.0007	118	81
NSr ₂	339	0.0007	48	65
Bi ₂ Se ₂	346	0.0007	50	49
Se ₂ Si ₂ Zr ₂	693	0.0008	61	85
Cl ₂ Zn	435	0.0008	64	81
F ₄ Sn	8	0.0008	1	1
Bi ₂ In ₂	631	0.0008	101	82
Cl ₄ Mn	571	0.0008	82	65
Hf ₂ Si ₂ Te ₂	531	0.0009	49	64
RhTe ₂	597	0.0009	81	118
O ₂ Sn ₂	570	0.0009	66	93
Fe ₂ SeTe	643	0.0009	81	100
Sn	371	0.0009	74	149
Bi ₂ Pd	882	0.0009	113	181
Se ₂ Sn	339	0.001	48	65
Ag ₂ K ₂ Te ₂	486	0.001	64	49
AlH ₄ Na	627	0.001	81	64
Fe ₂ Se ₂	410	0.001	50	65
Cu ₂ Se ₂	919	0.001	113	145
In	124	0.001	25	49
Cu ₂ Te ₂	523	0.001	65	82
Ca ₂ Cl ₂ F ₂	852	0.0011	82	101
C ₂ Br ₂ Y ₂	954	0.0011	88	115
HfLiS ₂	741	0.0011	79	126
PtS ₂	615	0.0011	79	126
Cl ₂ Y ₂	469	0.0011	48	65
Cu ₂ Rb ₂ Te ₂	795	0.0011	101	82
HgO	309	0.0011	49	81
C ₂ Br ₂ Y ₂	870	0.0012	80	105
O ₂ Sn ₂	570	0.0012	66	93
Br ₂ H ₂ Yb ₂	843	0.0012	81	100
As ₂ Fe ₂ Li ₂	843	0.0012	81	100

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Ba₂N (P-3m1 (164))

Structural and electronic properties

	Formula	Ba ₂ N
	Spacegroup	P-3m1 (164)
	Prototype	CdI ₂
	Parent 3D	Ba ₂ N
	Source DB	COD
	DB ID	8102920
DF2-C09	Binding energy [meV/ Å²]	44.04
RVV10	Binding energy [meV/ Å²]	45.22
	Band gap (PBE) [eV]	0.0

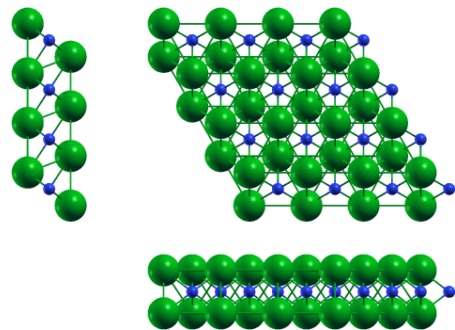


Band structure: Electronic band structure of Ba₂N (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ba₂N (P-3m1 (164)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.98318834	0.00000000	0.00000000
a₂		-1.99159417	3.44954229	0.00000000
a₃		0.00000000	0.00000000	22.98297273
		x [Å]	y [Å]	z [Å]
●	Ba	0.00000000	2.29969486	12.98928235
●	Ba	0.00000000	0.00000000	9.99369038
•	N	1.99159417	1.14984743	11.49148637



Orthographic projections: views of Ba₂N (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	4	2.9009	1	1
Na	4	0.2607	1	1
As ₂	5	0.2721	1	1
S ₂	5	0.009	1	1
CaCl	5	0.1301	1	1
Cl ₂ Zn	6	0.2706	1	1
MoTe ₂	6	0.2639	1	1
ReSe ₂	6	1.5891	1	1
CaI ₂	6	0.4778	1	1
HfTe ₂	6	0.0015	1	1
Te ₂ V	6	0.2667	1	1
CuTe ₂	6	0.2757	1	1
Ca ₂ Si	6	3.0298	1	1
I ₂ Yb	6	0.4713	1	1
Br ₂ Co	6	0.2715	1	1
Ca ₂ N	6	0.2729	1	1
AuTe ₂	6	0.0063	1	1
Cl ₂ Zn	6	0.1415	1	1
PdTe ₂	6	0.0038	1	1
S ₂ Ti	6	1.545	1	1
Te ₂ Zn	6	0.2637	1	1
Ba ₂ Hg	6	0.2057	1	1
Br ₂ Mn	6	0.2689	1	1
Cl ₂ Ni	6	1.5958	1	1
Cl ₂ Co	6	1.5425	1	1
CrTe ₂	6	0.2534	1	1
PtS ₂	6	0.2622	1	1
Br ₂ V	6	1.5831	1	1
Cl ₂ Fe	6	1.5373	1	1
CdClO	6	0.266	1	1
Se ₂ Ti	6	0.2585	1	1
Br ₂ Ti	6	1.6371	1	1
Te ₂ Zr	6	0.001	1	1
Te ₂ W	6	0.2641	1	1
AsSe ₂	6	0.2472	1	1
I ₂ Tm	6	0.4748	1	1
I ₂ Pb	6	2.9937	1	1
OTl ₂	6	0.2662	1	1
BiTe	6	0.4519	1	1
BrNZr	6	0.2489	1	1
NbSe ₂	6	1.5989	1	1
Br ₂ Fe	6	0.2716	1	1
GeS ₂	6	0.1222	1	1
MnSe ₂	6	0.13	1	1
DyI ₂	6	0.4851	1	1
Cl ₂ Zr	6	1.5401	1	1
Se ₂ Ta	6	1.5996	1	1
NbSe ₂	6	0.2475	1	1
F ₂ Ni	6	0.1381	1	1
Se ₂ Ta	6	1.6313	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

Formula	N° atoms	strain	cell size 1	cell size 2
MoS ₂	123	0.0	16	25
ReS ₂	294	0.0	37	61
I ₂ La ₂ Te	437	0.0001	64	49
Dy ₂ I ₂ S ₂	561	0.0001	73	57
S ₂ W	123	0.0001	16	25
Te ₂ W	492	0.0001	73	91
I ₂ Pb	255	0.0002	49	36
As ₂ Mg ₂ Na ₂	483	0.0002	65	48
MoS ₂	123	0.0002	16	25
Br ₂ Ca ₃ Si	486	0.0002	64	49
Tl	111	0.0002	25	36
BrNZr	339	0.0002	49	64
Cu ₃ Se ₃	9	0.0003	1	1
S ₂ Ti	255	0.0003	36	49
MoTe ₂	492	0.0003	73	91
CdH ₂ O ₂	674	0.0003	73	91
Se ₂ W	183	0.0003	25	36
CoH ₂ O ₂	552	0.0004	49	81
Se ₂ Sn ₂	599	0.0004	101	74
ReSe ₂	300	0.0004	43	57
Te ₂ Zn	492	0.0005	73	91
Cl ₂ Ni	300	0.0005	43	57
I ₂ Tm	435	0.0005	81	64
K	243	0.0005	65	48
MoSe ₂	183	0.0005	25	36
Se ₂ Ti	435	0.0006	64	81
Cl ₂ Co	255	0.0006	36	49
H ₄ Ti	833	0.0006	81	118
Te ₂ V	543	0.0006	81	100
Br ₂ Hf ₂	403	0.0007	49	64
I ₂ La ₂ Sb	386	0.0007	57	43
S ₂ V	123	0.0007	16	25
CaI ₂	435	0.0007	81	64
HgI ₂	597	0.0007	118	81
GeI ₂ La ₂	563	0.0007	81	64
HfLiS ₂	583	0.0007	73	91
DyI ₂	390	0.0007	73	57
CdO ₂	255	0.0007	36	49
Cd ₂ I ₃	705	0.0008	100	81
H ₂ Li ₂ Pd	833	0.0008	81	118
Cl ₂ N ₂ Zr ₂	414	0.0008	48	45
AsI ₂ La ₂	705	0.0008	100	81
Hg ₃ N ₂	227	0.0009	49	16
Br ₂ Mn	543	0.0009	81	100
NbSe ₂	300	0.0009	43	57
Ge ₂ I ₂ La ₂	786	0.0009	100	81
La ₂ S ₂	685	0.0009	115	85
Cl ₂ Hf ₂ N ₂	843	0.0009	81	100
Cl ₂ Zr	255	0.0009	36	49
OTl ₂	543	0.0009	81	100

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Ba₂Ni₃ (P-3m1 (164))

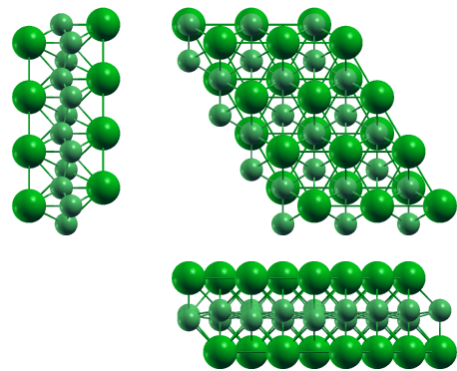
Structural and electronic properties

Formula	Ba ₂ Ni ₃
Spacegroup	P-3m1 (164)
Prototype	Ba ₂ Ni ₃
Parent 3D	Ba ₂ Ni ₃
Source DB	ICSD
DB ID	423734
DF2-C09 Binding energy [meV/ Å ²]	38.83
RVV10 Binding energy [meV/ Å ²]	40.89
Band gap (PBE) [eV]	0.0

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ba₂Ni₃ (P-3m1 (164)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		4.13546597	0.00000000	0.00000000
a₂		-2.06773298	3.58141858	0.00000000
a₃		0.00000000	0.00000000	24.86827794
		x [Å]	y [Å]	z [Å]
●	Ba	0.00000000	2.38761239	9.99736448
●	Ni	2.06773298	1.19380619	12.12387279
●	Ba	2.06773298	1.19380619	14.87091346
●	Ni	0.00000000	2.38761239	12.74440515
●	Ni	0.00000000	0.00000000	12.43413897



Orthographic projections: views of Ba₂Ni₃ (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	6	0.4563	1	1
Na	6	1.5504	1	1
AgTl	7	0.1653	1	1
Ag ₂	7	0.47	1	1
As ₂	7	0.2476	1	1
Sb ₂	7	0.0036	1	1
CaCl	7	0.1191	1	1
Cl ₂ Zn	8	0.2462	1	1
I ₂ Mg	8	0.0021	1	1
PSn ₂	8	0.2596	1	1
Ba ₂ Pt	8	0.4694	1	1
Br ₂ Zn	8	0.2749	1	1
HfS ₂	8	1.6292	1	1
AsSn ₂	8	0.2649	1	1
Te ₂ V	8	1.5808	1	1
I ₂ Pr	8	0.1471	1	1
CuTe ₂	8	0.2507	1	1
S ₂ Zr	8	0.2585	1	1
Br ₂ La	8	0.0024	1	1
Ca ₂ Si	8	0.4809	1	1
Br ₂ Co	8	0.247	1	1
Ca ₂ N	8	0.2483	1	1
BrCdI	8	0.0052	1	1
Cl ₂ Zn	8	0.1278	1	1
Te ₂ Ti	8	0.2753	1	1
I ₂ Zn	8	0.0068	1	1
BaF ₂	8	0.0087	1	1
RhTe ₂	8	0.2689	1	1
GeI ₂	8	0.0002	1	1
Br ₂ Mn	8	1.5921	1	1
PtS ₂	8	1.5579	1	1
CoTe ₂	8	1.6316	1	1
Se ₂ Ti	8	1.5389	1	1
AsKSn	8	0.0072	1	1
PbTe ₂	8	0.0042	1	1
I ₂ Nd	8	0.148	1	1
S ₂ Sn	8	0.2589	1	1
SnTe ₂	8	0.002	1	1
Sn	8	0.6342	1	3
Cl ₂ V	8	4.8691	1	1
I ₂ Pb	8	0.474	1	1
PtSe ₂	8	0.2658	1	1
Br ₂ Fe	8	0.2471	1	1
GeS ₂	8	0.1135	1	1
TaTe ₂	8	0.264	1	1
MnSe ₂	8	0.1191	1	1
Br ₂ Ni	8	0.2538	1	1
CeI ₂	8	0.1464	1	1
CuO ₂	8	0.1752	1	1
NbTe ₂	8	0.2582	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

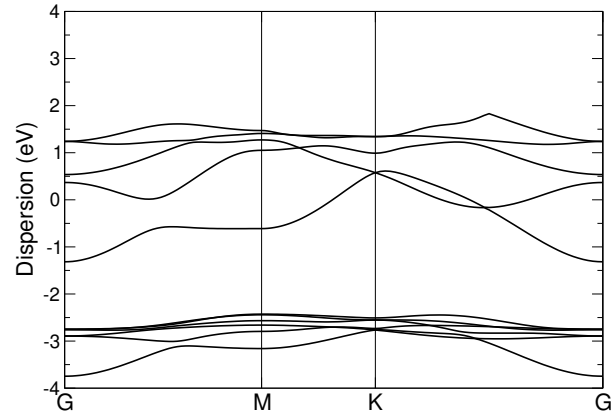
Formula	N° atoms	strain	cell size 1	cell size 2
Ga ₂ Te ₂	9	0.0	1	1
Br ₂ Mn	386	0.0	43	57
I ₂ Pr ₂ Si ₂	11	0.0001	1	1
ReS ₂	93	0.0001	9	16
Br ₂ Hf ₂ N ₂	629	0.0001	49	64
CdClHO	805	0.0002	81	100
PSn ₂	563	0.0002	64	81
TaTe ₂	638	0.0002	73	91
GeI ₂	8	0.0002	1	1
Cl ₂ Zr ₂	269	0.0002	25	36
HgI ₂	469	0.0002	65	48
AsCuLi ₂	9	0.0003	1	1
Cl ₂ V	488	0.0003	49	81
S ₂ Sn	563	0.0003	64	81
CrSe ₂	368	0.0003	37	61
KS ₂ Ti	443	0.0003	43	57
AsSn ₂	638	0.0004	73	91
Cl ₂ N ₂ Zr ₂	629	0.0004	49	64
Se ₂ Yb	8	0.0004	1	1
Na	229	0.0005	36	49
ClH ₃ O	500	0.0005	57	43
AgNO ₃	205	0.0006	25	16
S ₂ Zr	563	0.0006	64	81
Br ₂ V	233	0.0006	25	36
CCL ₂ Sc ₂	305	0.0006	25	36
Sb ₂ Te ₂	661	0.0006	81	64
CaH ₂ O ₂	565	0.0006	49	64
AgBrO ₂	373	0.0007	41	42
In	433	0.0007	65	108
BiTe ₂	8	0.0007	1	1
Br ₂ N ₂ Zr ₂	723	0.0007	57	73
Br ₂ HLa	9	0.0007	1	1
Hf ₂ I ₂ N ₂	911	0.0007	73	91
CdClHO	729	0.0008	73	91
Ca ₂ N	437	0.0008	49	64
I ₂ Pb	597	0.0008	81	64
CBr ₂ Lu ₂	650	0.0008	57	73
NbTe ₂	563	0.0008	64	81
MnO ₂	47	0.0008	4	9
Te ₄ W ₂	756	0.0008	84	56
Ga ₂ S ₃	425	0.0008	36	49
Cl ₂ H ₂ Lu ₂	723	0.0008	57	73
Ho ₂ S ₂	356	0.0008	40	39
Au ₂ I ₂	849	0.0008	105	81
Ce ₂ I ₂ S ₂	707	0.0009	73	57
Ca ₂ Si	536	0.0009	73	57
CoH ₂ O ₂	125	0.0009	9	16
NS ₂ Zr	376	0.0009	36	49
RhTe ₂	705	0.0009	81	100
Cl ₂ V	368	0.0009	37	61

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Ba₂Pt (P-3m1)

Structural and electronic properties

	Formula	Ba ₂ Pt
	Spacegroup	P-3m1
	Prototype	CdI2
	Parent 3D	Ba ₂ Pt
	Source DB	MPDS
	DB ID	S1420210
DF2-C09	Binding energy [meV/ Å²]	30.48
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

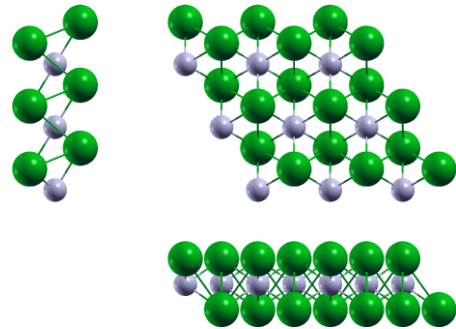


Band structure: Electronic band structure of Ba₂Pt (P-3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ba₂Pt (P-3m1) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		2.31340816	-4.00694047	0.00000000
a₂		2.31340816	4.00694047	0.00000000
a₃		0.00000000	0.00000000	18.62255301
		x [Å]	y [Å]	z [Å]
●	Ba	2.31340816	-1.33564682	1.61538460
●	Ba	2.31340816	1.33564682	-1.61538460
●	Pt	0.00000000	0.00000000	0.00000000



Orthographic projections: views of Ba₂Pt (P-3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	4	0.142	1	1
K	4	0.0052	1	1
AgTl	5	0.1212	1	1
Ag ₂	5	0.0003	1	1
Sb ₂	5	0.2579	1	1
I ₂ Mg	6	0.2659	1	1
I ₂ Pr	6	0.1126	1	1
Br ₂ La	6	0.2663	1	1
Ca ₂ Si	6	0.0046	1	1
AuTe ₂	6	0.2474	1	1
BrCdI	6	0.2704	1	1
I ₂ Zn	6	0.2534	1	1
BaF ₂	6	0.2753	1	1
GeI ₂	6	0.2632	1	1
Ba ₂ Hg	6	0.1302	1	1
AsKSn	6	0.2732	1	1
PbTe ₂	6	0.269	1	1
I ₂ Nd	6	0.113	1	1
Cl ₂ Cu	6	0.3122	1	1
SnTe ₂	6	0.2601	1	1
I ₂ Pb	6	0.0018	1	1
CeI ₂	6	0.1123	1	1
I ₂ Ti	6	1.4493	1	1
Se ₂ Yb	6	0.2636	1	1
BiTe ₂	6	0.2639	1	1
PtTe ₂	6	0.2469	1	1
I ₂ La	6	0.1149	1	1
F ₂ Zn	6	0.1112	1	1
Ba ₂ Cd	6	0.1321	1	1
Fe ₂ Te ₂	7	0.4266	1	1
Ca ₂ Cl ₂	7	0.4276	1	1
Cu ₂ I ₂	7	0.1233	1	1
Nd	7	0.1634	2	1
Cu ₂ Te ₂	7	0.1114	1	1
Ir ₂ P ₂	7	0.1129	1	1
Ag ₂ Br ₂	7	0.1151	1	1
Br ₂ Er ₂	7	0.2481	1	1
Tl	7	0.1548	2	1
O ₂ Sn ₂	7	0.112	1	1
Au ₂ Br ₂	7	0.1292	1	1
Br ₂ Cu ₂	7	0.4436	1	1
As ₂ Ir ₂	7	0.1162	1	1
O ₂ Pb ₂	7	0.1214	1	1
AgBrO ₂	7	0.2914	1	1
Cl ₂ La ₂	7	0.2503	1	1
Br ₂ Gd ₂	7	0.2488	1	1
MnNaTe ₂	7	0.2698	1	1
AsCuLi ₂	7	0.2626	1	1
Cu ₂ I ₂	7	0.2672	1	1
I ₂ La ₂	7	0.2724	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

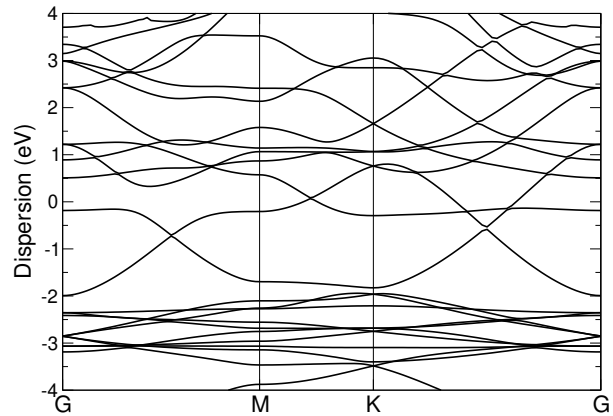
Formula	N° atoms	strain	cell size 1	cell size 2
F ₂ Lu ₂ Se ₂	609	0.0	57	73
Sb ₂ Se ₂ Te	674	0.0001	73	91
Se ₂ Sn	183	0.0001	25	36
TaTe ₂	123	0.0001	16	25
K ₂ PdSe ₂	345	0.0001	65	30
NSr ₂	183	0.0002	25	36
Pt ₂ Te ₂	304	0.0002	36	49
Br ₂ Tb ₂	357	0.0002	43	57
AgNO ₃	638	0.0002	91	73
As ₂ Sn ₂	403	0.0002	49	64
Br ₂ Co	294	0.0003	37	61
Br ₂ Gd ₂ Ge	743	0.0003	81	100
Cu ₂ I ₂	643	0.0003	81	100
Ag ₂	5	0.0003	1	1
Cl ₂ Y ₂	255	0.0003	25	36
Cl ₂ Zn	390	0.0003	49	81
BiTe ₂	492	0.0003	73	91
Er ₂ F ₂ Se ₂	402	0.0003	36	49
Br ₂ Fe	294	0.0003	37	61
Ga ₂ Ge ₂ Te ₂	678	0.0003	64	81
Br ₂ Gd ₂	403	0.0003	49	64
Cl ₂ Zn	294	0.0004	37	61
NaPSn	255	0.0004	36	49
PdTe ₂	300	0.0004	43	57
Br ₂ S ₂ Y ₂	228	0.0004	28	24
Hf ₂ I ₂ N ₂	198	0.0004	16	25
La ₂ S ₂	448	0.0004	64	64
CdClHO	148	0.0004	16	25
Bi ₂ S ₃	414	0.0004	43	57
Li ₂ P ₂ Pr	597	0.0004	64	81
Se ₂ Ta	75	0.0005	9	16
AsSe ₂	75	0.0005	9	16
Sb ₂ Se ₂ Te	674	0.0005	73	91
HfTe ₂	255	0.0005	36	49
KS ₂ Ti	471	0.0005	49	81
Se ₂ Yb	492	0.0005	73	91
SnTe ₂	435	0.0005	64	81
NbSe ₂	75	0.0005	9	16
CCL ₂ Lu ₂	416	0.0006	37	61
In ₂ Se ₃	353	0.0006	36	49
Gd ₂ I ₂	643	0.0006	81	100
Se ₂ Sn ₂	528	0.0006	76	75
H ₂ Li ₂ O ₂	951	0.0006	81	118
As ₂	233	0.0007	37	61
Br ₂ Ho ₂	357	0.0007	43	57
I ₂ Ti	183	0.0007	25	36
AsSn ₂	123	0.0007	16	25
NbSe ₂	75	0.0008	9	16
Br ₂ OV	241	0.0008	27	40
GeI ₂	492	0.0008	73	91

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

BaCu (P6/mmm (191))

Structural and electronic properties

Formula	BaCu
Spacegroup	P6/mmm (191)
Prototype	CuSr
Parent 3D	Ba ₄ Cu ₄
Source DB	ICSD
DB ID	58646
DF2-C09 Binding energy [meV/ Å²]	37.82
RVV10 Binding energy [meV/ Å²]	38.96
Band gap (PBE) [eV]	0.0

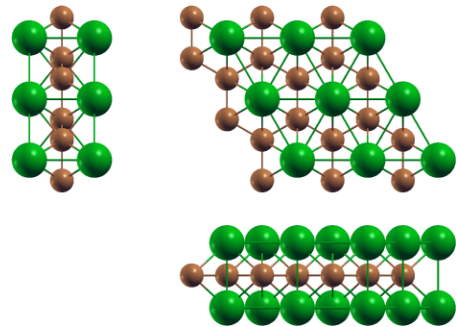


Band structure: Electronic band structure of BaCu (P6/mmm (191)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of BaCu (P6/mmm (191)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.46213759	0.00000000	0.00000000
a₂	-2.23106880	3.86432451	0.00000000
a₃	0.00000000	0.00000000	24.07421527
	x [Å]	y [Å]	z [Å]
● Ba	2.23106880	1.28810817	9.97647924
● Ba	2.23106880	1.28810817	14.09773603
● Cu	0.00000000	2.57621634	12.03710764
● Cu	0.00000000	0.00000000	12.03710764



Orthographic projections: views of BaCu (P6/mmm (191)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
GeTe	6	0.2475	1	1
S ₂	6	0.2496	1	1
In	6	0.2232	1	2
IrTe ₂	7	0.2487	1	1
CdCl ₂	7	1.6004	1	1
CaI ₂	7	0.0027	1	1
InSe ₂	7	0.2466	1	1
HfTe ₂	7	0.26	1	1
I ₂ Pr	7	0.1205	1	1
I ₂ Mn	7	0.2463	1	1
Br ₂ Cu	7	0.6379	1	1
I ₂ Yb	7	0.0002	1	1
Tl	7	0.6226	1	3
AuTe ₂	7	0.271	1	1
PdTe ₂	7	0.2675	1	1
FeI ₂	7	1.585	1	1
I ₂ Ni	7	1.5944	1	1
Ba ₂ Hg	7	0.1439	1	1
Cl ₂ Ni	7	4.8533	1	1
Ba ₂ N	7	0.2621	1	1
Te ₂ Zr	7	0.2606	1	1
I ₂ Nd	7	0.1211	1	1
I ₂ Tm	7	0.0015	1	1
I ₂ V	7	1.5297	1	1
Se ₂ Zr	7	1.5231	1	1
PtSe ₂	7	1.4485	1	1
BiTe	7	0.0075	1	1
NbSe ₂	7	4.8623	1	1
DyI ₂	7	0.0056	1	1
CeI ₂	7	0.1201	1	1
Se ₂ Ta	7	4.8643	1	1
Br ₂ Mg	7	1.584	1	1
F ₂ Ni	7	0.4306	1	1
PtTe ₂	7	0.2705	1	1
Br ₂ Cd	7	0.2662	1	1
I ₂ La	7	0.1238	1	1
F ₂ Zn	7	0.1184	1	1
Ba ₂ Cd	7	0.1463	1	1
NaPSn	7	0.2587	1	1
H ₂ Si ₂	8	0.247	1	1
Fe ₂ Te ₂	8	0.1143	1	1
Li ₂ Tl ₂	8	0.4836	1	1
Ca ₂ Cl ₂	8	0.1145	1	1
Cu ₂ I ₂	8	0.1352	1	1
Cl ₂ OOs	8	0.1088	1	1
Ir ₂ P ₂	8	0.1209	1	1
Ag ₂ Br ₂	8	0.1242	1	1
Br ₂ Er ₂	8	0.2718	1	1
O ₂ Sn ₂	8	0.4508	1	1
Cu ₂ S ₂	8	0.1168	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

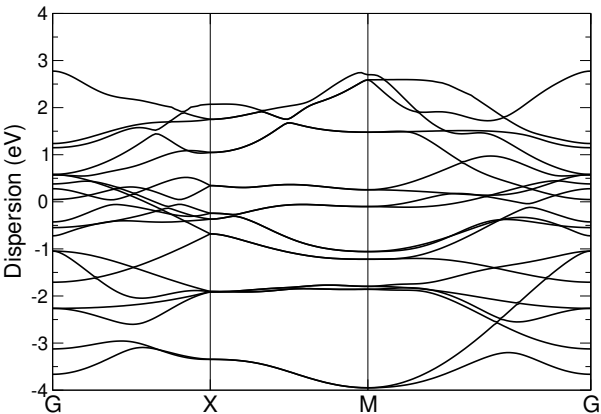
Formula	N° atoms	strain	cell size 1	cell size 2
S ₂ W	247	0.0	25	49
CdH ₂ O ₂	189	0.0	16	25
F ₂ Ho ₂ Se ₂	838	0.0	73	91
NbSe ₂	331	0.0001	37	61
PdTe ₂	624	0.0001	81	100
MoS ₂	247	0.0001	25	49
GeTe ₂	343	0.0001	43	57
Li ₂ Tl ₂	520	0.0001	73	57
MoS ₂	247	0.0001	25	49
I ₂ Yb	7	0.0002	1	1
AsSe ₂	331	0.0002	37	61
F ₂ Se ₂ Tm ₂	666	0.0002	57	73
S ₂	324	0.0002	49	64
Er ₂ F ₂ Se ₂	742	0.0002	64	81
Ga ₂ Se ₂	452	0.0002	49	64
Pt ₂ Te ₂	580	0.0002	64	81
PbS ₂	291	0.0003	36	49
I ₂ Ni	343	0.0003	43	57
Cl ₂ H ₂ Zr ₂	132	0.0003	9	16
LiMnSe ₂	520	0.0003	57	73
Ni ₂ SbTe ₂	516	0.0004	49	64
HNiO ₂	52	0.0004	4	9
Te ₂ W	139	0.0004	16	25
NaPSn	499	0.0004	64	81
IrTe ₂	388	0.0004	49	64
HfTe ₂	499	0.0005	64	81
Br ₂ Y ₂	340	0.0005	36	49
In ₂ Se ₃	661	0.0005	64	81
Se ₂ Ta	439	0.0005	49	81
Br ₂ Tb ₂	724	0.0005	81	100
NbS ₂	84	0.0006	9	16
MoTe ₂	139	0.0006	16	25
LiOS ₂ Ti	116	0.0006	9	16
CdClHO	244	0.0006	25	36
NbSe ₂	439	0.0006	49	81
Br ₂ Hf ₂	392	0.0007	37	61
Ge ₂ Te ₂	508	0.0007	66	61
Te ₂ Zn	139	0.0007	16	25
Bi ₂ S ₃	824	0.0008	81	100
S ₂ V	247	0.0008	25	49
PtSe ₂	208	0.0008	25	36
Ga ₂ Se ₂	340	0.0008	36	49
CdClO	139	0.0009	16	25
Cl ₂ Rb ₂	736	0.0009	130	54
O ₂ Sn ₂	792	0.0009	83	115
Ni ₂ Te ₂	400	0.0009	43	57
I ₂ Y ₂	520	0.0009	57	73
Te ₂ Zr	499	0.001	64	81
GeI ₃ Rb	404	0.001	81	16
Br ₂ Cd	624	0.001	81	100

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

BaMnGe (P4/nmm (129))

Structural and electronic properties

Formula	BaMnGe
Spacegroup	P4/nmm (129)
Prototype	PbClF
Parent 3D	Ba ₂ Ge ₂ Mn ₂
Source DB	COD
DB ID	9008362
DF2-C09 Binding energy [meV/ Å²]	42.77
RVV10 Binding energy [meV/ Å²]	44.56
Band gap (PBE) [eV]	0.0

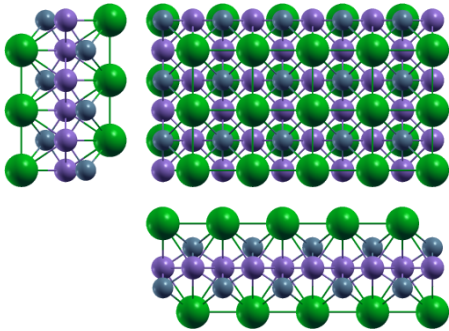


Band structure: Electronic band structure of BaMnGe (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of BaMnGe (P4/nmm (129)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.01503387	0.00000000	0.00000000
a₂	0.00000000	4.01503387	0.00000000
a₃	0.00000000	0.00000000	26.38225658
	x [Å]	y [Å]	z [Å]
● Ba	2.00751694	0.00000000	16.15423432
● Ge	0.00000000	2.00751694	14.53782815
● Ba	0.00000000	2.00751694	10.22802226
● Mn	0.00000000	0.00000000	13.19112829
● Mn	2.00751694	2.00751694	13.19112829
● Ge	2.00751694	0.00000000	11.84442843



Orthographic projections: views of BaMnGe (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	7	0.1685	1	1
Tl	7	0.1097	1	1
InSe	8	0.1346	1	1
Bi ₂	8	0.1393	1	1
AgTl	8	0.0134	1	1
Ag ₂	8	0.1749	1	1
P ₂	8	0.1109	1	1
PbTe	8	0.136	1	1
CaCl	8	0.2173	1	1
CdI ₂	9	0.1374	1	1
MoSe ₂	9	0.1099	1	1
Ba ₂ Pt	9	0.1746	1	1
Br ₂ Ca	9	0.1384	1	1
CaI ₂	9	0.1585	1	1
Br ₂ Cu	9	0.1006	1	1
Ca ₂ Si	9	0.18	1	1
I ₂ Yb	9	0.1559	1	1
BiClTe	9	0.1377	1	1
Cl ₂ Ti	9	0.1109	1	1
BrCdI	9	0.1294	1	1
HgI ₂	9	0.386	1	1
BaF ₂	9	0.1317	1	1
BiBrTe	9	0.1424	1	1
NbS ₂	9	0.1091	1	1
S ₂ Ta	9	0.1093	1	1
Se ₂ V	9	0.1096	1	1
AsKSn	9	0.1307	1	1
Cl ₂ Cu	9	0.0967	1	1
I ₂ Tm	9	0.1573	1	1
I ₂ V	9	0.1085	1	1
GeI ₂	9	0.1362	1	1
I ₂ Pb	9	0.1767	1	1
STl ₂	9	0.1324	1	1
BiI ₂	9	0.1483	1	1
GeS ₂	9	0.5932	1	1
MnSe ₂	9	0.2173	1	1
DyI ₂	9	0.1615	1	1
GdI ₂	9	0.1449	1	1
I ₂ La	9	0.0072	1	1
CdI ₂	9	0.1371	1	1
Sm	9	0.163	1	3
I ₂ Pr	9	0.1378	1	1
Se ₂ W	9	0.1099	1	1
Bi ₂ Te ₂	10	0.1963	1	1
Cu ₂ I ₂	10	0.0091	1	1
Cu ₂ Sr ₂	10	0.1433	1	1
Cl ₂ OOs	10	0.2238	1	1
LiMnTe ₂	10	0.1365	1	1
Cu ₂ Te ₂	10	0.0568	1	1
Ag ₂ Br ₂	10	0.0067	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

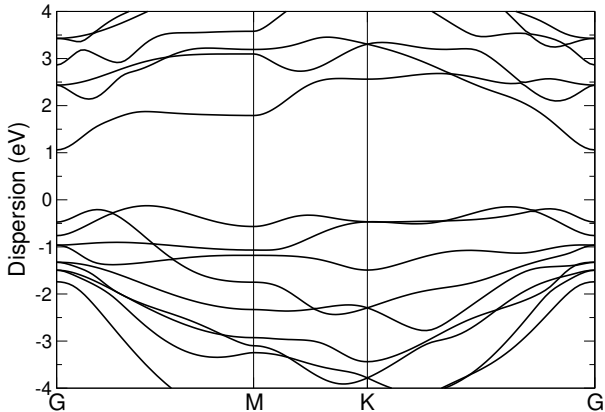
Formula	N° atoms	strain	cell size 1	cell size 2
Mg ₃	537	0.0002	49	81
AsSn ₂	483	0.0002	48	65
As ₂ Fe ₂	550	0.0003	49	64
H ₂ Li ₂ O ₂	870	0.0003	64	81
F ₂ I ₂ Yb ₂	12	0.0003	1	1
AgClO ₂	852	0.0003	80	93
Hf ₂ Se ₂ Si ₂	690	0.0003	50	65
HgO	806	0.0004	89	136
Ba ₂ F ₂ I ₂	870	0.0005	81	64
Cl ₄ Mn	474	0.0006	49	36
GeS ₂	486	0.0006	49	64
PtSe ₂	483	0.0006	48	65
O ₄ PTl	870	0.0006	81	64
CdClO	840	0.0007	81	118
TaTe ₂	483	0.0007	48	65
Eu ₂ H ₂ I ₂	12	0.0007	1	1
OTl ₂	840	0.0007	81	118
Hf ₂ Se ₂ Si ₂	678	0.0008	49	64
Ba ₂ H ₂ I ₂	678	0.0008	64	49
CoH ₂ O ₂	315	0.0009	20	39
Te ₂ V	840	0.0009	81	118
I ₃ Sn	866	0.001	109	53
I ₂ O ₂ Sm ₂	12	0.001	1	1
Cu ₂ K ₂ Te ₂	690	0.0011	65	50
Co ₂ S ₂	886	0.0011	81	100
S ₂ Ti	852	0.0012	79	126
Hf ₂ I ₂ N ₂	678	0.0012	48	65
Te ₂ W	840	0.0012	81	118
CdClHO	548	0.0012	48	65
F ₂ I ₂ Tm ₂	12	0.0012	1	1
Fe ₂ S ₂	718	0.0013	65	82
Hg ₄ O ₂	906	0.0013	120	31
AgClO ₂	384	0.0013	36	42
Tl	859	0.0014	113	181
MoTe ₂	840	0.0014	81	118
Cl ₂ Co	852	0.0014	79	126
H ₂ Na ₂ Pd	614	0.0014	49	64
Cu ₂ Na ₂ Se ₂	12	0.0014	1	1
Bi ₂ I ₂ O ₂	12	0.0014	1	1
Mg ₆	246	0.0014	16	25
Cl ₂ F ₂ Pb ₂	12	0.0014	1	1
Pb ₂ Se ₂	912	0.0014	98	81
I ₂ Pb	885	0.0015	103	89
Br ₂ Cr ₂ S ₂	558	0.0015	45	48
Ga ₂ S ₂	604	0.0015	52	73
PTe ₂ Ti ₂	677	0.0015	52	73
Br ₂ Ni	531	0.0016	52	73
Cl ₂ Mg	531	0.0016	52	73
Cl ₂ Zr	852	0.0016	79	126
I ₂ Pb	816	0.0016	95	82

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Bi₂S₃ (P-3m1 (164))

Structural and electronic properties

	Formula	Bi ₂ S ₃
	Spacegroup	P-3m1 (164)
	Prototype	As
	Parent 3D	Bi ₄ S ₃
	Source DB	COD
	DB ID	9013958
DF2-C09	Binding energy [meV/ Å²]	30.35
RVV10	Binding energy [meV/ Å²]	35.64
	Band gap (PBE) [eV]	1.19

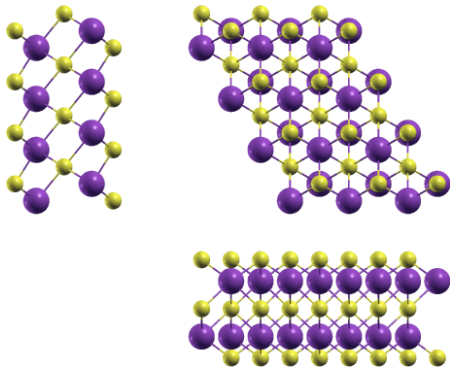


Band structure: Electronic band structure of Bi₂S₃ (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Bi₂S₃ (P-3m1 (164)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		4.02241151	0.00000000	0.00000000
a₂		-2.01120576	3.48351056	0.00000000
a₃		0.00000000	0.00000000	26.36194472
		x [Å]	y [Å]	z [Å]
●	Bi	2.01120576	1.16117019	11.28829463
●	S	2.01120576	1.16117019	16.53579853
●	Bi	0.00000000	0.00000000	15.07365009
●	S	0.00000000	2.32234037	13.18097236
●	S	0.00000000	0.00000000	9.82614619



Orthographic projections: views of Bi₂S₃ (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	6	2.8416	1	1
Na	6	0.2544	1	1
Gd	6	0.2369	1	1
As ₂	7	0.2654	1	1
CaCl	7	0.1269	1	1
Cl ₂ Zn	8	0.264	1	1
MoTe ₂	8	0.2575	1	1
ReSe ₂	8	1.5553	1	1
HfS ₂	8	0.2694	1	1
CaI ₂	8	0.466	1	1
HfTe ₂	8	0.0061	1	1
Te ₂ V	8	0.2601	1	1
CuTe ₂	8	0.2688	1	1
Ca ₂ Si	8	2.9679	1	1
I ₂ Yb	8	0.4597	1	1
Br ₂ Co	8	0.2648	1	1
Ca ₂ N	8	0.2662	1	1
AuTe ₂	8	0.0016	1	1
Cl ₂ Zn	8	0.1376	1	1
PdTe ₂	8	0.0008	1	1
I ₂ Zn	8	0.0063	1	1
Te ₂ Zn	8	0.2572	1	1
Bi ₂ Pd	8	0.4286	1	1
Br ₂ Mn	8	0.2623	1	1
Cl ₂ Ni	8	1.5619	1	1
CrTe ₂	8	0.2472	1	1
PtS ₂	8	0.2558	1	1
CoTe ₂	8	0.2699	1	1
Br ₂ V	8	1.5495	1	1
ClN ₂ Zr	8	1.5344	1	1
CdClO	8	0.2594	1	1
Ba ₂ N	8	0.0046	1	1
Se ₂ Ti	8	1.6351	1	1
Br ₂ Ti	8	0.2465	1	1
Te ₂ Zr	8	0.0056	1	1
Te ₂ W	8	0.2577	1	1
I ₂ Tm	8	0.4631	1	1
I ₂ Pb	8	2.9326	1	1
OTl ₂	8	0.2597	1	1
BrN ₂ Zr	8	1.5822	1	1
NbSe ₂	8	1.565	1	1
Br ₂ Fe	8	0.2649	1	1
GeS ₂	8	0.1196	1	1
MnSe ₂	8	0.1268	1	1
Br ₂ Cr	8	0.2469	1	1
DyI ₂	8	0.4732	1	1
Br ₂ Ni	8	0.2723	1	1
Se ₂ Ta	8	1.5657	1	1
Cl ₂ Mg	8	0.2724	1	1
F ₂ Ni	8	0.1344	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

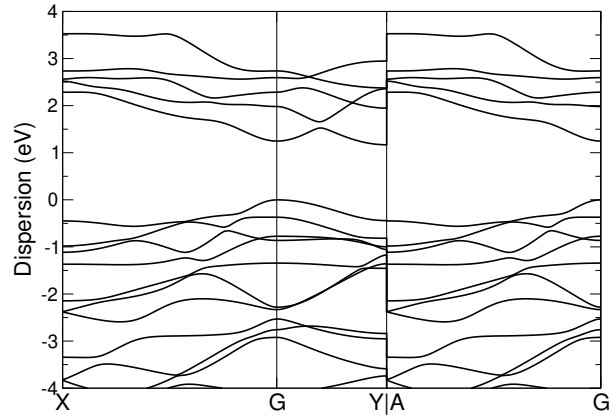
Formula	N° atoms	strain	cell size 1	cell size 2
I ₂ La ₂ Te	650	0.0001	73	57
CdClO	563	0.0001	64	81
FeO ₂	545	0.0001	49	100
AgNO ₃	490	0.0001	61	37
LiOS ₂ Ti	305	0.0002	25	36
Ag ₂	371	0.0002	57	43
GeI ₃ Rb	145	0.0002	25	4
PtS ₂	504	0.0002	57	73
Br ₂ Ho ₂	9	0.0002	1	1
Br ₂ Tb ₂	9	0.0002	1	1
Br ₂ Ca ₃ Si	707	0.0003	73	57
Cl ₂ Zn	638	0.0003	73	91
OTl ₂	563	0.0003	64	81
Cl ₂ Hf ₂ N ₂	806	0.0003	64	81
NiO ₂	432	0.0003	39	79
CaI ₂	674	0.0003	91	73
Br ₂ Co	638	0.0004	73	91
Br ₂ V	327	0.0004	36	49
NS ₂ Zr	577	0.0004	57	73
C ₄ Ca ₂	698	0.0004	70	58
N ₂ W	93	0.0004	9	16
Br ₂ Fe	638	0.0004	73	91
Cl ₂ Zr ₂	376	0.0004	36	49
CaH ₂ O ₂	905	0.0004	81	100
Ba ₂ Pt	414	0.0004	57	43
Ga ₂ S ₃	650	0.0004	57	73
Ag ₂ Te ₂	645	0.0005	73	70
Cl ₂ V	155	0.0005	16	25
GeI ₂ La ₂	905	0.0005	100	81
C ₂ Br ₂ La ₂	712	0.0005	68	62
I ₂ Pr ₂ S ₂	543	0.0005	57	43
Br ₂ O ₂ Sc ₂	698	0.0005	64	63
I ₂ Yb	743	0.0006	100	81
Te ₂ V	563	0.0006	64	81
Se ₂ Ta	386	0.0006	43	57
CCL ₂ Lu ₂	820	0.0007	73	91
I ₂ S ₂ Tb ₂	789	0.0007	81	64
Cu ₂ Na ₂ Te ₂	613	0.0007	65	48
CdH ₂ O ₂	725	0.0007	64	81
CrSe ₂	155	0.0008	16	25
Ba ₂ Cu ₂	824	0.0008	100	81
I ₂ Tm	743	0.0008	100	81
As ₂	547	0.0008	73	91
Na	358	0.0008	57	73
CCL ₂ Sc ₂	425	0.0008	36	49
Cl ₂ H ₂ Sc ₂	557	0.0008	43	57
PdTe ₂	8	0.0008	1	1
CuTe ₂	705	0.0009	81	100
CoO ₂	432	0.0009	39	79
BN	253	0.0009	25	64

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Bi₂Se₄ (C2/m)

Structural and electronic properties

	Formula	Bi ₂ Se ₄
	Spacegroup	C2/m
	Prototype	BiSe ₂
	Parent 3D	Bi ₄ Se ₈
	Source DB	ICSD
	DB ID	194720
DF2-C09	Binding energy [meV/ Å²]	40.41
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	1.17

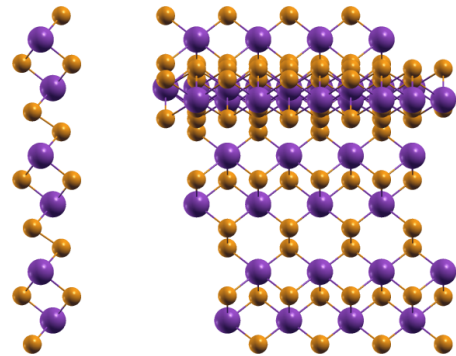


Band structure: Electronic band structure of Bi₂Se₄ (C2/m) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Bi₂Se₄ (C2/m) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		-0.00000524	4.20542098	0.00000000
a₂		7.91774134	2.10269868	0.00000000
a₃		0.00000000	0.00000000	17.91259602
		x [Å]	y [Å]	z [Å]
●	Bi	2.30376947	-0.00001218	0.41530199
●	Bi	-2.30376947	0.00001218	-0.41530199
●	Se	0.67880510	2.10269606	-0.98909113
●	Se	-0.67881033	2.10272492	0.98909113
●	Se	3.98485148	-0.00000746	-1.70247233
●	Se	3.93288986	2.10270614	1.70247233



Orthographic projections: views of Bi₂Se₄ (C2/m) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Br ₂ Ti	9	0.3058	1	1
Cl ₂ Cu	9	0.1632	1	1
BrNZr	9	0.3017	1	1
Se ₂ Ta	9	0.3047	1	1
O ₂ Sn ₂	10	0.1627	1	1
Br ₂ Hg ₃	11	1.1256	1	1
GeI ₃ Rb	11	1.1071	1	1
Nd	12	0.0907	1	6
I ₂ Pr	12	0.0589	1	2
Br ₂ Cu	12	0.0686	1	2
N ₂ W	12	0.1321	1	2
I ₂ Nd	12	0.059	1	2
Cl ₂ H ₂ Sc ₂	12	0.305	1	1
CeI ₂	12	0.0589	1	2
I ₂ La	12	0.0595	1	2
F ₂ Zn	12	0.0589	1	2
Fe ₂ Te ₂	14	0.0596	1	2
Ca ₂ Cl ₂	14	0.0596	1	2
HNiO ₂	14	0.1328	1	2
Ir ₂ P ₂	14	0.059	1	2
Ag ₂ Br ₂	14	0.0595	1	2
Cu ₂ S ₂	14	0.059	1	2
Ge ₂ Te ₂	14	0.0802	1	2
Br ₂ Cu ₂	14	0.0589	1	2
As ₂ Ir ₂	14	0.0599	1	2
Ge ₂ S ₂	14	0.0698	1	2
O ₂ Sn ₂	14	0.059	1	2
P ₂ Rh ₂	14	0.0591	1	2
F ₂ Tl ₂	14	0.0591	1	2
Ag ₂ Te ₂	14	0.0591	1	2
As ₂ Ru ₂	14	0.0595	1	2
C ₂	14	0.1474	1	4
La ₂ S ₂	14	0.0786	1	2
Ni ₂ Se ₂	14	0.0589	1	2
As ₂ Rh ₂	14	0.0595	1	2
NS ₂ Ta	14	0.1323	1	2
Na	16	0.2222	2	4
In	17	0.0998	2	5
Br ₂ Ca ₂ H ₂	18	0.0592	1	2
Er ₂ I ₂ O ₂	18	0.0591	1	2
Br ₂ O ₂ Tm ₂	18	0.0595	1	2
Cu ₄ Te ₂	18	0.06	1	2
Br ₂ O ₂ Y ₂	18	0.059	1	2
HfTe ₂	18	0.327	1	4
Cl ₂ F ₂ Pb ₂	18	0.0613	1	2
Ba ₂ Ge ₂ Mn ₂	18	0.0609	1	2
Br ₂ Ce ₂ O ₂	18	0.0603	1	2
Ca ₂ Ge ₂ Mn ₂	18	0.0589	1	2
PdTe ₂	18	0.338	1	4
Br ₂ F ₂ Tm ₂	18	0.0589	1	2

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

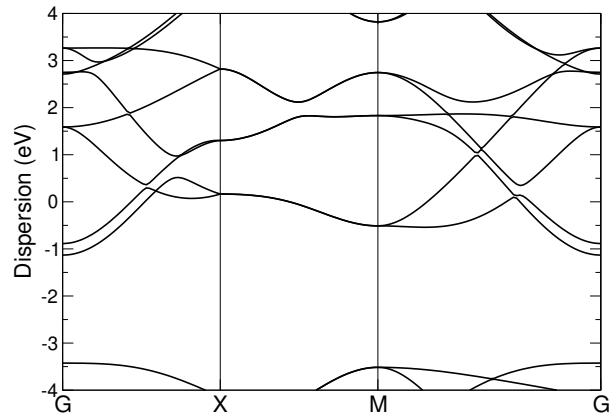
Formula	N° atoms	strain	cell size 1	cell size 2
CuGeO ₃	634	0.0008	39	80
Cl ₂ H ₂ Lu ₂	420	0.0008	18	52
Br ₂ O ₂ Pr ₂	318	0.0009	17	36
Cl ₂ Mg	264	0.0009	18	52
H ₂ Na ₂ O ₂	906	0.0009	39	112
Br ₂ Ni	264	0.0009	18	52
I ₂ La	990	0.0009	80	170
Ag ₂ Br ₂	942	0.001	65	138
PTe ₂ Ti ₂	368	0.001	18	52
Mg ₄	116	0.001	6	20
As ₂ Rh ₂	914	0.001	63	134
Ag ₂ Br ₂	914	0.001	63	134
Ge ₂ Mn ₂ Sr ₂	318	0.001	17	36
H ₂ I ₂ Yb ₂	282	0.001	15	32
I ₂ La	186	0.001	15	32
GeNi ₃ Te ₂	270	0.001	13	32
GeS ₂	282	0.001	20	54
Tl	56	0.0011	6	20
As ₂ Fe ₂	336	0.0011	20	54
Al ₂ Cl ₂ O ₂	324	0.0011	14	40
As ₂ Rh ₂	218	0.0012	15	32
Ag ₂ Br ₂	246	0.0012	17	36
Ga ₂ S ₂	316	0.0012	18	52
Cu ₂ Sr ₂	736	0.0012	52	106
Cl ₂ Fe	672	0.0012	42	140
I ₂ La ₂ P	842	0.0013	52	106
GeI ₂ Y ₂	686	0.0013	41	88
Ag ₂ Br ₂	218	0.0013	15	32
Hf ₂ Se ₂ Si ₂	444	0.0014	20	54
CeLi ₂ P ₂	865	0.0014	50	113
F ₂ Se ₂ Y ₂	126	0.0014	8	13
Br ₂ Nd ₂ O ₂	282	0.0014	15	32
NaPSn	174	0.0015	13	32
Br ₂ HLa	752	0.0015	50	113
BH ₄ Li	978	0.0015	50	113
H ₂ Na ₂ Pd	390	0.0015	20	54
F ₂ Se ₂ Tm ₂	270	0.0015	13	32
Cl ₂ Zr	672	0.0016	42	140
I ₂ O ₂ Y ₂	282	0.0016	15	32
LiMnSe ₂	206	0.0016	13	32
Pt ₂ Te ₂	206	0.0017	13	32
Br ₂ O ₂ Pr ₂	282	0.0017	15	32
NbSe ₂	591	0.0017	38	121
AsSe ₂	591	0.0017	38	121
Br ₂ Lu ₂ S ₂	78	0.0017	5	8
As ₂ Ir ₂	246	0.0017	17	36
Br ₂ N ₂ Zr ₂	420	0.0017	18	52
AsCuLi ₂	752	0.0017	50	113
Br ₂ Lu ₂ S ₂	78	0.0018	5	8
BiBrTe	630	0.0018	52	106

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

BiO (P4/nmm (129))

Structural and electronic properties

	Formula	BiO
	Spacegroup	P4/nmm (129)
	Prototype	FeSe
	Parent 3D	Cu ₂ Bi ₂ Te ₂ O ₂
	Source DB	ICSD
	DB ID	187824
DF2-C09	Binding energy [meV/ Å²]	107.87
RVV10	Binding energy [meV/ Å²]	102.13
	Band gap (PBE) [eV]	0.0

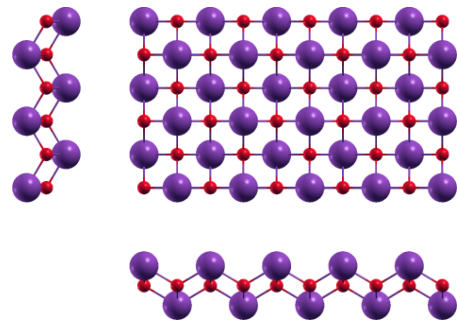


Band structure: Electronic band structure of BiO (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of BiO (P4/nmm (129)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		4.07454712	0.00000000	0.00000000
a₂		0.00000000	4.07454712	0.00000000
a₃		0.00000000	0.00000000	22.47747760
		x [Å]	y [Å]	z [Å]
●	Bi	2.03727356	0.00000000	12.44427896
●	Bi	0.00000000	2.03727356	10.03319864
●	O	0.00000000	0.00000000	11.23873880
●	O	2.03727356	2.03727356	11.23873880



Orthographic projections: views of BiO (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.1609	1	1
Tl	5	0.1113	1	1
InSe	6	0.1295	1	1
Bi ₂	6	0.1337	1	1
Ag ₂	6	0.1669	1	1
PbTe	6	0.1308	1	1
CaCl	6	0.2096	1	1
Cl ₂ Mn	7	0.11	1	1
CdI ₂	7	0.132	1	1
Nd	7	0.1737	1	3
MoSe ₂	7	0.1115	1	1
Ba ₂ Pt	7	0.1666	1	1
S ₂ Ta	7	0.1096	1	1
Br ₂ Ca	7	0.1329	1	1
CaI ₂	7	0.1515	1	1
Br ₂ Cu	7	0.0988	1	1
NSr ₂	7	0.1084	1	1
Ca ₂ Si	7	0.1717	1	1
I ₂ Yb	7	0.1491	1	1
BiClTe	7	0.1323	1	1
FeI ₂	7	0.1087	1	1
I ₂ Ni	7	0.109	1	1
NbS ₂	7	0.1096	1	1
CrI ₂	7	0.1086	1	1
BiBrTe	7	0.1366	1	1
NbS ₂	7	0.1106	1	1
Cl ₂ Fe	7	0.1088	1	1
S ₂ Ta	7	0.1108	1	1
Se ₂ V	7	0.1111	1	1
I ₂ Tm	7	0.1504	1	1
GeI ₂	7	0.1309	1	1
I ₂ Pb	7	0.1686	1	1
BiTe	7	0.142	1	1
MnSe ₂	7	0.2095	1	1
DyI ₂	7	0.1543	1	1
Cl ₂ Zr	7	0.1087	1	1
Br ₂ Mg	7	0.1087	1	1
GdI ₂	7	0.1389	1	1
CNNa	7	0.0689	1	1
F ₂ Ni	7	0.2214	1	1
CdI ₂	7	0.1317	1	1
I ₂ Pr	7	0.1323	1	1
Se ₂ W	7	0.1114	1	1
Bi ₂ Te ₂	8	0.1872	1	1
Bi ₂ In ₂	8	0.4067	1	1
Cu ₂ I ₂	8	0.002	1	1
Cu ₂ Sr ₂	8	0.1374	1	1
Cl ₂ OOs	8	0.2156	1	1
LiMnTe ₂	8	0.1312	1	1
AgCuTe ₂	8	0.1976	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

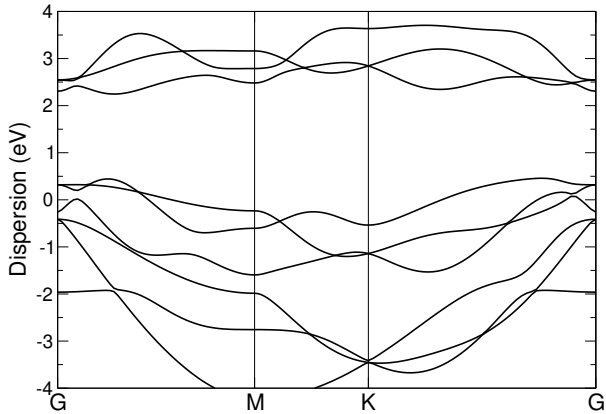
Formula	N° atoms	strain	cell size 1	cell size 2
Ba ₂ F ₂ I ₂	896	0.0	101	82
Mg ₂	68	0.0	9	16
H ₂ Li ₂ O ₂	580	0.0002	49	64
Br ₂ Zn	387	0.0002	48	65
CoO ₂	606	0.0002	54	130
Te ₂ Ti	387	0.0002	48	65
HfSe ₂	387	0.0003	48	65
Al ₂ Cl ₂ O ₂	792	0.0003	63	90
CCL ₂ Gd ₂	517	0.0003	48	65
MnSe ₂	887	0.0003	113	145
CaCl	742	0.0004	113	145
FeSe ₂	247	0.0004	25	49
NiO ₂	606	0.0004	54	130
Fe ₂ Li ₂ P ₂	924	0.0004	81	100
Br ₂ O ₂ Ti ₂	56	0.0004	5	6
Br ₂ La ₂ O ₂	10	0.0005	1	1
Eu ₂ F ₂ I ₂	10	0.0005	1	1
C ₂ Br ₂ Tb ₂	804	0.0005	72	86
Ba ₂ F ₂ I ₂	886	0.0005	100	81
O ₄ PTl	896	0.0006	101	82
Fe ₂ Se ₂	732	0.0006	82	101
Cl ₂ ORu	580	0.0006	64	81
Mg ₃	775	0.0007	85	145
Ge ₂ Se ₂ Zr ₂	752	0.0007	65	82
Ca ₂ Cl ₂	588	0.0007	65	82
HfS ₂	678	0.0007	81	118
C ₂ Br ₂ Gd ₂	804	0.0007	72	86
Cl ₄ Mn	877	0.0008	113	85
CaH ₂ O ₂	914	0.0008	81	118
CBr ₂ Y ₂	517	0.0008	48	65
CoTe ₂	678	0.0009	81	118
Tl	277	0.0009	49	81
O ₄ PTl	886	0.0009	100	81
Cl ₄ Mg ₂	576	0.0009	93	34
Cu ₂ K ₂ Te ₂	718	0.0009	82	65
I ₃ Sn	892	0.001	149	74
Ga ₂ S ₂	796	0.001	81	118
Se ₂ Ta	694	0.001	79	126
NbSe ₂	694	0.001	79	126
Cl ₂ OOs	724	0.0011	81	100
Br ₂ Pr ₂	452	0.0011	48	65
Cl ₄ KTl	560	0.0011	89	34
AgTe ₂	578	0.0011	65	106
P ₄	936	0.0011	112	122
Sn ₂ Te ₂	648	0.0011	90	72
Cu ₂ Se ₂ Tl ₂	10	0.0011	1	1
Bi ₂ In ₂	460	0.0011	65	50
Cl ₂ Ni	694	0.0012	79	126
C ₄ Ca ₂	534	0.0012	54	53
Si ₂ Te ₂ Zr ₂	934	0.0012	82	101

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

BiTe₂ (P-3m1 (164))

Structural and electronic properties

	Formula	BiTe ₂
	Spacegroup	P-3m1 (164)
	Prototype	CdI ₂
	Parent 3D	Ag ₃ Bi ₃ Te ₆
	Source DB	COD
	DB ID	9001316
DF2-C09	Binding energy [meV/ Å²]	81.74
RVV10	Binding energy [meV/ Å²]	83.08
	Band gap (PBE) [eV]	0.0

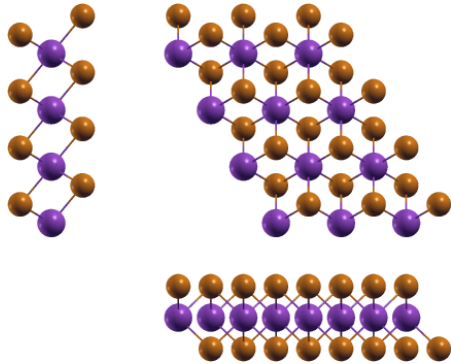


Band structure: Electronic band structure of BiTe₂ (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of BiTe₂ (P-3m1 (164)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.14159985	0.00000000	0.00000000
a₂	-2.07079993	3.58673068	0.00000000
a₃	0.00000000	0.00000000	24.03805260
	x [Å]	y [Å]	z [Å]
● Te	2.07079993	1.19557689	14.00417611
● Bi	0.00000000	0.00000000	12.01902630
● Te	0.00000000	2.39115379	10.03387649



Orthographic projections: views of BiTe₂ (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	4	0.4546	1	1
Na	4	1.5454	1	1
AgTl	5	0.1645	1	1
Ag ₂	5	0.4682	1	1
As ₂	5	0.2467	1	1
Sb ₂	5	0.0043	1	1
CaCl	5	0.1187	1	1
Cl ₂ Zn	6	1.5957	1	1
I ₂ Mg	6	0.0014	1	1
MoTe ₂	6	1.5617	1	1
PSn ₂	6	0.2586	1	1
Ba ₂ Pt	6	0.4676	1	1
Br ₂ Zn	6	0.2739	1	1
HfS ₂	6	0.2502	1	1
AsSn ₂	6	0.2639	1	1
I ₂ Pr	6	0.1465	1	1
CuTe ₂	6	0.2498	1	1
S ₂ Zr	6	0.2575	1	1
Br ₂ La	6	0.0017	1	1
Ca ₂ Si	6	0.4791	1	1
Br ₂ Co	6	1.6003	1	1
Ca ₂ N	6	0.2473	1	1
BrCdI	6	0.0045	1	1
Cl ₂ Zn	6	0.1273	1	1
Te ₂ Ti	6	0.2743	1	1
I ₂ Zn	6	0.0075	1	1
BaF ₂	6	0.0079	1	1
RhTe ₂	6	0.2679	1	1
GeI ₂	6	0.0005	1	1
Br ₂ Mn	6	1.5869	1	1
PtS ₂	6	1.5528	1	1
CoTe ₂	6	0.2507	1	1
Se ₂ Ti	6	1.5339	1	1
AsKSn	6	0.0065	1	1
Te ₂ W	6	1.5629	1	1
PbTe ₂	6	0.0035	1	1
I ₂ Nd	6	0.1474	1	1
S ₂ Sn	6	0.2579	1	1
SnTe ₂	6	0.0027	1	1
Sn	6	0.6319	1	3
Cl ₂ V	6	4.8542	1	1
I ₂ Pb	6	0.4722	1	1
STl ₂	6	0.0089	1	1
PtSe ₂	6	0.2648	1	1
Br ₂ Fe	6	0.2462	1	1
GeS ₂	6	0.1132	1	1
TaTe ₂	6	0.2631	1	1
MnSe ₂	6	0.1187	1	1
Br ₂ Ni	6	1.6389	1	1
CeI ₂	6	0.1458	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

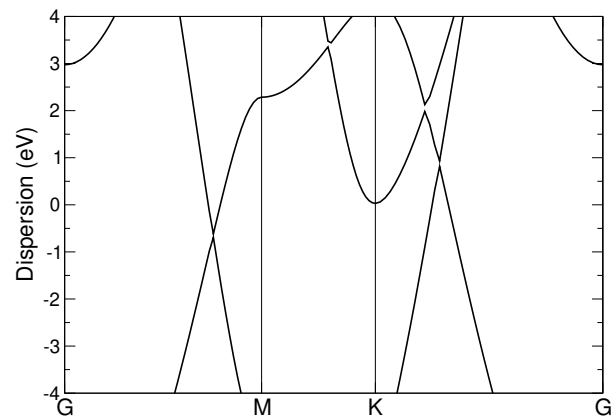
Formula	N° atoms	strain	cell size 1	cell size 2
Br ₂ N ₂ Zr ₂	609	0.0	57	73
CaH ₂ O ₂	467	0.0001	49	64
Sb ₂ Te ₂	499	0.0001	81	64
CBr ₂ Lu ₂	536	0.0001	57	73
MnO ₂	39	0.0001	4	9
Br ₂ V	183	0.0001	25	36
Ga ₂ S ₃	353	0.0001	36	49
ClH ₃ O	386	0.0002	57	43
NS ₂ Zr	304	0.0002	36	49
Na	157	0.0002	36	49
RhTe ₂	543	0.0002	81	100
Se ₂ Yb	6	0.0003	1	1
CrSe ₂	390	0.0003	49	81
Ba ₂ Pt	492	0.0003	91	73
Ag ₂ I ₂	387	0.0003	65	48
Cl ₂ N ₂ Zr ₂	531	0.0003	49	64
AsSn ₂	492	0.0003	73	91
PtSe ₂	492	0.0003	73	91
Sb ₂ Se ₂ Te	8	0.0003	1	1
KS ₂ Ti	357	0.0003	43	57
MoSe ₂	123	0.0004	16	25
CrSe ₂	294	0.0004	37	61
AgBrO ₂	526	0.0004	74	76
CuTe ₂	339	0.0004	49	64
Cl ₂ Zn	300	0.0005	43	57
GeI ₂	6	0.0005	1	1
N ₃ W ₂	512	0.0005	39	79
AgBrO ₂	519	0.0005	73	75
PSn ₂	435	0.0005	64	81
Se ₂ W	123	0.0005	16	25
Ag ₂	419	0.0005	91	73
CdClHO	643	0.0005	81	100
ReS ₂	75	0.0006	9	16
AgBrO ₂	291	0.0006	41	42
I ₂ Nd ₂ S ₂	786	0.0006	100	81
ReSe ₂	183	0.0007	25	36
Ba ₂ Ni ₃	8	0.0007	1	1
C ₂ Cl ₂ Y ₂	576	0.0007	58	67
Ga ₂ Te ₂	7	0.0007	1	1
Br ₂ Mn	300	0.0007	43	57
HfS ₂	339	0.0007	49	64
Sb ₂ Se ₂ Te	8	0.0008	1	1
I ₂ Pr ₂ Si ₂	9	0.0008	1	1
PtS ₂	255	0.0008	36	49
HgI ₂	339	0.0008	65	48
Br ₂ Hf ₂ N ₂	531	0.0008	49	64
TaTe ₂	492	0.0009	73	91
LiO	233	0.0009	37	61
Cl ₂ Zr ₂	219	0.0009	25	36
AsCuLi ₂	7	0.001	1	1

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

C (P6/mmm)

Structural and electronic properties

	Formula	C
	Spacegroup	P6/mmm
	Prototype	In
	Parent 3D	C ₂
	Source DB	ICSD
	DB ID	252268
DF2-C09	Binding energy [meV/ Å²]	39.32
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

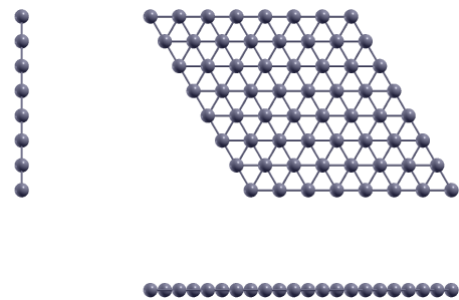


Band structure: Electronic band structure of C (P6/mmm) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of C (P6/mmm) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	-0.85952845	1.48874695	0.00000000
a₂	-0.85952845	-1.48874695	0.00000000
a₃	0.00000000	0.00000000	12.00000000
	x [Å]	y [Å]	z [Å]
• C	-0.42976422	0.74437347	0.00000000



Orthographic projections: views of C (P6/mmm) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
In	5	0.0413	4	1
Mg ₂	6	0.1248	4	1
ReSe ₂	7	0.0025	4	1
S ₂ Ta	7	0.0084	4	1
S ₂ Ti	7	0.0035	4	1
NbS ₂	7	0.0088	4	1
Cl ₂ Ni	7	0.0034	4	1
Cl ₂ Co	7	0.0039	4	1
Br ₂ V	7	0.0017	4	1
ClNZr	7	0.0004	4	1
Cl ₂ Fe	7	0.0046	4	1
Br ₂ Ti	7	0.0091	4	1
AsSe ₂	7	0.0049	4	1
CdO ₂	7	0.004	4	1
BrNZr	7	0.0063	4	1
NbSe ₂	7	0.0039	4	1
GeS ₂	7	0.3423	4	1
Br ₂ Cr	7	0.0094	4	1
Cl ₂ Zr	7	0.0042	4	1
Se ₂ Ta	7	0.0039	4	1
NbSe ₂	7	0.0052	4	1
Se ₂ Ta	7	0.0083	4	1
Cl ₂ Hf ₂	8	0.0072	4	1
Br ₂ Hf ₂	8	0.0058	4	1
Cl ₂ Zr ₂	8	0.0009	4	1
As ₂ Fe ₂	8	0.344	4	1
O ₂ Sn ₂	8	0.0895	4	1
LiNbS ₂	8	0.0083	4	1
Cl ₂ Sc ₂	8	0.0096	4	1
H ₂ Na ₂ Pd	9	0.3407	4	1
CCL ₂ Sc ₂	9	0.0005	4	1
Cl ₂ Cu	9	0.0602	6	1
Hf ₂ Se ₂ Si ₂	10	0.3449	4	1
Br ₂ H ₂ Zr ₂	10	0.0093	4	1
Cu ₂ O ₂	10	0.1378	6	1
Br ₂ H ₂ Zr ₂	10	0.0001	4	1
H ₂ Na ₂ O ₂	10	0.3185	4	1
AgBrO ₂	10	0.0802	6	1
Ge ₂ S ₂	10	0.0572	6	1
Cl ₂ H ₂ Sc ₂	10	0.0085	4	1
H ₂ MnO ₂	11	6.131	1	2
N ₃ W ₂	11	6.0677	1	2
Sn	13	0.0108	10	3
Sm	13	0.0065	9	4
NaO ₄	14	0.0003	9	1
AgNO ₃	14	0.0006	9	1
O ₂ Sn ₂	15	0.2438	7	2
K	17	0.011	15	2
H ₂ Li ₂ Pt	17	0.078	7	2
C ₂	17	0.0447	9	4

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

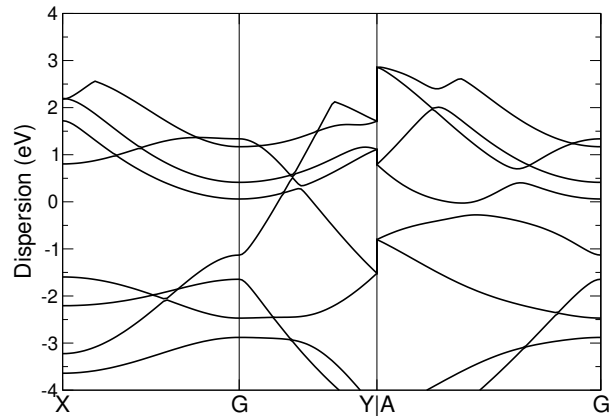
Formula	N° atoms	strain	cell size 1	cell size 2
Bi ₂	33	0.0	25	4
FeI ₂	129	0.0001	81	16
Br ₂ H ₂ Zr ₂	10	0.0001	4	1
Br ₂ Mg	129	0.0002	81	16
CoH ₂ O ₂	206	0.0002	81	25
NaO ₄	14	0.0003	9	1
CrO ₂	139	0.0004	64	25
ClNZr	7	0.0004	4	1
Br ₂ Cd	76	0.0004	49	9
CrI ₂	129	0.0004	81	16
Ga ₂ Gd ₂ I ₂	49	0.0004	25	4
NS ₂ Ta	113	0.0005	49	16
I ₂ La ₂ Sb	109	0.0005	64	9
PdTe ₂	76	0.0005	49	9
CCL ₂ Sc ₂	9	0.0005	4	1
AgNO ₃	14	0.0006	9	1
Bi ₂ SeTe ₂	45	0.0006	25	4
Br ₂ PY ₂	94	0.0006	49	9
Ga ₂ I ₂ Tb ₂	49	0.0007	25	4
N ₂ Re	52	0.0007	25	9
K	73	0.0008	64	9
Cl ₂ Fe ₂ O ₂	127	0.0009	55	12
Cl ₂ Zr ₂	8	0.0009	4	1
Te ₄ TiZr	129	0.0009	81	8
GeTe ₂	129	0.001	81	16
K ₂ PdSe ₂	83	0.0011	63	4
Br ₂ Tb ₂	85	0.0011	49	9
Br ₂ Ca	37	0.0011	25	4
Cu ₂ Te ₂	113	0.0012	65	12
I ₂ S ₂ Sm ₂	118	0.0012	64	9
Cl ₂ Hg ₂ N ₂	122	0.0012	80	7
I ₂ Ni	129	0.0012	81	16
ReS ₂	156	0.0012	81	25
Bi ₂ S ₃	94	0.0013	49	9
NSr ₂	129	0.0013	81	16
PbS ₂ Sn	110	0.0014	70	10
Cl ₂ Zn	101	0.0014	65	12
Se ₂ Sn	129	0.0016	81	16
Br ₂ Ho ₂	85	0.0016	49	9
As ₂ Co ₂ Li ₂	137	0.0016	65	12
Cl ₂ Cr ₂ O ₂	372	0.0016	162	35
F ₂ Ho ₂ Se ₂	103	0.0017	49	9
Br ₂ V	7	0.0017	4	1
Sb ₂ Te ₃	45	0.0017	25	4
Cl ₂ Y ₂	161	0.0017	81	16
N ₂ W	97	0.0017	49	16
C ₂ Br ₂ La ₂	205	0.0018	103	17
Ni ₂ Te ₂	145	0.0018	81	16
C ₂ Cl ₂ Y ₂	88	0.0018	40	8
I ₂ Pr	37	0.0019	25	4

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Ca₂C₄ (C2/m)

Structural and electronic properties

	Formula	Ca ₂ C ₄
	Spacegroup	C2/m
	Prototype	C2Ca
	Parent 3D	C ₄ Ca ₂
	Source DB	ICSD
	DB ID	252716
DF2-C09	Binding energy [meV/ Å²]	33.43
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

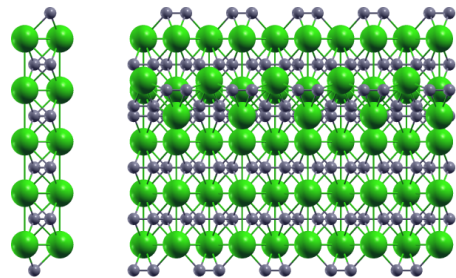


Band structure: Electronic band structure of Ca₂C₄ (C2/m) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ca₂C₄ (C2/m) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		-1.44914731	4.42920074	0.00000000
a₂		3.45310759	1.13224780	0.00000000
a₃		0.00000000	0.00000000	18.05621020
		x [Å]	y [Å]	z [Å]
●	Ca	2.08884510	-0.54146282	-7.78687541
●	Ca	1.36426249	1.67371062	-10.26933480
•	C	-0.14570336	0.44384896	-8.46322791
•	C	0.14570336	-0.44384896	-9.59298230
•	C	-0.57931449	1.77050327	-8.46321915
•	C	-0.86983283	2.65869747	-9.59299106



Orthographic projections: views of Ca₂C₄ (C2/m) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	7	0.1157	1	1
Na	7	0.4122	1	1
S ₂	8	0.5227	1	1
P ₂	8	0.1167	1	1
Cl ₂ Mn	9	0.1147	1	1
MoSe ₂	9	0.1158	1	1
Br ₂ Cu	9	0.1882	1	1
Cl ₂ Ti	9	0.1166	1	1
BiBrTe	9	0.15	1	1
S ₂ Ta	9	0.1153	1	1
Se ₂ V	9	0.1155	1	1
Se ₂ Ti	9	0.4088	1	1
GdI ₂	9	0.1525	1	1
Se ₂ W	9	0.1158	1	1
K	10	3.5978	1	4
Li ₂ Tl ₂	10	0.9615	1	1
InSe	10	0.7845	1	2
Cu ₂ Sr ₂	10	0.1509	1	1
AlLiTe ₂	10	0.1548	1	1
Br ₂ Zr ₂	10	0.4079	1	1
P ₂ Sn ₂	10	0.5253	1	1
PbTe	10	0.7915	1	2
Gd	10	0.2005	1	4
CS ₂ Ta ₂	11	0.1166	1	1
I ₂ La ₂ P	11	0.1517	1	1
Cl ₂ NSe ₂	11	0.1147	1	1
Sn	11	1.1263	1	5
Ni ₂ SbTe ₂	11	0.5231	1	1
CNb ₂ S ₂	11	0.1168	1	1
CdI ₂	12	0.7984	1	2
Cu ₄ Te ₂	12	0.1489	1	1
BiClTe	12	0.7999	1	2
HgI ₂	12	1.0221	1	2
GeI ₂	12	0.7376	1	2
CNRb	12	1.0909	1	2
CKN	12	0.8773	1	2
HN ₃ OZn	12	0.1164	1	1
AsKSn	12	0.7638	1	2
GeI ₂	12	0.7925	1	2
STl ₂	12	0.7731	1	2
CuO ₂	12	0.6233	1	2
Se ₂ Yb	12	0.7385	1	2
BiTe ₂	12	0.7395	1	2
F ₂ Se ₂ Yb ₂	12	0.5257	1	1
Sm	12	0.7227	1	6
Ba ₂ Cd	12	1.4201	1	2
I ₂ Pr	12	0.8002	1	2
Na	13	0.1543	2	1
LiMnTe ₂	14	0.7937	1	2
AsLi ₃	14	0.7857	1	2

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

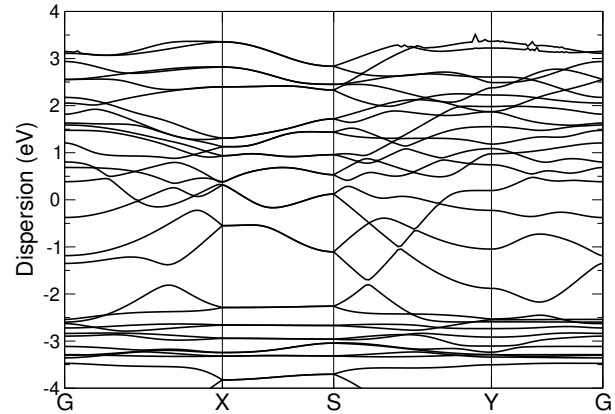
Formula	N° atoms	strain	cell size 1	cell size 2
K	624	0.0002	90	84
Br ₂ Ho ₂	628	0.0003	58	70
CBr ₂ Lu ₂	957	0.0003	72	105
I ₂ La ₂ Sb	960	0.0003	90	84
HfLiS ₂	852	0.0003	70	108
AgTe ₂	540	0.0004	49	82
CrSe ₂	738	0.0004	63	120
Bi ₂ S ₃	698	0.0004	58	70
C ₂ Li ₂	584	0.0005	56	62
Br ₂ La ₂	970	0.0005	91	106
HfSe ₂	831	0.0006	82	113
CaI ₂	312	0.0006	35	34
Cu ₂ K ₂ Te ₂	816	0.0006	75	61
PtS ₂	744	0.0006	70	108
Te ₂ Ti	831	0.0006	82	113
GdI ₂	309	0.0006	34	35
F ₂ Se ₂ Tm ₂	990	0.0006	73	92
Gd ₂ GeI ₂	954	0.0006	84	90
Br ₂ Lu ₂ S ₂	966	0.0006	89	72
Br ₂ Lu ₂ S ₂	966	0.0006	89	72
Br ₂ Tb ₂	628	0.0006	58	70
Br ₂ Cr ₂ S ₂	636	0.0006	50	56
F ₂ Se ₂ Y ₂	768	0.0007	70	58
Br ₂ Er ₂ O ₂	906	0.0007	70	81
MoTe ₂	744	0.0007	70	108
Sn	143	0.0007	18	35
I ₂ Y ₂	806	0.0007	73	92
Br ₂ Ca ₂ H ₂	906	0.0008	70	81
CoH ₂ O ₂	730	0.0008	45	92
Sb ₂	758	0.0008	91	106
Fe ₂ SeTe	820	0.0008	76	91
Br ₂ Zn	831	0.0008	82	113
Cu ₂ Se ₂	494	0.0008	45	56
S ₂ Sn ₂	732	0.0008	74	72
Te ₂ W	744	0.0009	70	108
Cl ₄ Mn	907	0.0009	92	71
MoSe ₂	420	0.0009	37	66
PtTe ₂	558	0.0009	58	70
Ca ₂ Mn ₂ Si ₂	906	0.0009	70	81
I ₂ N ₂ Zr ₂	942	0.0009	75	82
Br ₂ Ho ₂ S ₂	846	0.001	79	62
I ₂ S ₂ Tl ₂	606	0.001	45	56
Ag ₂ F ₄	678	0.001	73	40
C ₂ Br ₂ Gd ₂	744	0.001	56	68
K ₂ O ₂ Tl ₂	720	0.001	70	50
Se ₂ W	420	0.001	37	66
P ₂ Rh ₂	636	0.001	60	69
Br ₂ Ho ₂ O ₂	906	0.001	70	81
Br ₂ Ho ₂ O ₂	774	0.0011	60	69
Cl ₂ Er ₂ S ₂	660	0.0011	61	49

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Ca₂Cu (P-1 (2))

Structural and electronic properties

	Formula	Ca ₂ Cu
	Spacegroup	P-1 (2)
	Prototype	WTe ₂
	Parent 3D	Ca ₈ Cu ₄
	Source DB	ICSD
	DB ID	108865
DF2-C09	Binding energy [meV/ Å²]	61.94
RVV10	Binding energy [meV/ Å²]	62.65
	Band gap (PBE) [eV]	0.0

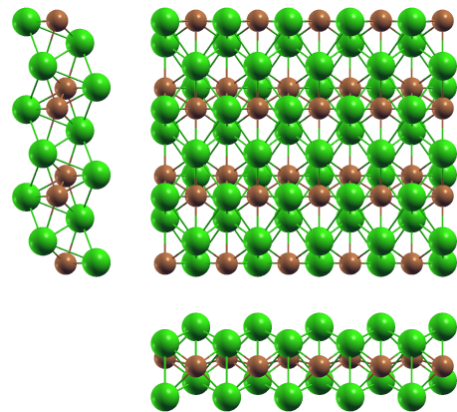


Band structure: Electronic band structure of Ca₂Cu (P-1 (2)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ca₂Cu (P-1 (2)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		4.19246586	−0.00017952	0.00000000
a₂		0.00020762	5.94055593	0.00000000
a₃		0.00000000	0.00000000	24.70845014
		x [Å]	y [Å]	z [Å]
●	Ca	3.14448005	2.18910931	13.61469115
●	Ca	1.04826108	5.18670664	14.73110162
●	Cu	3.14470511	5.26888438	12.64497186
●	Ca	1.04819342	3.75126710	11.09375898
●	Ca	3.14441240	0.75366977	9.97734851
●	Cu	1.04796837	0.67149203	12.06347828



Orthographic projections: views of Ca₂Cu (P-1 (2)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	8	0.2943	1	2
Sn	8	0.1241	1	2
Na	8	0.1466	1	2
In	8	0.1254	1	2
Ba ₂ Hg	9	0.2485	1	1
CKN	9	0.0424	1	1
Ba ₂ Cd	9	0.2519	1	1
Br ₃ Cs	10	0.3491	1	1
As ₂	10	0.1528	1	2
S ₂	10	0.5999	1	2
Au ₂ Se ₂	10	0.1618	1	1
SbSe ₂ Tl	10	0.0306	1	1
F ₄ Sn	11	0.2475	1	1
Hg ₃ N ₂	11	0.3766	1	1
ClKO ₃	11	0.3563	1	1
Cl ₄ Mn	11	0.972	1	1
Br ₂ Ho ₂ S ₂	12	0.3709	1	1
I ₂ Lu ₂ Se ₂	12	0.0102	1	1
PSn ₂	12	0.1604	1	2
MoSe ₂	12	0.1281	1	2
ReSe ₂	12	0.1383	1	2
Ho ₂ I ₂ S ₂	12	0.0336	1	1
S ₂ Ta	12	0.1321	1	2
Br ₂ Zn	12	0.1706	1	2
HfS ₂	12	0.1551	1	2
AsSn ₂	12	0.1639	1	2
GeTe ₂	12	0.5889	1	2
SiTe ₂	12	0.1748	1	2
CuTe ₂	12	0.1548	1	2
S ₂ Zr	12	0.1598	1	2
PbS ₂	12	0.5692	1	2
Br ₂ Co	12	0.1525	1	2
Br ₂ Cr ₂ S ₂	12	1.8724	1	1
Br ₂ Ca ₃ Si	12	0.2488	1	1
Cl ₂ Rh ₂ Te ₂	12	0.267	1	1
Ca ₂ N	12	0.1532	1	2
K ₂ O ₂ Tl ₂	12	0.1631	1	1
S ₂ Ti	12	0.1347	1	2
Te ₂ Ti	12	0.1709	1	2
NbS ₂	12	0.1318	1	2
Br ₂ S ₂ Y ₂	12	0.3764	1	1
I ₄ Zr ₂	12	0.6193	1	1
RhTe ₂	12	0.1666	1	2
Gd ₂ I ₂ S ₂	12	0.3863	1	1
Cl ₂ Ni	12	0.1388	1	2
Cl ₂ Co	12	0.1345	1	2
Br ₂ Er ₂ Se ₂	12	0.0201	1	1
PtS ₂	12	0.1474	1	2
CoTe ₂	12	0.1553	1	2
Br ₂ V	12	0.1378	1	2

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

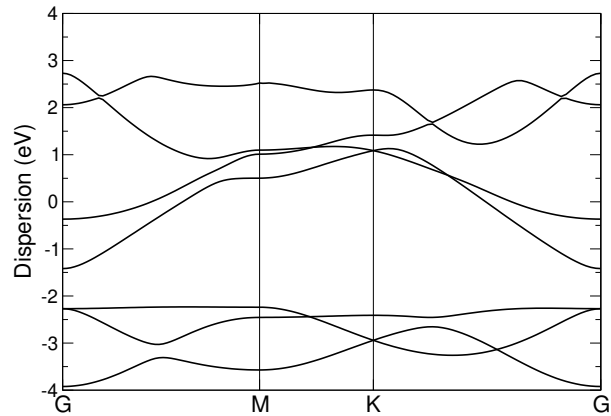
Formula	N° atoms	strain	cell size 1	cell size 2
I ₂ S ₂ Sm ₂	342	0.0001	24	33
K	177	0.0003	24	33
Cl ₂ O ₂ Y ₂	894	0.0003	50	99
Cl ₂ Ho ₂ O ₂	894	0.0004	50	99
Bi ₂ Te ₂	616	0.0006	56	70
I ₂ La ₂ Sb	309	0.0006	24	33
CrI ₂	624	0.0007	53	102
Br ₂ Mg	624	0.0007	53	102
ClNZr	120	0.0007	9	22
FeI ₂	624	0.0007	53	102
I ₂ V	597	0.0007	50	99
Ga ₂ Se ₂	696	0.0008	50	99
O ₂ Zn	489	0.0011	32	99
I ₂ Ni	669	0.0011	57	109
Br ₂ Y ₂	696	0.0012	50	99
CBr ₂ Lu ₂	973	0.0012	58	125
NSr ₂	624	0.0013	53	102
Ge ₂ Te ₂	34	0.0013	3	4
Ni ₂ Te ₂	778	0.0013	57	109
LiO ₂	534	0.0013	40	98
Cl ₂ Zn	456	0.0013	40	72
I ₄ Zr ₂	738	0.0014	63	60
AgClO ₄	828	0.0014	67	71
Hg ₃ S ₂	935	0.0014	110	55
Cl ₂ N ₂ Ti ₂	246	0.0014	14	27
CdCl ₂	669	0.0014	57	109
PbS ₂	597	0.0014	50	99
Cl ₂ Rh ₂ Te ₂	852	0.0014	70	72
K ₂ PtS ₂	454	0.0015	49	32
Se ₂ Sn	624	0.0015	53	102
I ₂ Mn	669	0.0015	57	109
GeTe ₂	624	0.0015	53	102
Cl ₂ Er ₂ H ₂	996	0.0015	57	109
Br ₂ CsF	812	0.0015	76	89
Cl ₂ Fe ₂ O ₂	282	0.0016	15	32
N ₃ Na	552	0.0016	50	63
Cl ₂ Y ₂	828	0.0016	53	102
CCl ₂ Sc ₂	164	0.0016	9	22
I ₂ Ni	624	0.0016	53	102
Br ₂ In ₂ O ₂	942	0.0016	59	98
InSe ₂	669	0.0016	57	109
Se ₂ Zr	597	0.0017	50	99
Bi ₂ Se ₂	116	0.0017	10	14
Hf ₂ Si ₂ Te ₂	912	0.0017	53	99
Co ₂ Se ₂	714	0.0017	53	99
NiTe ₂	648	0.0017	54	108
Ca ₂ Cl ₂ H ₂	672	0.0017	40	72
SiTe ₂	648	0.0017	54	108
Cu ₂ Rb ₂ Te ₂	948	0.0017	73	85
Ho ₂ I ₂ S ₂	102	0.0018	8	9

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Ca₂N (P-3m1 (164))

Structural and electronic properties

	Formula	Ca ₂ N
	Spacegroup	P-3m1 (164)
	Prototype	CdI ₂
	Parent 3D	Ca ₂ N
	Source DB	COD
	DB ID	2200084
DF2-C09	Binding energy [meV/ Å²]	71.71
RVV10	Binding energy [meV/ Å²]	71.39
	Band gap (PBE) [eV]	0.0

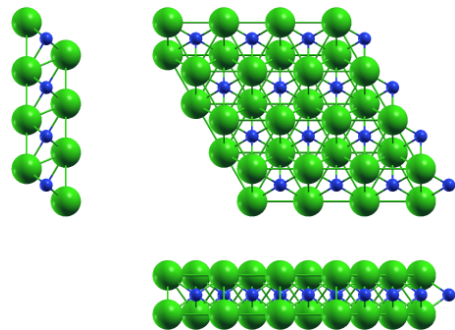


Band structure: Electronic band structure of Ca₂N (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ca₂N (P-3m1 (164)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.61269773	0.00000000	0.00000000
a₂		-1.80634887	3.12868801	0.00000000
a₃		0.00000000	0.00000000	22.51508558
		x [Å]	y [Å]	z [Å]
●	Ca	0.00000000	2.08579201	12.51395478
●	Ca	0.00000000	0.00000000	10.00113080
•	N	1.80634887	1.04289600	11.25754279



Orthographic projections: views of Ca₂N (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	4	0.1206	1	1
Na	4	0.0083	1	1
In	4	0.4311	1	1
In	4	0.2491	1	1
InSe	5	3.0422	1	1
HgO	5	0.1281	1	1
As ₂	5	0.0005	1	1
LiO	5	0.2635	1	1
P ₂	5	0.2745	1	1
Mg ₂	5	0.1129	1	1
Sb ₂	5	2.8329	1	1
Cl ₂ Zn	6	0.0016	1	1
I ₂ Mg	6	2.9057	1	1
S ₂ V	6	0.2534	1	1
MoS ₂	6	0.2543	1	1
MoTe ₂	6	0.0061	1	1
AgTe ₂	6	0.1223	1	1
PSn ₂	6	0.0085	1	1
HfS ₂	6	0.0022	1	1
HfTe ₂	6	0.4484	1	1
Te ₂ V	6	0.0043	1	1
CuTe ₂	6	0.0018	1	1
S ₂ Zr	6	0.0077	1	1
Br ₂ La	6	2.9101	1	1
Br ₂ Co	6	0.001	1	1
ReS ₂	6	1.5533	1	1
Cl ₂ Ti	6	0.2748	1	1
AuTe ₂	6	0.4676	1	1
PdTe ₂	6	0.4615	1	1
Mg ₃	6	0.1175	1	1
I ₂ Zn	6	0.4794	1	1
Te ₂ Zn	6	0.0063	1	1
S ₂ W	6	0.2544	1	1
Bi ₂ Pd	6	0.1351	1	1
GeI ₂	6	0.498	1	1
Br ₂ Mn	6	0.0027	1	1
PtS ₂	6	0.0073	1	1
CoTe ₂	6	0.0025	1	1
CdClO	6	0.0047	1	1
Ba ₂ N	6	0.4521	1	1
AsKSn	6	2.9715	1	1
Te ₂ Zr	6	0.4496	1	1
Te ₂ W	6	0.006	1	1
Cl ₂ Cu	6	0.5782	1	1
S ₂ Sn	6	0.008	1	1
Cl ₂ V	6	0.26	1	1
I ₂ Pb	6	13.6039	1	1
STl ₂	6	3.0033	1	1
OTl ₂	6	0.0046	1	1
Br ₂ Fe	6	0.0009	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

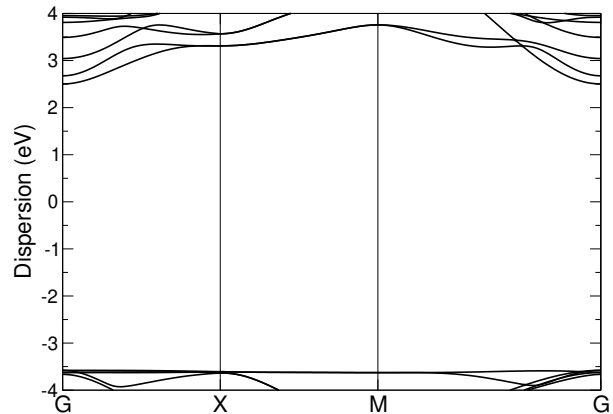
Formula	N° atoms	strain	cell size 1	cell size 2
F ₂ Lu ₂ Se ₂	561	0.0	73	57
I ₂ Pb	390	0.0	81	49
Gd ₂ I ₂	343	0.0	57	43
Br ₂ HLa	388	0.0	64	49
PtTe ₂	492	0.0001	91	73
In	211	0.0001	49	64
DyI ₂	123	0.0001	25	16
CoH ₂ O ₂	353	0.0001	36	49
PdTe ₂	543	0.0001	100	81
Ir ₂ P ₂	387	0.0002	65	48
In ₂ Se ₂	499	0.0002	81	64
AgNO ₃	545	0.0002	100	49
Br ₂ O ₂ Sm ₂	483	0.0002	65	48
I ₂ Pr ₂ S ₂	405	0.0002	61	37
Bi ₂ Se ₃	386	0.0003	57	43
I ₂ Nd	339	0.0003	65	48
Cu ₂ I ₂	343	0.0003	57	43
Br ₂ Gd ₂ Ge	386	0.0003	57	43
AuTe ₂	492	0.0003	91	73
I ₂ S ₂ Tb ₂	171	0.0003	25	16
Br ₂ La	300	0.0003	57	43
CeLi ₂ P ₂	437	0.0004	64	49
I ₂ O ₂ Yb ₂	483	0.0004	65	48
Nd	43	0.0005	9	16
BaF ₂	255	0.0005	49	36
Cl ₂ V	435	0.0005	64	81
Cu ₂ Sr ₂	208	0.0005	36	25
FeO ₂	294	0.0005	37	61
AsCuLi ₂	388	0.0005	64	49
STl ₂	255	0.0005	49	36
Cl ₄ Mn	217	0.0005	39	20
As ₂	5	0.0005	1	1
BiBrTe	183	0.0005	36	25
H ₂ NiO ₂	536	0.0005	57	73
LiO	401	0.0006	73	91
FHOZn	516	0.0006	64	81
MoS ₂	390	0.0006	57	73
Li ₂ Tl ₂	247	0.0006	49	25
NaO ₄	545	0.0006	100	49
Br ₂ Hf ₂ N ₂	9	0.0006	1	1
I ₂ Pb	294	0.0006	61	37
CCL ₂ Lu ₂	8	0.0007	1	1
I ₂ Pr ₂ Si ₂	486	0.0007	64	49
I ₂ Mg	300	0.0007	57	43
Ga ₂ I ₂ Y ₂	363	0.0007	49	36
CrSe ₂	435	0.0007	64	81
Br ₂ Tb ₂	624	0.0007	100	81
Ga ₂ Te ₂	388	0.0007	64	49
S ₂ W	390	0.0008	57	73
Ba ₂ Ni ₃	437	0.0008	64	49

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CaClF (P4/nmm (129))

Structural and electronic properties

Formula	CaClF
Spacegroup	P4/nmm (129)
Prototype	PbClF
Parent 3D	Ca ₂ Cl ₂ F ₂
Source DB	COD
DB ID	9011173
DF2-C09 Binding energy [meV/ Å²]	32.31
RVV10 Binding energy [meV/ Å²]	39.07
Band gap (PBE) [eV]	6.08

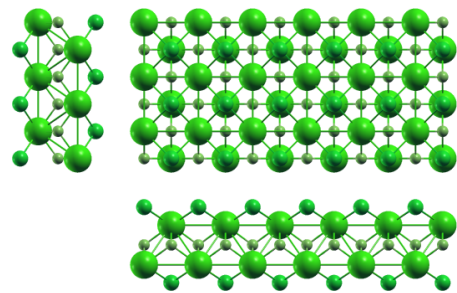


Band structure: Electronic band structure of CaClF (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CaClF (P4/nmm (129)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.77746812	0.00000000	0.00000000
a₂		0.00000000	3.77746812	0.00000000
a₃		0.00000000	0.00000000	24.87228356
		x [Å]	y [Å]	z [Å]
●	Ca	0.00000000	1.88873406	13.81155281
●	Cl	1.88873406	0.00000000	15.06091160
●	Ca	1.88873406	0.00000000	11.06073075
●	Cl	0.00000000	1.88873406	9.81137197
●	F	1.88873406	1.88873406	12.43614178
●	F	0.00000000	0.00000000	12.43614178



Orthographic projections: views of CaClF (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	7	1.11	1	1
K	7	0.7725	1	1
InSe	8	0.1612	1	1
HgO	8	0.5698	1	1
Bi ₂	8	0.1676	1	1
PbTe	8	0.1631	1	1
Sb ₂	8	0.1454	1	1
I ₂ Mg	9	0.1508	1	1
CdI ₂	9	0.165	1	1
Br ₂ Ca	9	0.1664	1	1
CaI ₂	9	0.1925	1	1
HfTe ₂	9	0.1325	1	1
Te ₂ V	9	0.1085	1	1
Br ₂ La	9	0.1511	1	1
Br ₂ Cu	9	0.114	1	1
I ₂ Yb	9	0.1892	1	1
BiClTe	9	0.1654	1	1
ReS ₂	9	0.1105	1	1
AuTe ₂	9	0.1386	1	1
BrCdI	9	0.1538	1	1
Cl ₂ Zn	9	0.0081	1	1
PdTe ₂	9	0.1366	1	1
I ₂ Zn	9	0.1425	1	1
BaF ₂	9	0.1572	1	1
BiBrTe	9	0.1717	1	1
Bi ₂ Pd	9	0.5977	1	1
GeI ₂	9	0.149	1	1
Ba ₂ Hg	9	0.3789	1	1
Br ₂ Mn	9	0.1089	1	1
CdClO	9	0.1084	1	1
Ba ₂ N	9	0.1337	1	1
AsKSn	9	0.1557	1	1
Te ₂ Zr	9	0.1329	1	1
PbTe ₂	9	0.1529	1	1
Cl ₂ Cu	9	0.1032	1	1
I ₂ Tm	9	0.191	1	1
SnTe ₂	9	0.1469	1	1
GeI ₂	9	0.1634	1	1
STl ₂	9	0.1582	1	1
OTl ₂	9	0.1085	1	1
BiTe	9	0.1794	1	1
DyI ₂	9	0.1963	1	1
Se ₂ Yb	9	0.1492	1	1
BiTe ₂	9	0.1495	1	1
GdI ₂	9	0.175	1	1
PtTe ₂	9	0.1383	1	1
Br ₂ Cd	9	0.1359	1	1
O ₂ Pt	9	0.109	1	1
CdI ₂	9	0.1645	1	1
Ba ₂ Cd	9	0.3845	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

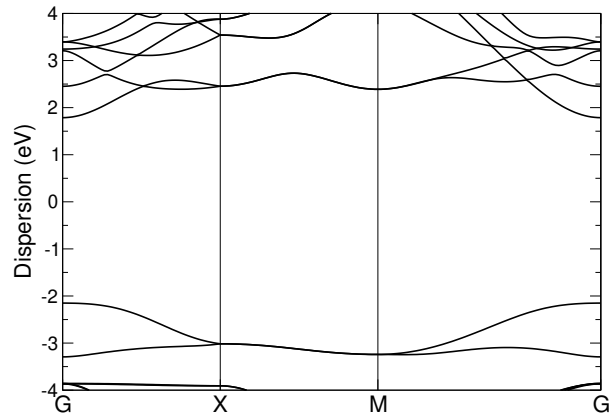
Formula	N° atoms	strain	cell size 1	cell size 2
Mg ₂	806	0.0	89	136
F ₄ Pb	474	0.0	49	36
K	433	0.0001	64	49
Bi ₂ Pd	495	0.0002	50	65
As ₂ Mg ₂ Na ₂	678	0.0002	64	49
Mg ₆	876	0.0004	61	85
Ag ₂ K ₂ Se ₂	876	0.0004	85	61
Sm	454	0.0004	54	130
In	859	0.0005	113	181
AlH ₄ Na	246	0.0006	25	16
Cl ₂ Mn	840	0.0007	81	118
BrNZr	483	0.0007	48	65
Sn	496	0.0007	65	106
Au ₂ Br ₂	732	0.0007	80	63
O ₂ Sn ₂	922	0.0008	87	100
As ₂ Cd ₂ K ₂	366	0.0009	36	25
O ₂ Sn ₂	922	0.0009	87	100
Bi ₂ Pd	486	0.0009	49	64
FeH ₂ O ₂	541	0.001	36	65
Ba ₂ Cd	843	0.001	100	81
N ₃ W ₂	315	0.001	20	39
Cl ₂ V	852	0.001	79	126
Ba ₂ Hg	852	0.001	101	82
Br ₂ Hf ₂	548	0.0011	48	65
C ₂ Br ₂ Y ₂	858	0.0011	69	74
La ₂ S ₂	580	0.0011	64	49
Ca ₂ O ₂	560	0.0011	50	65
AgNO ₂	938	0.0011	99	86
Ba ₂ F ₂ I ₂	366	0.0011	36	25
HgO	314	0.0011	36	49
O ₂ Sn ₂	646	0.0012	61	70
AgClO ₄	780	0.0012	81	49
O ₂ Sn ₂	646	0.0012	61	70
Ho ₂ I ₂ S ₂	690	0.0013	70	45
FeSe ₂	639	0.0013	58	97
AgCuTe ₂	602	0.0013	59	62
C ₂ Br ₂ Y ₂	756	0.0013	61	65
Se ₂ Ta	483	0.0014	48	65
Au ₂ I ₂	968	0.0014	108	80
O ₄ PTl	366	0.0014	36	25
FHOZn	978	0.0015	79	126
Ge ₂ Te ₂ Zr ₂	12	0.0015	1	1
CrSe ₂	852	0.0015	79	126
NbS ₂	840	0.0016	81	118
Cl ₂ H ₂ Sc ₂	678	0.0016	48	65
Ba ₂ Hg	843	0.0016	100	81
Ga ₂ S ₂	680	0.0016	62	77
PTe ₂ Ti ₂	757	0.0016	62	77
H ₂ I ₂ Sr ₂	690	0.0016	65	50
Br ₂ Ni	603	0.0016	62	77

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CaHCl (P4/nmm (129))

Structural and electronic properties

Formula	CaHCl
Spacegroup	P4/nmm (129)
Prototype	PbClF
Parent 3D	Ca ₂ H ₂ Cl ₂
Source DB	COD
DB ID	9009165
DF2-C09 Binding energy [meV/ Å²]	30.85
RVV10 Binding energy [meV/ Å²]	35.6
Band gap (PBE) [eV]	3.94

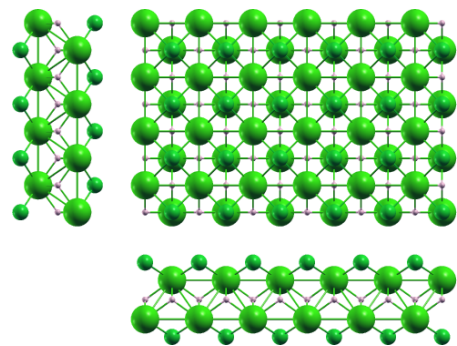


Band structure: Electronic band structure of CaHCl (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CaHCl (P4/nmm (129)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.70805224	0.00000000	0.00000000
a₂		0.00000000	3.70805224	0.00000000
a₃		0.00000000	0.00000000	24.80016906
		x [Å]	y [Å]	z [Å]
●	Ca	0.00000000	1.85402612	13.74134648
●	Cl	1.85402612	0.00000000	14.95183761
●	Ca	1.85402612	0.00000000	11.05882258
•	H	0.00000000	0.00000000	12.40008453
•	H	1.85402612	1.85402612	12.40008453
●	Cl	0.00000000	1.85402612	9.84833145



Orthographic projections: views of CaHCl (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	7	1.1575	1	1
Tl	7	0.5596	1	1
InSe	8	0.1709	1	1
HgO	8	0.595	1	1
Bi ₂	8	0.1778	1	1
GeTe	8	0.1321	1	1
AgTl	8	0.3784	1	1
S ₂	8	0.1333	1	1
PbTe	8	0.173	1	1
Sb ₂	8	0.1538	1	1
IrTe ₂	9	0.1328	1	1
CrS ₂	9	0.1099	1	1
I ₂ Mg	9	0.1596	1	1
CdCl ₂	9	0.1314	1	1
CdI ₂	9	0.175	1	1
AgTe ₂	9	0.5683	1	1
Br ₂ Ca	9	0.1765	1	1
CaI ₂	9	0.7709	1	1
InSe ₂	9	0.1316	1	1
GeTe ₂	9	0.1306	1	1
HfTe ₂	9	0.1395	1	1
I ₂ Mn	9	0.1314	1	1
Br ₂ La	9	0.1599	1	1
Br ₂ Cu	9	0.1199	1	1
BiClTe	9	0.1754	1	1
AuTe ₂	9	0.1463	1	1
BrCdI	9	0.1629	1	1
Cl ₂ Zn	9	0.0005	1	1
PdTe ₂	9	0.1441	1	1
FeI ₂	9	0.1299	1	1
I ₂ Ni	9	0.1308	1	1
CrI ₂	9	0.1295	1	1
I ₂ Zn	9	0.1506	1	1
BaF ₂	9	0.1666	1	1
BiBrTe	9	0.1822	1	1
Bi ₂ Pd	9	0.2152	1	1
GeI ₂	9	0.1577	1	1
Ba ₂ Hg	9	0.3979	1	1
N ₂ W	9	0.1114	1	1
Ba ₂ N	9	0.1407	1	1
AsKSn	9	0.165	1	1
Te ₂ Zr	9	0.1399	1	1
PbTe ₂	9	0.1619	1	1
Cl ₂ Cu	9	0.1069	1	1
I ₂ Tm	9	0.7664	1	1
SnTe ₂	9	0.1553	1	1
GeI ₂	9	0.1733	1	1
STl ₂	9	0.1676	1	1
BiTe	9	0.1905	1	1
DyI ₂	9	0.7818	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

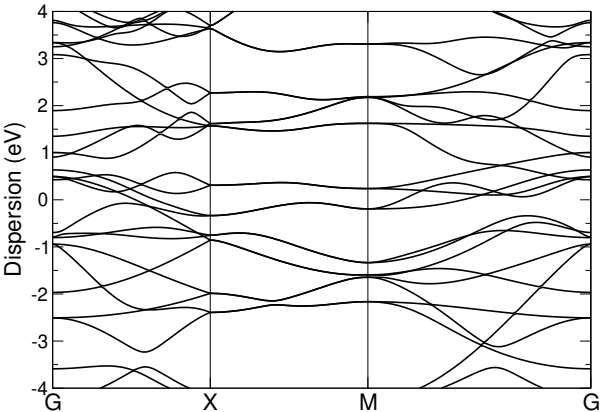
Formula	N° atoms	strain	cell size 1	cell size 2
Bi ₂ In ₂	214	0.0001	25	16
Ba ₂ F ₂ I ₂	612	0.0001	61	41
HgO	422	0.0002	49	64
Ag ₂ K ₂ Te ₂	780	0.0003	81	49
Cu ₂ Rb ₂ Te ₂	246	0.0004	25	16
I ₂ La ₂ O ₂	882	0.0004	82	65
F ₄ Sn	806	0.0005	81	64
Cl ₂ Zn	9	0.0005	1	1
Er ₂ I ₂ S ₂	876	0.0005	90	56
Hf ₃ Te ₂	11	0.0006	1	1
Se ₂ Sn ₂	876	0.0007	98	72
AgTe ₂	363	0.0008	36	49
Cu ₂ F ₄	894	0.0009	100	49
K	330	0.0009	49	36
I ₂ S ₂ Yb ₂	978	0.0011	100	63
Cl ₄ Cu ₂	204	0.0011	25	9
I ₂ S ₂ Yb ₂	948	0.0011	97	61
Gd ₂ I ₂ S ₂	972	0.0011	101	61
N ₂ Re	237	0.0012	20	39
I ₂ La ₂ O ₂	870	0.0012	81	64
As ₂ Mg ₂ Na ₂	510	0.0012	49	36
O ₂ Pt	852	0.0013	79	126
Ba ₂ Hg	678	0.0013	81	64
In	600	0.0013	79	126
Br ₂ Er ₂ Se ₂	288	0.0014	30	18
Ag ₂ K ₂ Se ₂	366	0.0014	36	25
I ₂ S ₂ Tm ₂	948	0.0014	97	61
AgNO ₂	336	0.0014	36	30
Br ₂ Ca	885	0.0014	103	89
Bi ₂ Pd	636	0.0015	65	82
Br ₂ Dy ₂ S ₂	978	0.0015	100	63
FeSe ₂	708	0.0015	65	106
Cl ₂ Mn	531	0.0015	52	73
ClN ₂ Zr	483	0.0015	48	65
Br ₂ Ca ₃ Si	870	0.0015	81	64
Cl ₂ N ₂ Sc ₂	677	0.0015	52	73
Ho ₂ I ₂ S ₂	846	0.0016	87	54
I ₂ Pr	885	0.0016	103	89
AgClO ₂	856	0.0016	86	85
I ₂ Pr	765	0.0016	89	77
BiClTe	885	0.0016	103	89
CdClO	603	0.0016	62	77
BiClTe	765	0.0016	89	77
Br ₂ Ca	765	0.0016	89	77
OTl ₂	603	0.0016	62	77
Cl ₂ Hf ₂ N ₂	834	0.0016	62	77
S ₂ Ti	483	0.0016	48	65
NSr ₂	975	0.0016	106	113
I ₂ Se ₂ Tm ₂	228	0.0017	24	14
NaO ₄	973	0.0017	108	65

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CaMnGe (P4/nmm (129))

Structural and electronic properties

	Formula	CaMnGe
	Spacegroup	P4/nmm (129)
	Prototype	PbClF
	Parent 3D	Ca ₂ Ge ₂ Mn ₂
	Source DB	cod
	DB ID	1539711
DF2-C09	Binding energy [meV/ Å²]	64.43
RVV10	Binding energy [meV/ Å²]	65.88
	Band gap (PBE) [eV]	0.0

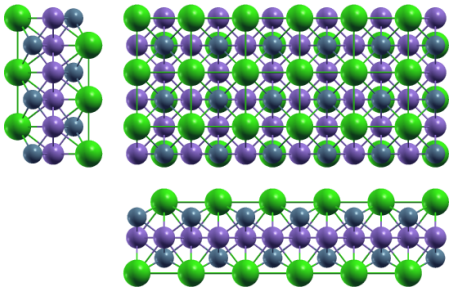


Band structure: Electronic band structure of CaMnGe (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CaMnGe (P4/nmm (129)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.88289667	0.00000000	0.00000000
a₂		0.00000000	3.88289667	0.00000000
a₃		0.00000000	0.00000000	24.86542606
		x [Å]	y [Å]	z [Å]
●	Ca	0.00000000	1.94144833	14.97848679
●	Ge	1.94144833	0.00000000	13.89481422
●	Ca	1.94144833	0.00000000	9.88693927
●	Mn	1.94144833	1.94144833	12.43271303
●	Mn	0.00000000	0.00000000	12.43271303
●	Ge	0.00000000	1.94144833	10.97061184



Orthographic projections: views of CaMnGe (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	7	0.3831	1	1
K	7	0.1876	1	1
In	7	0.1115	1	1
InSe	8	0.1482	1	1
Bi ₂	8	0.1538	1	1
AgTl	8	0.025	1	1
Ag ₂	8	0.1948	1	1
LiO	8	0.1091	1	1
PbTe	8	0.1499	1	1
Sb ₂	8	0.1345	1	1
I ₂ Mg	9	0.1391	1	1
S ₂ V	9	0.1107	1	1
MoS ₂	9	0.1105	1	1
CdI ₂	9	0.1515	1	1
Nd	9	0.7667	1	3
PSn ₂	9	0.1085	1	1
Ba ₂ Pt	9	0.1944	1	1
Br ₂ Ca	9	0.1527	1	1
CaI ₂	9	0.1762	1	1
I ₂ Pr	9	0.0028	1	1
Br ₂ La	9	0.1394	1	1
Br ₂ Cu	9	0.1068	1	1
I ₂ Yb	9	0.1732	1	1
BiClTe	9	0.1519	1	1
BrCdI	9	0.1417	1	1
HgI ₂	9	1.1323	1	1
I ₂ Zn	9	0.132	1	1
BaF ₂	9	0.1447	1	1
BiBrTe	9	0.1574	1	1
S ₂ W	9	0.1105	1	1
Bi ₂ Pd	9	0.5593	1	1
GeI ₂	9	0.1375	1	1
AsKSn	9	0.1434	1	1
PbTe ₂	9	0.1409	1	1
I ₂ Nd	9	0.0038	1	1
Cl ₂ Cu	9	0.0991	1	1
I ₂ Tm	9	0.1748	1	1
SnTe ₂	9	0.1357	1	1
Cl ₂ V	9	0.1097	1	1
GeI ₂	9	0.1501	1	1
I ₂ Pb	9	0.1969	1	1
STl ₂	9	0.1455	1	1
BiTe	9	0.1644	1	1
DyI ₂	9	0.1796	1	1
CeI ₂	9	0.0021	1	1
Se ₂ Yb	9	0.1377	1	1
MoS ₂	9	0.1105	1	1
BiTe ₂	9	0.138	1	1
GdI ₂	9	0.1604	1	1
CrSe ₂	9	0.1099	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

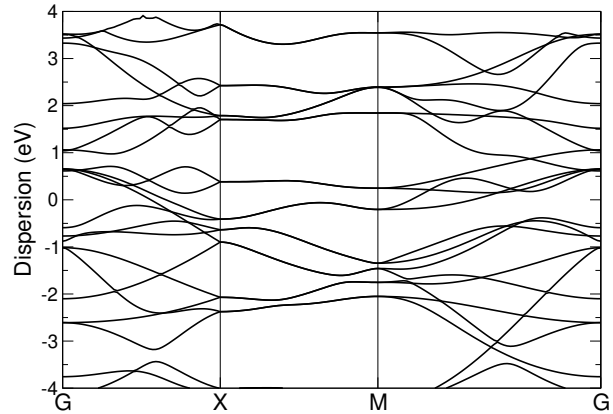
Formula	N° atoms	strain	cell size 1	cell size 2
AgTe ₂	429	0.0	41	61
HgI ₂	933	0.0	113	85
FeSe ₂	102	0.0001	9	16
Br ₂ F ₂ Tm ₂	12	0.0002	1	1
I ₂ Lu ₂ O ₂	12	0.0002	1	1
K	681	0.0004	100	81
Br ₂ O ₂ V ₂	66	0.0004	5	6
Bi ₂ Cl ₂ O ₂	12	0.0006	1	1
H ₂ Na ₂ Pd	997	0.0006	82	101
ReSe ₂	840	0.0006	81	118
Te ₂ V	483	0.0008	48	65
Br ₂ Mn	483	0.0008	48	65
Ba ₂ F ₂ I ₂	510	0.0008	49	36
Br ₂ Gd ₂ O ₂	12	0.0009	1	1
Br ₂ Cr ₂ S ₂	504	0.0009	42	42
AgClO ₄	246	0.0009	25	16
Pd ₂ S ₄	708	0.001	79	39
Ca ₂ O ₂	412	0.001	36	49
Cl ₂ Hf ₂ N ₂	678	0.001	48	65
Cl ₂ Ni	840	0.001	81	118
OTl ₂	483	0.001	48	65
Pb ₂ Se ₂	292	0.0011	32	25
Br ₂ V	840	0.0011	81	118
H ₂ Na ₂ Pd	986	0.0011	81	100
F ₂ Zn	9	0.0012	1	1
As ₂ Cd ₂ K ₂	510	0.0012	49	36
O ₄ PTl	510	0.0012	49	36
KS ₂ Ti	548	0.0012	48	65
Cu ₂ Na ₂ Te ₂	882	0.0012	82	65
Cl ₂ Rb ₂	186	0.0012	25	9
CdClO	483	0.0012	48	65
Ba ₂ H ₂ I ₂	876	0.0013	85	61
C ₂ I ₂ Y ₂	864	0.0013	70	74
In	655	0.0013	85	145
GeS ₂	795	0.0014	82	101
Cl ₄ Cu ₂	534	0.0014	64	25
Br ₂ Ca ₃ Si	198	0.0014	21	12
NbSe ₂	840	0.0014	81	118
H ₂ NiO ₂	929	0.0014	64	109
C ₂ I ₂ Y ₂	666	0.0014	54	57
CaI ₂	885	0.0014	103	89
HgO	222	0.0015	25	36
Se ₂ Ta	840	0.0015	81	118
H ₂ Na ₂ O ₂	690	0.0015	50	65
Br ₂ Ca ₂ F ₂	12	0.0015	1	1
CuO ₂	678	0.0015	63	100
Cl ₂ S ₂ Tl ₂	780	0.0015	81	49
CaI ₂	765	0.0016	89	77
Ga ₂ Se ₂	680	0.0016	62	77
Cu ₂ K ₂ Te ₂	876	0.0017	85	61

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CaMnSi (P4/nmm (129))

Structural and electronic properties

Formula	CaMnSi
Spacegroup	P4/nmm (129)
Prototype	PbClF
Parent 3D	Ca ₂ Mn ₂ Si ₂
Source DB	cod
DB ID	1539705
DF2-C09 Binding energy [meV/ Å²]	67.58
RVV10 Binding energy [meV/ Å²]	67.54
Band gap (PBE) [eV]	0.0

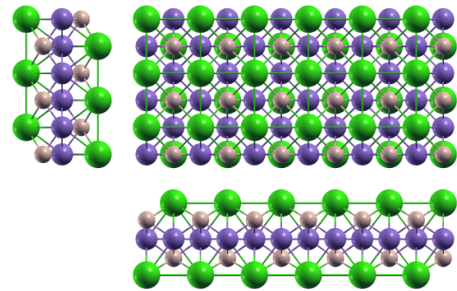


Band structure: Electronic band structure of CaMnSi (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CaMnSi (P4/nmm (129)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.83101623	0.00000000	0.00000000
a₂		0.00000000	3.83101623	0.00000000
a₃		0.00000000	0.00000000	24.79726510
		x [Å]	y [Å]	z [Å]
●	Ca	0.00000000	1.91550812	14.94800939
●	Si	1.91550812	0.00000000	13.75295014
●	Ca	1.91550812	0.00000000	9.84925571
●	Mn	1.91550812	1.91550812	12.39863255
●	Mn	0.00000000	0.00000000	12.39863255
●	Si	0.00000000	1.91550812	11.04431496



Orthographic projections: views of CaMnSi (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	7	0.397	1	1
K	7	0.1959	1	1
In	7	0.11	1	1
InSe	8	0.1543	1	1
Bi ₂	8	0.1603	1	1
Ag ₂	8	0.768	1	1
PbTe	8	0.1561	1	1
Sb ₂	8	0.1396	1	1
I ₂ Mg	9	0.1446	1	1
S ₂ V	9	0.1093	1	1
MoS ₂	9	0.1092	1	1
CdI ₂	9	0.1579	1	1
Ba ₂ Pt	9	0.767	1	1
Br ₂ Ca	9	0.1592	1	1
HfS ₂	9	0.1085	1	1
CaI ₂	9	0.184	1	1
I ₂ Pr	9	0.0093	1	1
Br ₂ La	9	0.1449	1	1
Br ₂ Cu	9	0.1101	1	1
Ca ₂ Si	9	0.7845	1	1
I ₂ Yb	9	0.1808	1	1
BiClTe	9	0.1583	1	1
AuTe ₂	9	0.1333	1	1
BrCdI	9	0.1474	1	1
PdTe ₂	9	0.1315	1	1
HgI ₂	9	1.1671	1	1
I ₂ Zn	9	0.1369	1	1
BaF ₂	9	0.1506	1	1
BiBrTe	9	0.1642	1	1
S ₂ W	9	0.1092	1	1
GeI ₂	9	0.1429	1	1
CoTe ₂	9	0.1086	1	1
AsKSn	9	0.1492	1	1
PbTe ₂	9	0.1465	1	1
Cl ₂ Cu	9	0.1009	1	1
I ₂ Tm	9	0.1825	1	1
SnTe ₂	9	0.141	1	1
GeI ₂	9	0.1564	1	1
I ₂ Pb	9	0.7741	1	1
STl ₂	9	0.1515	1	1
BiTe	9	0.1715	1	1
DyI ₂	9	0.1876	1	1
Br ₂ Ni	9	0.109	1	1
CeI ₂	9	0.0085	1	1
Se ₂ Yb	9	0.1431	1	1
MoS ₂	9	0.1091	1	1
Cl ₂ Mg	9	0.109	1	1
BiTe ₂	9	0.1434	1	1
GdI ₂	9	0.1673	1	1
PtTe ₂	9	0.133	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

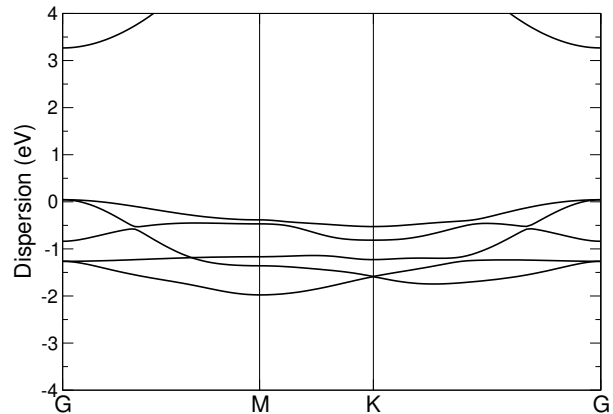
Formula	N° atoms	strain	cell size 1	cell size 2
Ba ₂ F ₂ I ₂	876	0.0	85	61
Ba ₂ H ₂ I ₂	366	0.0001	36	25
Br ₂ Ho ₂ O ₂	12	0.0002	1	1
HgO	536	0.0002	61	85
Br ₂ Ca ₂ H ₂	12	0.0002	1	1
Ca ₂ O ₂	962	0.0002	85	113
Se ₂ Ti	483	0.0003	48	65
In	375	0.0003	49	81
Cl ₄ Cu ₂	738	0.0003	89	34
C ₂ Li ₂	246	0.0004	25	24
H ₂ Li ₂ Pd	221	0.0005	16	25
As ₂ Mg ₂ Na ₂	870	0.0005	81	64
O ₄ PTl	876	0.0006	85	61
Br ₂ Zr ₂	548	0.0006	48	65
Cl ₂ Co	840	0.0006	81	118
CuGeO ₃	735	0.0006	70	63
S ₂ Ti	840	0.0007	81	118
Bi ₂ Se ₂	912	0.0007	98	81
Ag ₂ K ₂ Se ₂	510	0.0007	49	36
Cl ₂ Zr	840	0.0008	81	118
HgI ₂	402	0.0008	49	36
K	550	0.0009	81	64
C ₄ Ca ₂	906	0.0009	81	70
Br ₂ Er ₂ O ₂	12	0.0011	1	1
Cl ₂ Fe	840	0.0011	81	118
H ₄ Ti	221	0.0011	16	25
Au ₂ Br ₂	914	0.0011	99	80
H ₂ I ₂ Sr ₂	882	0.0012	82	65
C ₄ Ca ₂	774	0.0012	69	60
C ₂ I ₂ La ₂	138	0.0012	12	11
Ge ₂ Te ₂	712	0.0013	78	61
H ₂ Na ₂ O ₂	882	0.0013	65	82
AgTe ₂	258	0.0013	25	36
AgNO ₂	602	0.0014	63	56
P ₂ Rh ₂	10	0.0014	1	1
Mg ₂	146	0.0014	16	25
Sn	445	0.0014	58	97
Pb ₂ Se ₂	874	0.0014	97	73
Na	353	0.0014	48	65
Mo ₂ Te ₄	450	0.0015	45	30
Mg ₆	366	0.0015	25	36
F ₂ Tl ₂	10	0.0015	1	1
C ₂	510	0.0015	44	123
AsSe ₂	531	0.0015	52	73
NbSe ₂	531	0.0015	52	73
H ₂ Na ₂ O ₂	870	0.0015	64	81
O ₂ Pt	711	0.0015	64	109
Bi ₂ Pd	849	0.0016	85	113
In	493	0.0017	64	109
CdClHO	680	0.0017	62	77

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CaOHCl (P3m1)

Structural and electronic properties





Formula	CaOHCl
Spacegroup	P3m1
Prototype	FHOZn
Parent 3D	Ca ₂ Cl ₂ H ₂ O ₂
Source DB	MPDS
DB ID	S1600224
DF2-C09 Binding energy [meV/ Å²]	81.58
RVV10 Binding energy [meV/ Å²]	N/A
Band gap (PBE) [eV]	3.22

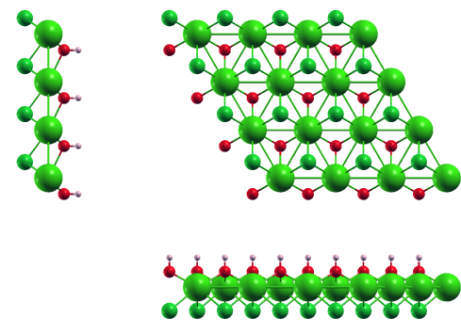


Band structure: Electronic band structure of CaOHCl (P3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CaOHCl (P3m1) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	-1.89235074	-3.27764762	0.00000000
a₂	3.78470148	0.00000000	0.00000000
a₃	0.00000000	0.00000000	18.87331597
	x [Å]	y [Å]	z [Å]
 Ca	-0.00000000	-2.18509842	0.37275892
 H	0.00000000	0.00000000	-1.66039006
 Cl	1.89235074	-1.09254921	1.97873724
 O	0.00000000	0.00000000	-0.69110610



Orthographic projections: views of CaOHCl (P3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	5	0.111	1	1
InSe	6	0.4724	1	1
HgO	6	0.1156	1	1
AsSb	6	0.0074	1	1
Bi ₂	6	0.4873	1	1
LiO	6	1.5341	1	1
PbTe	6	0.4769	1	1
CaCl	6	0.1503	1	1
Cl ₂ Mn	7	0.2588	1	1
CdI ₂	7	0.4813	1	1
AgTe ₂	7	0.112	1	1
MoSe ₂	7	0.25	1	1
S ₂ Ta	7	0.2617	1	1
Br ₂ Zn	7	0.0029	1	1
Br ₂ Ca	7	0.4845	1	1
SiTe ₂	7	0.0012	1	1
Br ₂ La	7	0.4476	1	1
NSr ₂	7	0.0091	1	1
PbS ₂	7	0.0048	1	1
BiClTe	7	0.4823	1	1
BrCdI	7	0.4545	1	1
S ₂ Ti	7	0.2688	1	1
Mg ₃	7	0.4314	1	1
Te ₂ Ti	7	0.0026	1	1
NbS ₂	7	0.2611	1	1
BaF ₂	7	0.4627	1	1
BiBrTe	7	0.4968	1	1
RhTe ₂	7	0.0069	1	1
Bi ₂ Pd	7	0.1204	1	1
Cl ₂ Co	7	0.2683	1	1
NbS ₂	7	0.2551	1	1
ClNZr	7	0.2734	1	1
Cl ₂ Fe	7	0.2673	1	1
S ₂ Ta	7	0.254	1	1
AsKSn	7	0.4591	1	1
PbTe ₂	7	0.4521	1	1
NiTe ₂	7	0.0006	1	1
I ₂ V	7	0.0026	1	1
GeI ₂	7	0.4775	1	1
Se ₂ Zr	7	0.0016	1	1
STl ₂	7	0.4651	1	1
PtSe ₂	7	0.009	1	1
CdO ₂	7	0.2681	1	1
CoI ₂	7	0.0079	1	1
GeS ₂	7	0.1394	1	1
MnSe ₂	7	0.1502	1	1
Cl ₂ Zr	7	0.2678	1	1
I ₂ Ti	7	0.0082	1	1
F ₂ Na	7	0.0009	1	1
CdI ₂	7	0.4802	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

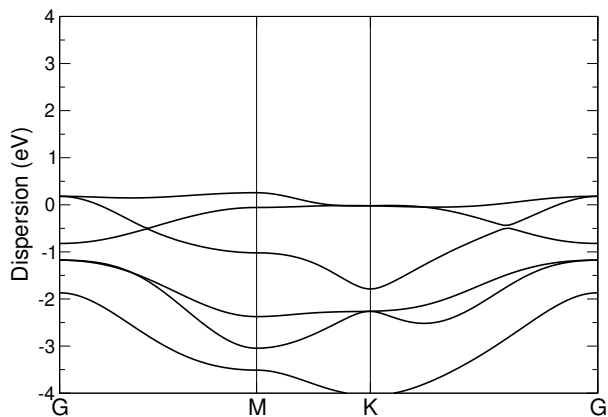
Lattice matching - minimal strain

Formula	N° atoms	strain	cell size 1	cell size 2
Cl ₂ H ₂ Zr ₂	666	0.0	57	73
FeH ₂ O ₂	189	0.0001	16	25
GdI ₂	357	0.0001	57	43
Cl ₂ NSc ₂	661	0.0001	64	81
Cl ₂ O ₂ Tm ₂	10	0.0001	1	1
Cl ₂ Zr	624	0.0002	81	100
CS ₂ Ta ₂	457	0.0002	43	57
Br ₂ Ca ₃ Si	294	0.0002	36	25
Cl ₂ Fe	624	0.0002	81	100
NbS ₂	447	0.0002	57	73
Cu ₄ Te ₂	498	0.0003	57	45
Cl ₂ Ti	343	0.0003	43	57
I ₂ Pr	463	0.0003	73	57
AsI ₂ La ₂	376	0.0003	49	36
Cd ₂ I ₃	376	0.0003	49	36
Cl ₂ Mn	499	0.0003	64	81
CdO ₂	624	0.0003	81	100
PbTe	452	0.0004	81	64
BiClTe	463	0.0004	73	57
In ₂ Te ₃	729	0.0004	91	73
As ₂ CeLi ₂	644	0.0004	81	64
Br ₂ H ₂ Sr ₂	548	0.0004	65	48
Ga ₂ I ₂ Y ₂	886	0.0004	100	81
P ₂	286	0.0004	43	57
Gd ₂ I ₂ S ₂	294	0.0004	36	25
Sb ₂ SeTe ₂	729	0.0004	91	73
Li ₂ Tl ₂	100	0.0005	16	9
Bi ₂ STe ₂	644	0.0005	81	64
Cl ₂ Co	624	0.0005	81	100
Br ₂ Ca	463	0.0005	73	57
N ₄	740	0.0005	77	108
BiBrTe	403	0.0005	64	49
O ₂ Pt	208	0.0006	25	36
GeI ₂	516	0.0006	81	64
MoSe ₂	388	0.0006	49	64
Gd ₂ GeI ₂	577	0.0006	73	57
NiTe ₂	7	0.0006	1	1
BaF ₂	643	0.0006	100	81
Nd	149	0.0006	25	49
Cl ₂ Hf ₂	656	0.0006	73	91
C ₂ Br ₂ Gd ₂	860	0.0007	92	82
STl ₂	583	0.0007	91	73
CdI ₂	463	0.0007	73	57
HN ₃ OZn	514	0.0007	43	57
Cu ₄ Te ₂	550	0.0008	64	49
F ₂ Se ₂ Y ₂	466	0.0008	61	37
Se ₂ W	388	0.0008	49	64
Cu ₂ I ₂	452	0.0008	65	48
ClKO ₃	449	0.0008	81	25
Bi ₂ Se ₂ Te	729	0.0008	91	73

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Structural and electronic properties




DF2-C09 Binding energy [meV/ Å ²]	58.23
RVV10 Binding energy [meV/ Å ²]	N/A
Band gap (PBE) [eV]	0.0

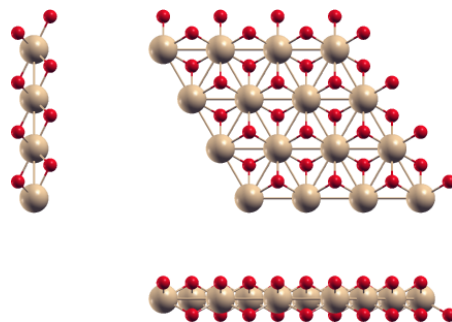


Band structure: Electronic band structure of CdO₂ (P-3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CdO₂ (P-3m1) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		1.70437257	-2.95205989	0.00000000
a₂		1.70437257	2.95205989	0.00000000
a₃		0.00000000	0.00000000	16.09818573
		x [Å]	y [Å]	z [Å]
	O	1.70437257	-0.98401996	0.96141042
	Cd	0.00000000	0.00000000	0.00000000
	O	1.70437257	0.98401996	-0.96141042



Orthographic projections: views of CdO₂ (P-3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	4	0.1398	1	1
Sn	4	0.118	1	1
In	4	0.1203	1	1
HgO	5	0.1507	1	1
AsSb	5	0.4788	1	1
GeTe	5	0.4947	1	1
S ₂	5	0.4988	1	1
Mg ₂	5	0.1274	1	1
IrTe ₂	6	0.4971	1	1
CrS ₂	6	0.2666	1	1
Cl ₂ Mn	6	0.0065	1	1
AgTe ₂	6	0.1423	1	1
ReSe ₂	6	0.0066	1	1
S ₂ Ta	6	0.0044	1	1
Br ₂ Zn	6	0.4531	1	1
InSe ₂	6	0.4928	1	1
GeTe ₂	6	2.8393	1	1
SiTe ₂	6	0.4633	1	1
NSr ₂	6	0.483	1	1
PbS ₂	6	0.4722	1	1
ReS ₂	6	0.2753	1	1
LiO ₂	6	2.8115	1	1
FeI ₂	6	0.4863	1	1
S ₂ Ti	6	0.0005	1	1
Mg ₃	6	0.135	1	1
Te ₂ Ti	6	0.4538	1	1
NbS ₂	6	0.0049	1	1
CrI ₂	6	0.4852	1	1
N ₂ W	6	0.257	1	1
Cl ₂ Ni	6	0.0076	1	1
Cl ₂ Co	6	0.0001	1	1
NbS ₂	6	0.0091	1	1
Br ₂ V	6	0.0058	1	1
ClN ₂ Zr	6	0.0037	1	1
Cl ₂ Fe	6	0.0006	1	1
AsSe ₂	6	0.0091	1	1
NiTe ₂	6	0.4618	1	1
Cl ₂ Cu	6	0.1081	1	1
I ₂ V	6	0.4667	1	1
Se ₂ Zr	6	0.4644	1	1
NbSe ₂	6	0.008	1	1
CoI ₂	6	0.4799	1	1
O ₂ Zn	6	0.2618	1	1
Cl ₂ Zr	6	0.0002	1	1
FeSe ₂	6	0.1149	1	1
Se ₂ Ta	6	0.0081	1	1
Br ₂ Mg	6	0.486	1	1
I ₂ Ti	6	0.4808	1	1
NbSe ₂	6	0.0093	1	1
F ₂ Na	6	0.458	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

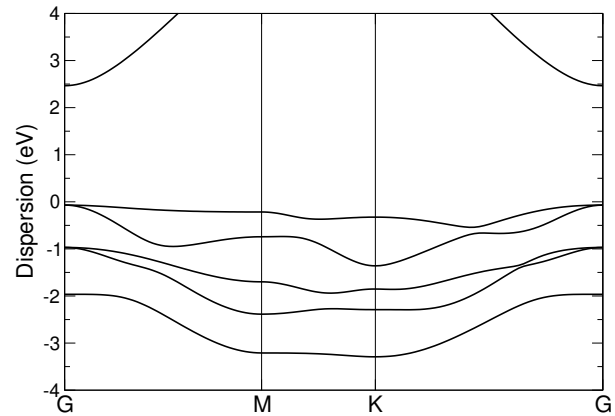
Formula	N° atoms	strain	cell size 1	cell size 2
PbTe	107	0.0	25	16
Cl ₂ Gd ₂	343	0.0	57	43
F ₂ Se ₂ Y ₂	471	0.0	79	39
As ₂ CeLi ₂	155	0.0	25	16
NSr ₂	390	0.0001	73	57
In ₂ S ₃	437	0.0001	64	49
I ₂ V	492	0.0001	91	73
Cl ₂ Co	6	0.0001	1	1
Cl ₂ Zr	6	0.0002	1	1
F ₂ Lu ₂ Se ₂	258	0.0002	36	25
GeI ₂	123	0.0002	25	16
NiTe ₂	543	0.0003	100	81
Cl ₂ Ho ₂ O ₂	711	0.0003	91	73
AlLiTe ₂	439	0.0003	81	49
GeTe	290	0.0003	64	49
Te ₂ Zr	255	0.0003	49	36
Se ₂ Sn	390	0.0003	73	57
CaClHO	624	0.0003	100	81
AlLiTe ₂	331	0.0004	61	37
PTe ₂ Zr ₂	563	0.0004	81	64
FeH ₂ O ₂	597	0.0004	64	81
ClKO ₃	17	0.0005	4	1
Cl ₂ O ₂ Tm ₂	786	0.0005	100	81
S ₂ Ti	6	0.0005	1	1
Cu ₃ Se ₃	363	0.0005	49	36
Cl ₂ Y ₂	504	0.0005	73	57
Br ₂ Ca ₃ Si	102	0.0005	16	9
LiMnTe ₂	139	0.0005	25	16
I ₂ N ₂ Zr ₂	531	0.0006	77	50
ClH ₃ O	272	0.0006	49	25
Cl ₂ Fe	6	0.0006	1	1
IrTe ₂	339	0.0006	64	49
H ₂ Si ₂	388	0.0007	64	49
CrS ₂	543	0.0007	81	100
Cl ₂ Tb ₂	343	0.0007	57	43
Ba ₂ N	255	0.0007	49	36
LiO ₂	705	0.0008	118	117
In ₂ Se ₃	327	0.0008	49	36
Gd ₂ I ₂ S ₂	102	0.0008	16	9
HfTe ₂	255	0.0008	49	36
Bi ₂ Te ₃	488	0.0008	81	49
Ga ₂ Se ₂	388	0.0008	64	49
I ₂ La ₂ Te	93	0.0008	16	9
CrI ₂	390	0.0008	73	57
Bi ₂ STe ₂	155	0.0008	25	16
Cu ₂ Se ₂	387	0.0008	65	48
SiTe ₂	543	0.0009	100	81
BiTe	390	0.0009	81	49
Bi ₂ STe ₂	155	0.0009	25	16
S ₂ Zn ₂	343	0.0009	57	43

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CdOHCl (P3m1 (156))

Structural and electronic properties





	Formula	CdOHCl
	Spacegroup	P3m1 (156)
	Prototype	FHOZn
	Parent 3D	Cd ₂ O ₂ H ₂ Cl ₂
	Source DB	ICSD
	DB ID	91087
DF2-C09	Binding energy [meV/ Å²]	53.04
RVV10	Binding energy [meV/ Å²]	60.79
	Band gap (PBE) [eV]	2.54

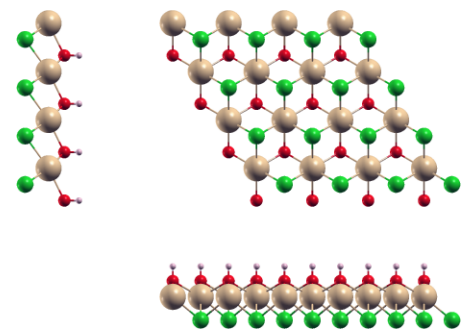


Band structure: Electronic band structure of CdOHCl (P3m1 (156)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CdOHCl (P3m1 (156)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.69798850	0.00000000	0.00000000
a₂		-1.84899425	3.20255199	0.00000000
a₃		0.00000000	0.00000000	23.49687376
		x [Å]	y [Å]	z [Å]
	Cd	0.00000000	2.13503466	11.94737786
	H	0.00000000	0.00000000	9.92936094
	O	0.00000000	0.00000000	10.89984688
	Cl	1.84899425	1.06751733	13.49579496



Orthographic projections: views of CdOHCl (P3m1 (156)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	5	0.1151	1	1
Tl	5	0.2661	1	1
In	5	1.5369	1	1
InSe	6	0.501	1	1
HgO	6	0.1212	1	1
Bi ₂	6	2.9721	1	1
LiO	6	0.2485	1	1
P ₂	6	0.2587	1	1
PbTe	6	2.9192	1	1
Mg ₂	6	0.4326	1	1
Sb ₂	6	0.4597	1	1
Sm	6	0.222	1	2
I ₂ Mg	7	0.4741	1	1
S ₂ V	7	1.5599	1	1
MoS ₂	7	1.5652	1	1
Cl ₂ Mn	7	0.2745	1	1
AgTe ₂	7	0.1165	1	1
PSn ₂	7	0.0026	1	1
MoSe ₂	7	0.2651	1	1
Br ₂ Zn	7	0.0082	1	1
HfS ₂	7	0.0086	1	1
AsSn ₂	7	0.0011	1	1
I ₂ Pr	7	0.2096	1	1
CuTe ₂	7	0.009	1	1
S ₂ Zr	7	0.0034	1	1
Br ₂ La	7	0.4749	1	1
Br ₂ Cu	7	0.9898	1	1
Cl ₂ Ti	7	0.259	1	1
BrCdI	7	0.4821	1	1
HgI ₂	7	0.322	1	1
Mg ₃	7	0.1127	1	1
Te ₂ Ti	7	0.0085	1	1
I ₂ Zn	7	0.4517	1	1
RhTe ₂	7	0.004	1	1
S ₂ W	7	1.5657	1	1
Bi ₂ Pd	7	0.1271	1	1
GeI ₂	7	0.4693	1	1
NbS ₂	7	0.2706	1	1
CoTe ₂	7	0.0083	1	1
S ₂ Ta	7	0.2693	1	1
Se ₂ V	7	0.2674	1	1
AsKSn	7	0.487	1	1
PbTe ₂	7	0.4796	1	1
S ₂ Sn	7	0.0031	1	1
SnTe ₂	7	0.4636	1	1
Cl ₂ V	7	1.5952	1	1
GeI ₂	7	2.9223	1	1
STl ₂	7	0.4933	1	1
PtSe ₂	7	0.0018	1	1
GeS ₂	7	0.1492	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

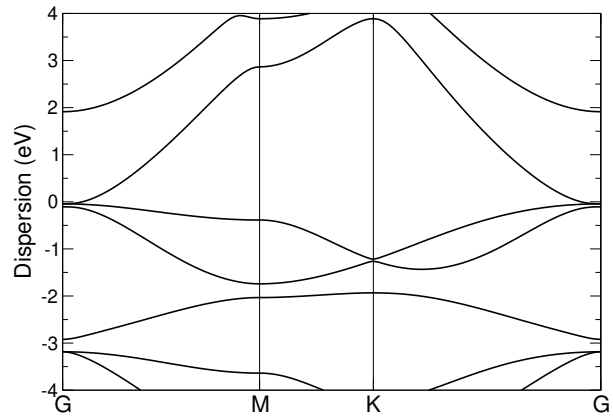
Formula	N° atoms	strain	cell size 1	cell size 2
Li ₂ P ₂ Pr	805	0.0	100	81
Hf ₂ I ₂ N ₂	10	0.0	1	1
Br ₂ HLa	656	0.0	91	73
Ga ₂ Ge ₂ Te ₂	886	0.0001	100	81
C ₂	34	0.0001	4	9
Gd ₂ I ₂	580	0.0001	81	64
Sb ₂ Te ₃	376	0.0001	49	36
Se ₂ V	624	0.0002	81	100
CS ₂ Ta ₂	661	0.0002	64	81
Cu ₂ I ₂	580	0.0002	81	64
Br ₂ Gd ₂ Ge	644	0.0002	81	64
Cl ₂ Ti	499	0.0003	64	81
I ₂ O ₂ Sm ₂	548	0.0003	65	48
Gd ₂ I ₂ S ₂	820	0.0003	115	60
In ₂ Te ₃	501	0.0003	64	49
Ge ₂ I ₂ La ₂	294	0.0003	36	25
Bi ₂ Se ₃	644	0.0004	81	64
CeLi ₂ P ₂	729	0.0004	91	73
PbTe	314	0.0004	57	43
Sb ₂ SeTe ₂	501	0.0004	64	49
Cl ₂ V	343	0.0004	43	57
As ₂ CeLi ₂	443	0.0004	57	43
P ₂	418	0.0004	64	81
BrCdI	463	0.0004	73	57
Br ₂ La	516	0.0004	81	64
Ba ₂ Pt	148	0.0004	25	16
Cu ₄ Te ₂	412	0.0004	49	36
Bi ₂ STe ₂	443	0.0005	57	43
SSb ₂ Te ₂	577	0.0005	73	57
AsCuLi ₂	656	0.0005	91	73
MoSe ₂	565	0.0005	73	91
Se ₂ Sn ₂	620	0.0005	95	60
Eu ₂ H ₂ I ₂	548	0.0006	65	48
TaTe ₂	7	0.0006	1	1
Sb ₂	562	0.0006	100	81
LiO	324	0.0006	49	64
GeI ₂	357	0.0006	57	43
I ₂ Pr ₂ Si ₂	802	0.0007	91	73
Se ₂ W	565	0.0007	73	91
Ag ₂	132	0.0007	25	16
FHOZn	400	0.0007	43	57
Bi ₂ Se ₂ Te	501	0.0007	64	49
Ga ₂ Te ₂	656	0.0007	91	73
HN ₃ OZn	742	0.0007	64	81
I ₂ Mg	516	0.0008	81	64
Ba ₂ Ni ₃	729	0.0008	91	73
Eu ₂ I ₂ O ₂	548	0.0008	65	48
Al ₂ Cl ₂ O ₂	486	0.0008	48	49
STl ₂	403	0.0008	64	49
Br ₂ La ₂	724	0.0008	100	81

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CdOHCl (P3m1)

Structural and electronic properties





	Formula	CdOHCl
	Spacegroup	P3m1
	Prototype	CdClHO
	Parent 3D	Cd ₂ Cl ₂ H ₂ O ₂
	Source DB	MPDS
	DB ID	S1503863
DF2-C09	Binding energy [meV/ Å²]	120.43
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

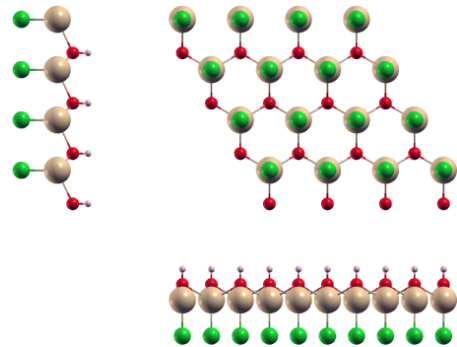


Band structure: Electronic band structure of CdOHCl (P3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CdOHCl (P3m1) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		-1.86156617	-3.22432720	0.00000000
a₂		3.72313235	-0.00000000	0.00000000
a₃		0.00000000	0.00000000	19.79320306
		x [Å]	y [Å]	z [Å]
	Cd	1.86156617	-1.07477573	0.16564226
	H	0.00000000	0.00000000	-1.80426114
	Cl	1.86156617	-1.07477573	2.47006324
	O	0.00000000	0.00000000	-0.83144436



Orthographic projections: views of CdOHCl (P3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	5	0.1138	1	1
Tl	5	0.2616	1	1
HgO	6	0.1195	1	1
LiO	6	1.5902	1	1
P ₂	6	0.2544	1	1
PbTe	6	0.4972	1	1
Mg ₂	6	0.4253	1	1
Sb ₂	6	0.4519	1	1
I ₂ Mg	7	0.4659	1	1
Cl ₂ Mn	7	0.2698	1	1
AgTe ₂	7	0.115	1	1
PSn ₂	7	0.0058	1	1
MoSe ₂	7	0.2606	1	1
S ₂ Ta	7	0.2729	1	1
Br ₂ Zn	7	0.0049	1	1
AsSn ₂	7	0.002	1	1
SiTe ₂	7	0.0091	1	1
S ₂ Zr	7	0.0065	1	1
Br ₂ La	7	0.4668	1	1
Cl ₂ Ti	7	0.2546	1	1
BrCdI	7	0.4739	1	1
HgI ₂	7	0.3154	1	1
Mg ₃	7	0.1116	1	1
Te ₂ Ti	7	0.0052	1	1
NbS ₂	7	0.2722	1	1
BaF ₂	7	0.4824	1	1
BiBrTe	7	2.9773	1	1
RhTe ₂	7	0.0008	1	1
Bi ₂ Pd	7	0.125	1	1
GeI ₂	7	0.4613	1	1
NbS ₂	7	0.2659	1	1
S ₂ Ta	7	0.2647	1	1
Se ₂ V	7	0.2628	1	1
AsKSn	7	0.4787	1	1
PbTe ₂	7	0.4714	1	1
I ₂ Nd	7	0.2064	1	1
NiTe ₂	7	0.0085	1	1
Cl ₂ Cu	7	2.945	1	1
S ₂ Sn	7	0.0062	1	1
SnTe ₂	7	0.4557	1	1
GeI ₂	7	0.4978	1	1
Se ₂ Zr	7	0.0095	1	1
STl ₂	7	0.4849	1	1
PtSe ₂	7	0.0014	1	1
GeS ₂	7	0.1462	1	1
TaTe ₂	7	0.0026	1	1
NbTe ₂	7	0.0067	1	1
Se ₂ Yb	7	0.4619	1	1
BiTe ₂	7	0.4625	1	1
F ₂ Na	7	0.0069	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

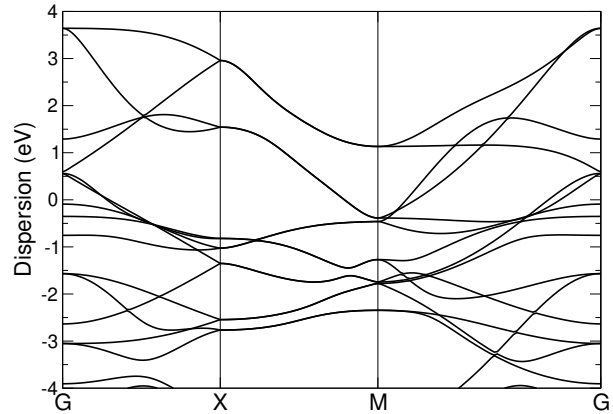
Formula	N° atoms	strain	cell size 1	cell size 2
LiOS ₂ Ti	824	0.0	81	100
Bi ₂ Se ₃	729	0.0	91	73
ReS ₂	208	0.0	25	36
Br ₂ La	583	0.0	91	73
GeI ₂	643	0.0	100	81
Br ₂ Ca	357	0.0001	57	43
C ₂ F ₂	596	0.0001	49	100
Ba ₂ Ni ₃	805	0.0002	100	81
Bi ₂ STe ₂	501	0.0002	64	49
Ga ₂ Te ₂	724	0.0002	100	81
Gd ₂ I ₂	656	0.0003	91	73
I ₂ Pr ₂ Si ₂	886	0.0003	100	81
S ₂ Ta	565	0.0003	73	91
Se ₂ Yb	643	0.0003	100	81
LiO	286	0.0003	43	57
BaF ₂	463	0.0003	73	57
HN ₃ OZn	666	0.0003	57	73
I ₂ Nd ₂ O ₂	548	0.0004	65	48
Sm	235	0.0004	39	79
I ₂ Mg	583	0.0004	91	73
I ₂ Yb	219	0.0004	36	25
AsCuLi ₂	724	0.0004	100	81
Cu ₂ Sr ₂	340	0.0004	49	36
MoS ₂	291	0.0005	36	49
Sb ₂ Te ₂	164	0.0005	25	16
Ga ₂ I ₂ Tb ₂	486	0.0005	57	43
I ₂ La ₂ P	376	0.0005	49	36
Cl ₂ O ₂ Ti ₂	332	0.0005	35	32
Ga ₂ I ₂ Y ₂	634	0.0005	73	57
I ₂ La ₂	580	0.0005	81	64
BiTe ₂	643	0.0005	100	81
Cu ₂ I ₂	656	0.0006	91	73
Br ₂ Gd ₂ Ge	729	0.0006	91	73
CS ₂ Ta ₂	593	0.0006	57	73
Cl ₂ F ₂ Pb ₂	548	0.0006	65	48
Ba ₂ Cu ₂	244	0.0006	36	25
AgClO ₄	276	0.0006	39	20
Ce ₂ I ₂ Si ₂	802	0.0006	91	73
S ₂ W	291	0.0006	36	49
Bi ₂ I ₂ O ₂	548	0.0006	65	48
Cu ₂ Na ₂ Se ₂	548	0.0006	65	48
Ba ₂ Hg	715	0.0006	118	81
STl ₂	463	0.0006	73	57
Cl ₂ Ti	447	0.0007	57	73
I ₂ Pr	357	0.0007	57	43
PbTe	354	0.0007	64	49
MoS ₂	291	0.0007	36	49
GeI ₂ La ₂	269	0.0007	36	25
As ₂ CeLi ₂	501	0.0007	64	49
H ₂ NiO ₂	389	0.0007	36	49

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CoAs (P4mm (99))

Structural and electronic properties

	Formula	CoAs
	Spacegroup	P4mm (99)
	Prototype	FeSe
	Parent 3D	KCo ₂ As ₂
	Source DB	ICSD
	DB ID	610072
DF2-C09	Binding energy [meV/ Å²]	90.35
RVV10	Binding energy [meV/ Å²]	86.3
	Band gap (PBE) [eV]	0.0

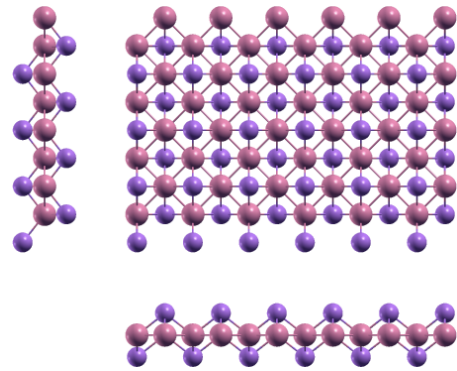


Band structure: Electronic band structure of CoAs (P4mm (99)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CoAs (P4mm (99)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.63817576	0.00000000	0.00000000
a₂		0.00000000	3.63817576	0.00000000
a₃		0.00000000	0.00000000	22.67745109
		x [Å]	y [Å]	z [Å]
●	As	0.00000000	0.00000000	12.75674724
●	Co	0.00000000	1.81908788	11.33873763
●	Co	1.81908788	3.63817576	11.33873763
●	As	1.81908788	1.81908788	9.92067967



Orthographic projections: views of CoAs (P4mm (99)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	5	0.5859	1	1
InSe	6	0.1817	1	1
HgO	6	0.2145	1	1
AsSb	6	0.1344	1	1
Bi ₂	6	0.189	1	1
GeTe	6	0.1392	1	1
AgTl	6	0.3979	1	1
S ₂	6	0.1406	1	1
PbTe	6	0.1839	1	1
Sb ₂	6	0.1631	1	1
CaCl	6	0.0049	1	1
IrTe ₂	7	0.14	1	1
I ₂ Mg	7	0.1694	1	1
CdCl ₂	7	0.1383	1	1
CdI ₂	7	0.186	1	1
AgTe ₂	7	0.5949	1	1
ReSe ₂	7	0.1088	1	1
Br ₂ Ca	7	0.1876	1	1
InSe ₂	7	0.1387	1	1
GeTe ₂	7	0.1375	1	1
SiTe ₂	7	0.1298	1	1
HfTe ₂	7	0.1474	1	1
I ₂ Mn	7	0.1384	1	1
Br ₂ La	7	0.1698	1	1
Br ₂ Cu	7	0.1268	1	1
NSr ₂	7	0.1356	1	1
PbS ₂	7	0.1324	1	1
BiClTe	7	0.1865	1	1
AuTe ₂	7	0.1549	1	1
BrCdI	7	0.1731	1	1
PdTe ₂	7	0.1525	1	1
FeI ₂	7	0.1366	1	1
I ₂ Ni	7	0.1377	1	1
Mg ₃	7	0.5685	1	1
CrI ₂	7	0.1363	1	1
I ₂ Zn	7	0.1596	1	1
BaF ₂	7	0.177	1	1
BiBrTe	7	0.1937	1	1
GeI ₂	7	0.1673	1	1
Ba ₂ Hg	7	1.1249	1	1
N ₂ W	7	0.1094	1	1
Cl ₂ Ni	7	0.109	1	1
Br ₂ V	7	0.1086	1	1
Ba ₂ N	7	0.1488	1	1
AsKSn	7	0.1753	1	1
Te ₂ Zr	7	0.1478	1	1
PbTe ₂	7	0.1719	1	1
NiTe ₂	7	0.1294	1	1
SnTe ₂	7	0.1648	1	1
I ₂ V	7	0.1308	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

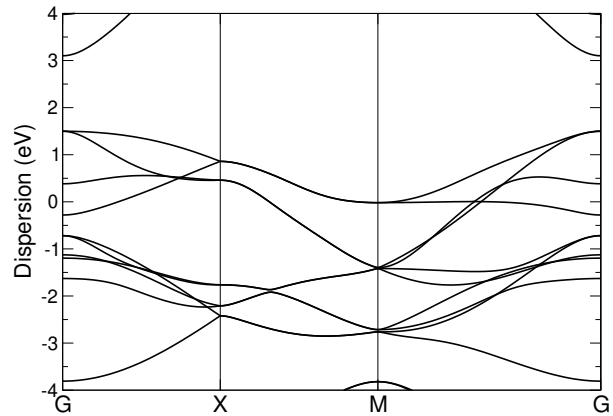
Formula	N° atoms	strain	cell size 1	cell size 2
AgTe ₂	388	0.0	49	64
Cu ₂ I ₂	580	0.0001	81	64
Cu ₂ Se ₂ Tl ₂	718	0.0002	82	65
H ₂ I ₂ Sr ₂	706	0.0003	85	61
Br ₂ H ₂ Sr ₂	708	0.0003	81	64
I ₂ La ₂ O ₂	550	0.0003	64	49
Cl ₂ Mn	387	0.0003	48	65
I ₂ Nd ₂ O ₂	896	0.0004	101	82
FeSe ₂	139	0.0004	16	25
O ₄ PSn	196	0.0004	25	16
AgClO ₄	118	0.0007	16	9
As ₂ Cd ₂ K ₂	196	0.0007	25	16
Ca ₂ Cl ₂	8	0.0007	1	1
Ge ₂ Se ₂ Zr ₂	10	0.0007	1	1
Br ₂ Ca ₃ Si	280	0.0007	40	20
Pb ₂ Se ₂	484	0.0008	72	49
S ₂ Sn ₂	872	0.0008	124	94
Cl ₂ NSc ₂	517	0.0008	48	65
Mg ₃	291	0.0008	36	49
Mg ₄	792	0.0008	85	113
Ge ₂ Te ₂	568	0.0009	83	59
I ₂ Nd ₂ O ₂	886	0.0009	100	81
HgO	424	0.001	65	82
Cu ₂ Se ₂ Tl ₂	708	0.001	81	64
CoH ₂ O ₂	946	0.001	79	126
AlH ₄ Na	736	0.0011	97	58
Ag ₂ I ₂	900	0.0011	136	89
Br ₂ Ca ₃ Si	962	0.0011	113	85
Li ₂ Tl ₂	692	0.0011	108	65
I ₂ O ₂ Pr ₂	886	0.0012	100	81
Bi ₂ In ₂	684	0.0012	106	65
Tl	453	0.0012	85	113
Cl ₂ F ₂ Pb ₂	896	0.0012	101	82
Cl ₄ Mn	569	0.0012	81	49
LiO	560	0.0012	81	118
LiOS ₂ Ti	517	0.0012	48	65
Bi ₂ I ₂ O ₂	896	0.0013	101	82
Au ₂ I ₂	236	0.0013	35	24
Ba ₂ Cd	707	0.0013	113	85
Cu ₂ Na ₂ Se ₂	896	0.0013	101	82
N ₃ Na	420	0.0013	63	42
Ba ₂ Hg	707	0.0013	113	85
Bi ₂ O ₂	588	0.0014	82	65
Co ₂ Se ₂	8	0.0014	1	1
F ₂ I ₂ Pb ₂	962	0.0014	113	85
F ₂ I ₂ Tm ₂	896	0.0014	101	82
Ga ₂ I ₂ Y ₂	946	0.0015	103	89
ReS ₂	694	0.0015	79	126
Cu ₂ Te ₂	788	0.0015	98	99
Cu ₂ Rb ₂ Te ₂	814	0.0015	106	65

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CoS (P4/nmm (129))

Structural and electronic properties

	Formula	CoS
	Spacegroup	P4/nmm (129)
	Prototype	FeSe
	Parent 3D	Co ₂ TlS ₂
	Source DB	COD
	DB ID	1524706
DF2-C09	Binding energy [meV/ Å²]	51.0
RVV10	Binding energy [meV/ Å²]	51.83
	Band gap (PBE) [eV]	0.0

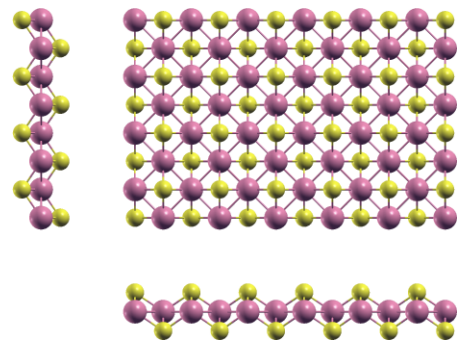


Band structure: Electronic band structure of CoS (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CoS (P4/nmm (129)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.60500358	0.00000000	0.00000000
a₂		0.00000000	3.60500358	0.00000000
a₃		0.00000000	0.00000000	22.48514586
		x [Å]	y [Å]	z [Å]
●	S	0.00000000	0.00000000	10.01635236
●	Co	1.80250179	0.00000000	11.24257293
●	Co	0.00000000	1.80250179	11.24257293
●	S	1.80250179	1.80250179	12.46879351



Orthographic projections: views of CoS (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	5	0.2062	1	1
InSe	6	0.1871	1	1
HgO	6	0.2195	1	1
AsSb	6	0.1378	1	1
Bi ₂	6	0.1947	1	1
GeTe	6	0.1429	1	1
AgTl	6	0.4076	1	1
S ₂	6	0.1443	1	1
PbTe	6	0.1894	1	1
Sb ₂	6	0.1679	1	1
CaCl	6	0.0007	1	1
IrTe ₂	7	0.1437	1	1
I ₂ Mg	7	0.1744	1	1
CdCl ₂	7	0.142	1	1
CdI ₂	7	0.1916	1	1
AgTe ₂	7	0.2093	1	1
Br ₂ Zn	7	0.13	1	1
Br ₂ Ca	7	0.1932	1	1
InSe ₂	7	0.1423	1	1
GeTe ₂	7	0.1411	1	1
SiTe ₂	7	0.133	1	1
HfTe ₂	7	0.1515	1	1
I ₂ Mn	7	0.1421	1	1
Br ₂ La	7	0.1748	1	1
Br ₂ Cu	7	0.1305	1	1
NSr ₂	7	0.1391	1	1
PbS ₂	7	0.1357	1	1
BiClTe	7	0.1921	1	1
AuTe ₂	7	0.1593	1	1
BrCdI	7	0.1782	1	1
LiO ₂	7	0.3479	1	1
PdTe ₂	7	0.1568	1	1
FeI ₂	7	0.1402	1	1
I ₂ Ni	7	0.1413	1	1
S ₂ Ti	7	0.1084	1	1
Te ₂ Ti	7	0.1302	1	1
CrI ₂	7	0.1398	1	1
I ₂ Zn	7	0.1643	1	1
BaF ₂	7	0.1823	1	1
GeI ₂	7	0.1723	1	1
Ba ₂ N	7	0.153	1	1
AsKSn	7	0.1805	1	1
Te ₂ Zr	7	0.152	1	1
PbTe ₂	7	0.177	1	1
NiTe ₂	7	0.1326	1	1
SnTe ₂	7	0.1697	1	1
I ₂ V	7	0.134	1	1
GeI ₂	7	0.1897	1	1
Se ₂ Zr	7	0.1333	1	1
STl ₂	7	0.1835	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

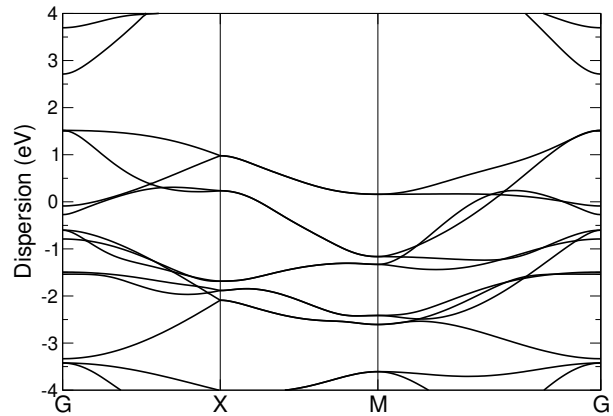
Formula	N° atoms	strain	cell size 1	cell size 2
Bi ₂ In ₂	520	0.0	81	49
Ba ₂ Cd	304	0.0	49	36
I ₂ O ₂ Sm ₂	886	0.0001	100	81
Br ₂ F ₂ Sr ₂	560	0.0001	65	50
Mg ₄	460	0.0001	50	65
AgTe ₂	887	0.0001	113	145
I ₃ Sn	356	0.0002	64	25
F ₂ I ₂ Pb ₂	412	0.0002	49	36
Tl	265	0.0002	50	65
HgO	524	0.0002	81	100
Sn ₂ Te ₂	884	0.0003	136	85
Mg ₂	414	0.0003	61	85
Mg ₆	742	0.0003	64	81
Eu ₂ I ₂ O ₂	896	0.0003	101	82
Se ₂ V	387	0.0003	48	65
Br ₂ F ₂ Pb ₂	560	0.0004	65	50
I ₂ O ₂ Pr ₂	718	0.0004	82	65
Cu ₂ Rb ₂ Te ₂	618	0.0004	81	49
I ₂ O ₂ Pr ₂	708	0.0004	81	64
Mg ₃	679	0.0004	85	113
Au ₂ Br ₂	576	0.0004	84	60
Eu ₂ H ₂ I ₂	886	0.0004	100	81
I ₂ La ₂ O ₂	962	0.0005	113	85
FeSe ₂	764	0.0005	89	136
F ₄ Nb	501	0.0005	64	49
CaCl	6	0.0007	1	1
FHOZn	796	0.0007	81	118
F ₂ I ₂ Sm ₂	708	0.0007	81	64
MnSe ₂	7	0.0007	1	1
Ce ₂ I ₂ S ₂	958	0.0008	118	81
Ca ₂ Si	715	0.0008	118	81
Ba ₂ H ₂ I ₂	814	0.0008	106	65
CrSe ₂	678	0.0008	81	118
F ₂ I ₂ Yb ₂	886	0.0008	100	81
K ₂ Mn ₂ Sb ₂	896	0.0008	101	82
Br ₂ Ce ₂ O ₂	896	0.0008	101	82
Eu ₂ I ₂ O ₂	886	0.0009	100	81
O ₂ Pb ₂	580	0.0009	81	64
K	169	0.0009	36	25
Cl ₂ V	678	0.001	81	118
Mg ₄	452	0.001	49	64
Br ₂ Ga ₂ Te ₂	286	0.0011	40	21
S ₂ Ta	387	0.0011	48	65
H ₂ Li ₂ Pt	489	0.0011	46	61
Ba ₂ Ge ₂ Mn ₂	886	0.0011	100	81
Tl	257	0.0011	48	65
Br ₂ CsF	684	0.0011	106	65
CrS ₂	694	0.0012	79	126
Br ₂ F ₂ Sr ₂	550	0.0012	64	49
As ₂ Mg ₂ Na ₂	294	0.0012	36	25

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CoSe (P4/nmm (129))

Structural and electronic properties

	Formula	CoSe
	Spacegroup	P4/nmm (129)
	Prototype	FeSe
	Parent 3D	Co ₂ TlSe ₂
	Source DB	COD
	DB ID	1531163
DF2-C09	Binding energy [meV/ Å²]	46.9
RVV10	Binding energy [meV/ Å²]	49.38
	Band gap (PBE) [eV]	0.0

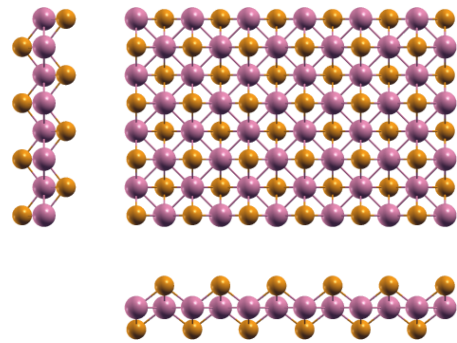


Band structure: Electronic band structure of CoSe (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CoSe (P4/nmm (129)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.64876326	0.00000000	0.00000000
a₂		0.00000000	3.64876326	0.00000000
a₃		0.00000000	0.00000000	22.89992937
		x [Å]	y [Å]	z [Å]
●	Se	3.64876326	0.00000000	12.87235869
●	Co	0.00000000	1.82438163	11.44996468
●	Co	1.82438163	3.64876326	11.44996468
●	Se	1.82438163	1.82438163	10.02757068



Orthographic projections: views of CoSe (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	5	0.5818	1	1
InSe	6	0.18	1	1
HgO	6	0.213	1	1
AsSb	6	0.1333	1	1
Bi ₂	6	0.1872	1	1
GeTe	6	0.1381	1	1
AgTl	6	0.3949	1	1
S ₂	6	0.1394	1	1
PbTe	6	0.1822	1	1
Sb ₂	6	0.1616	1	1
CaCl	6	0.0063	1	1
IrTe ₂	7	0.1388	1	1
I ₂ Mg	7	0.1679	1	1
CdCl ₂	7	0.1372	1	1
CdI ₂	7	0.1843	1	1
AgTe ₂	7	0.5908	1	1
ReSe ₂	7	0.1085	1	1
Br ₂ Ca	7	0.1859	1	1
InSe ₂	7	0.1375	1	1
GeTe ₂	7	0.1364	1	1
HfTe ₂	7	0.1461	1	1
I ₂ Mn	7	0.1373	1	1
Br ₂ La	7	0.1683	1	1
Br ₂ Cu	7	0.1257	1	1
NSr ₂	7	0.1346	1	1
PbS ₂	7	0.1314	1	1
BiClTe	7	0.1848	1	1
AuTe ₂	7	0.1535	1	1
BrCdI	7	0.1715	1	1
Cl ₂ Zn	7	0.0082	1	1
PdTe ₂	7	0.1511	1	1
FeI ₂	7	0.1356	1	1
I ₂ Ni	7	0.1366	1	1
Mg ₃	7	0.5645	1	1
CrI ₂	7	0.1352	1	1
I ₂ Zn	7	0.1582	1	1
BaF ₂	7	0.1753	1	1
BiBrTe	7	0.1919	1	1
GeI ₂	7	0.1658	1	1
Ba ₂ Hg	7	1.1175	1	1
N ₂ W	7	0.1097	1	1
Cl ₂ Ni	7	0.1087	1	1
Ba ₂ N	7	0.1475	1	1
AsKSn	7	0.1736	1	1
Te ₂ Zr	7	0.1466	1	1
PbTe ₂	7	0.1703	1	1
AsSe ₂	7	0.1091	1	1
SnTe ₂	7	0.1633	1	1
I ₂ V	7	0.1298	1	1
GeI ₂	7	0.1824	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

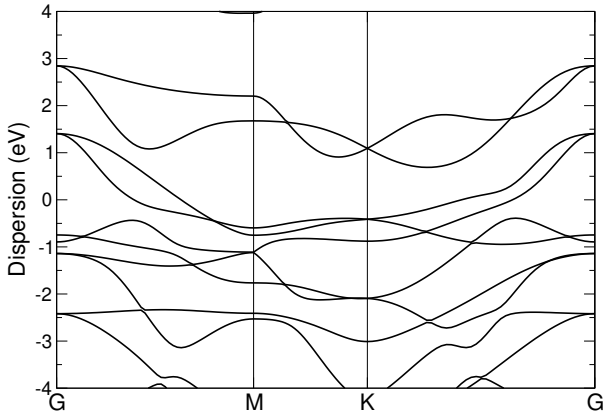
Formula	N° atoms	strain	cell size 1	cell size 2
F ₂ I ₂ Pb ₂	962	0.0	113	85
I ₂ La ₂ O ₂	560	0.0001	65	50
Ba ₂ Cd	707	0.0001	113	85
Cl ₄ Mn	569	0.0001	81	49
Tl	453	0.0002	85	113
I ₂ O ₂ Pr ₂	886	0.0002	100	81
Br ₂ F ₂ Pb ₂	708	0.0003	81	64
Br ₂ H ₂ Sr ₂	718	0.0003	82	65
AlH ₄ Na	736	0.0003	97	58
Sn	492	0.0003	89	136
Li ₂ Tl ₂	692	0.0003	108	65
Mg ₆	590	0.0003	50	65
HgO	418	0.0004	64	81
Br ₂ F ₂ Sr ₂	708	0.0005	81	64
Mg ₄	792	0.0005	85	113
Mg ₃	291	0.0005	36	49
NbS ₂	387	0.0006	48	65
Hf ₂ Si ₂ Te ₂	10	0.0006	1	1
Cl ₂ NSc ₂	517	0.0006	48	65
Cu ₂ K ₂ Te ₂	196	0.0007	25	16
F ₄ Sn	501	0.0007	64	49
Cl ₄ KTl	474	0.0007	81	25
Cu ₂ I ₂	588	0.0007	82	65
Ge ₂ Te ₂	568	0.0008	83	59
As ₂ Mg ₂ Na ₂	706	0.0008	85	61
AgCuTe ₂	888	0.0009	112	110
F ₂ I ₂ Sm ₂	886	0.0009	100	81
FeSe ₂	139	0.001	16	25
Au ₂ Br ₂	340	0.001	49	36
Br ₂ Ca ₃ Si	280	0.001	40	20
S ₂ Ta	387	0.001	48	65
I ₂ La ₂ O ₂	550	0.001	64	49
Br ₂ H ₂ Sr ₂	708	0.0011	81	64
O ₂ Pb ₂	724	0.0011	100	81
Cl ₂ Mn	387	0.0011	48	65
ReS ₂	694	0.0011	79	126
LiNbS ₂	452	0.0011	48	65
Ag ₂ F ₄	626	0.0011	95	41
K	401	0.0012	85	61
O ₄ PSn	196	0.0012	25	16
Cr ₂ O ₄	46	0.0013	4	5
Cu ₄ Te ₂	718	0.0013	79	67
As ₂ Co ₂	8	0.0014	1	1
AgTe ₂	388	0.0014	49	64
CKN	329	0.0014	56	35
NS ₂ Ta	692	0.0014	64	109
STl ₂	679	0.0014	103	89
Mg ₆	580	0.0014	49	64
Cu ₂ I ₂	580	0.0015	81	64
Ba ₂ Hg	403	0.0015	64	49

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CoTe₂ (P-3m1 (164))

Structural and electronic properties

	Formula	CoTe ₂
	Spacegroup	P-3m1 (164)
	Prototype	CdI ₂
	Parent 3D	CoTe ₂
	Source DB	ICSD
	DB ID	625401
DF2-C09	Binding energy [meV/ Å²]	51.44
RVV10	Binding energy [meV/ Å²]	50.67
	Band gap (PBE) [eV]	0.0

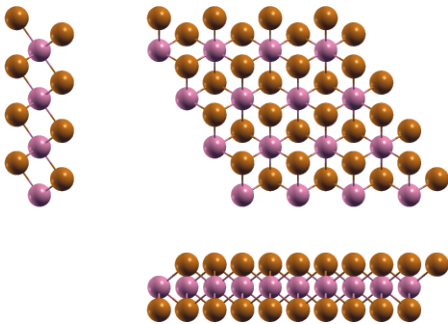


Band structure: Electronic band structure of CoTe₂ (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CoTe₂ (P-3m1 (164)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.63214496	0.00000000	0.00000000
a₂	-1.81607248	3.14552981	0.00000000
a₃	0.00000000	0.00000000	22.73658785
	x [Å]	y [Å]	z [Å]
● Te	0.00000000	2.09701987	12.84835660
● Co	0.00000000	0.00000000	11.36829392
● Te	1.81607248	1.04850994	9.88823125



Orthographic projections: views of CoTe₂ (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	4	0.1192	1	1
In	4	0.4254	1	1
In	4	1.5986	1	1
InSe	5	3.008	1	1
HgO	5	0.1264	1	1
As ₂	5	0.003	1	1
LiO	5	0.2599	1	1
P ₂	5	0.2708	1	1
PbTe	5	3.0318	1	1
Mg ₂	5	0.112	1	1
Sb ₂	5	0.4813	1	1
Cl ₂ Zn	6	0.0041	1	1
I ₂ Mg	6	0.4962	1	1
S ₂ V	6	0.25	1	1
MoS ₂	6	1.6279	1	1
MoTe ₂	6	0.0086	1	1
AgTe ₂	6	0.1208	1	1
PSn ₂	6	0.0059	1	1
HfS ₂	6	0.0003	1	1
Te ₂ V	6	0.0067	1	1
CuTe ₂	6	0.0007	1	1
S ₂ Zr	6	0.0051	1	1
Br ₂ La	6	0.4971	1	1
Br ₂ Cu	6	1.0312	1	1
NiO ₂	6	4.8724	1	1
Ca ₂ Si	6	13.6126	1	1
Br ₂ Co	6	0.0035	1	1
ReS ₂	6	1.5351	1	1
Ca ₂ N	6	0.0025	1	1
Cl ₂ Ti	6	0.271	1	1
AuTe ₂	6	0.4613	1	1
PdTe ₂	6	0.4552	1	1
Mg ₃	6	0.1163	1	1
I ₂ Zn	6	0.4729	1	1
Te ₂ Zn	6	0.0087	1	1
S ₂ W	6	1.6284	1	1
Bi ₂ Pd	6	0.1331	1	1
GeI ₂	6	2.8492	1	1
N ₂ W	6	1.4463	1	1
Br ₂ Mn	6	0.0052	1	1
CdClO	6	0.0072	1	1
Te ₂ W	6	0.0084	1	1
S ₂ Sn	6	0.0054	1	1
SnTe ₂	6	0.4853	1	1
Cl ₂ V	6	0.2565	1	1
GeI ₂	6	3.035	1	1
STl ₂	6	2.9696	1	1
OTl ₂	6	0.007	1	1
Br ₂ Fe	6	0.0034	1	1
TaTe ₂	6	0.0092	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

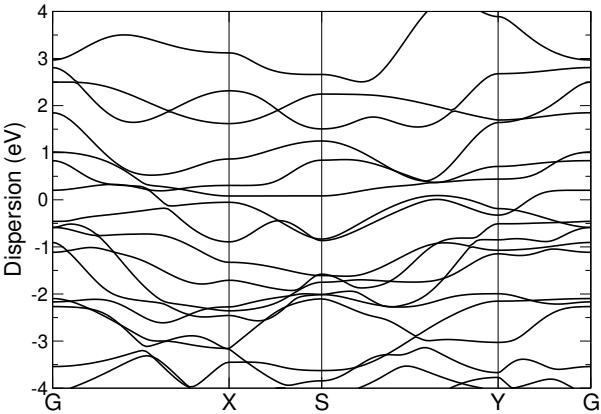
Formula	N° atoms	strain	cell size 1	cell size 2
Cl ₂ La ₂	565	0.0	91	73
AuTe ₂	543	0.0	100	81
GeI ₂ Y ₂	327	0.0001	49	36
FeH ₂ O ₂	255	0.0001	25	36
Ce ₂ I ₂ Si ₂	486	0.0001	64	49
BrCdI	300	0.0001	57	43
Ga ₂ Ge ₂ Te ₂	561	0.0001	73	57
Br ₂ Ca ₃ Si	171	0.0001	25	16
SSb ₂ Te ₂	386	0.0001	57	43
NiO ₂	390	0.0001	49	81
Ga ₂ S ₂	7	0.0001	1	1
Ca ₂ Si	390	0.0001	81	49
Ce ₂ I ₂ S ₂	537	0.0001	81	49
As ₂ Li ₂ Nd	327	0.0002	49	36
Li ₂ P ₂ Pr	504	0.0002	73	57
Br ₂ O ₂ V ₂	558	0.0002	66	60
Bi ₂ Br ₂ O ₂	483	0.0002	65	48
GdI ₂	183	0.0002	36	25
F ₂ Lu ₂ Se ₂	627	0.0003	81	64
Gd ₂ I ₂ S ₂	171	0.0003	25	16
Sb ₂ Se ₂ Te	437	0.0003	64	49
I ₂ Mg	339	0.0003	64	49
HfS ₂	6	0.0003	1	1
H ₂ MgO ₂	467	0.0003	49	64
PtTe ₂	543	0.0003	100	81
Gd	253	0.0003	52	97
FHOZn	463	0.0004	57	73
LiO	354	0.0005	64	81
MnNaTe ₂	343	0.0005	57	43
CrSe ₂	390	0.0005	57	73
AlH ₄ Na	237	0.0005	39	20
Au ₂ K ₂ S ₂	390	0.0005	90	20
Bi ₂ Se ₂ Te	327	0.0005	49	36
Sb ₂ Te ₂	331	0.0005	61	37
Cl ₂ OV	496	0.0005	72	70
S ₂ V	339	0.0005	49	64
Er ₂ I ₂ O ₂	483	0.0006	65	48
AgNO ₃	432	0.0006	79	39
Br ₂ Eu ₂ F ₂	483	0.0006	65	48
Br ₂ Er ₂	624	0.0006	100	81
Br ₂ La	339	0.0006	64	49
CoO ₂	390	0.0007	49	81
CuTe ₂	6	0.0007	1	1
O ₂ Pt	300	0.0007	43	57
Bi ₂ Se ₃	437	0.0007	64	49
Sb ₂ Se ₂ Te	437	0.0007	64	49
Al ₂ Cl ₂ O ₂	435	0.0007	49	48
Cl ₂ V	390	0.0007	57	73
Sb ₂	333	0.0007	73	57
NiO ₂	294	0.0008	37	61

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CrAuTe₄ (Pm (6))

Structural and electronic properties

	Formula	CrAuTe ₄
	Spacegroup	Pm (6)
	Prototype	ZrTiTe ₄
	Parent 3D	CrAuTe ₄
	Source DB	ICSD
	DB ID	150279
DF2-C09	Binding energy [meV/ Å²]	46.05
RVV10	Binding energy [meV/ Å²]	48.44
	Band gap (PBE) [eV]	0.0

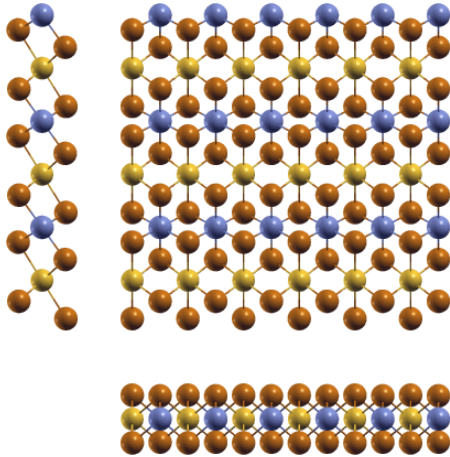


Band structure: Electronic band structure of CrAuTe₄ (Pm (6)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CrAuTe₄ (Pm (6)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.70150785	0.00000000	0.00000000
a₂		0.00000000	7.04897575	0.00000000
a₃		0.00000000	0.00000000	23.18197542
		x [Å]	y [Å]	z [Å]
●	Te	1.85075393	4.59696914	10.05200541
●	Te	0.00000000	0.66981502	10.00375355
●	Cr	1.85075393	6.73444447	11.59101914
●	Te	1.85075393	1.82303291	13.12991756
●	Te	0.00000000	5.75013678	13.17827061
●	Au	0.00000000	3.21000331	11.59096001



Orthographic projections: views of CrAuTe₄ (Pm (6)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Nd	9	0.0845	1	3
CrTe ₂	9	0.3512	1	1
Bi ₂	10	0.1944	1	2
Ag ₂	10	1.0523	1	2
Br ₂ Zr ₂	10	0.3573	1	1
Au ₂ Se ₂	10	0.6044	1	1
PbTe	10	0.1891	1	2
Cl ₂ Sc ₂	10	0.351	1	1
Sb ₂	10	0.0383	1	2
I ₂ Mg	12	0.1742	1	2
I ₂ Lu ₂ Se ₂	12	0.597	1	1
CdI ₂	12	0.1913	1	2
PSn ₂	12	0.0307	1	2
Ba ₂ Pt	12	1.051	1	2
Br ₂ Ca	12	0.1929	1	2
AsSn ₂	12	0.0284	1	2
CuTe ₂	12	0.5936	1	2
Br ₂ La	12	0.1746	1	2
BiClTe	12	0.1918	1	2
Cl ₂ Rh ₂ Te ₂	12	0.0206	1	1
AuTe ₂	12	0.0316	1	2
K ₂ O ₂ Tl ₂	12	0.5956	1	1
BrCdI	12	0.178	1	2
Cl ₂ Zn	12	0.0182	1	2
PdTe ₂	12	0.0298	1	2
I ₂ Zn	12	0.0354	1	2
BaF ₂	12	0.182	1	2
Te ₂ Zn	12	0.569	1	2
I ₄ Zr ₂	12	0.0089	1	1
RhTe ₂	12	0.0268	1	2
Bi ₂ Pd	12	0.1059	1	2
GeI ₂	12	0.1721	1	2
AsKSn	12	0.1802	1	2
PbTe ₂	12	0.1768	1	2
Cl ₂ Cu	12	0.1079	1	2
S ₂ Sn	12	0.031	1	2
SnTe ₂	12	0.0398	1	2
GeI ₂	12	0.1894	1	2
STl ₂	12	0.1832	1	2
PtSe ₂	12	0.028	1	2
AuI ₄ Li	12	0.0774	1	1
GeS ₂	12	0.017	1	2
TaTe ₂	12	0.0287	1	2
DyI ₂	12	0.9937	1	2
CuO ₂	12	0.0771	1	2
Se ₂ Yb	12	0.1723	1	2
BiTe ₂	12	0.1726	1	2
Se ₄ TiZr	12	0.0308	1	1
Mo ₂ Te ₄	12	0.6005	1	1
I ₂ Sb ₂ Te ₂	12	0.1077	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

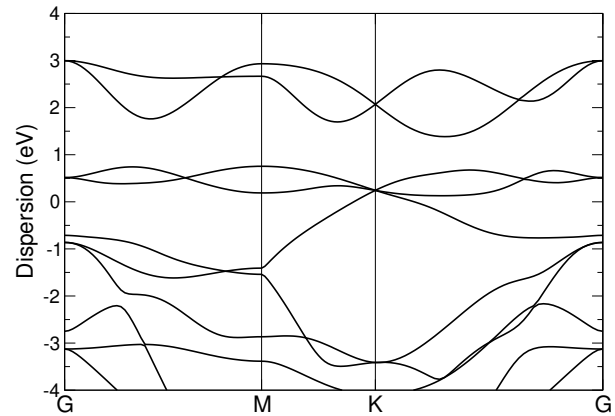
Formula	N° atoms	strain	cell size 1	cell size 2
Gd ₂ I ₂ Se ₂	348	0.0006	28	30
I ₄ Sr ₂	630	0.0009	63	42
AgNO ₂	778	0.0011	63	100
Au ₂ I ₂	596	0.0012	52	71
Er ₂ I ₂ S ₂	354	0.0012	27	32
As ₂ O ₃	912	0.0013	82	84
I ₂ Pr ₂ S ₂	576	0.0013	40	56
La ₂ S ₂	464	0.0015	40	56
CuGeO ₃	393	0.0015	28	45
Bi ₂ Te ₂	822	0.0015	73	96
I ₂ S ₂ Tm ₂	354	0.0015	27	32
Ag ₂	352	0.0016	40	56
I ₂ Se ₂ Tb ₂	348	0.0016	28	30
Br ₂ Dy ₂ S ₂	396	0.0016	30	36
As ₄	24	0.0016	2	3
Cl ₄ Pd ₂	828	0.0017	70	68
Ba ₂ Pt	408	0.0017	40	56
Cu ₂ F ₄	348	0.0018	30	28
I ₂ S ₂ Yb ₂	396	0.0019	30	36
Ga ₂ Gd ₂ I ₂	960	0.0019	61	99
Cl ₄ Cu ₂	354	0.002	35	24
Br ₂ Ga ₂ Te ₂	738	0.002	60	63
Nd	81	0.002	8	33
As ₂ O ₃	555	0.002	50	51
CKN	717	0.0021	74	91
AgCuTe ₂	286	0.0021	21	40
Ga ₂ I ₂ Tb ₂	960	0.0022	61	99
Br ₂ Er ₂ S ₂	876	0.0022	66	80
Cu ₂ Te ₂	836	0.0022	60	119
Br ₂ Ho ₂ S ₂	876	0.0022	66	80
Ag ₂ F ₄	942	0.0022	85	72
I ₂ S ₂ Tb ₂	312	0.0023	24	28
Cl ₂ O ₂ Ti ₂	504	0.0023	28	56
Br ₂ Ca ₃ Si	816	0.0023	55	81
Sb ₂ Te ₂	464	0.0023	40	56
AsI ₂ La ₂	491	0.0024	36	55
Cu ₂ Te ₂	392	0.0024	28	56
Au ₂ K ₂ Se ₂	570	0.0024	63	32
Dy ₂ I ₂ S ₂	312	0.0024	24	28
Br ₂ Ho ₂ S ₂	834	0.0024	63	76
Cl ₄ Mn	999	0.0025	84	99
F ₄ Nb	917	0.0025	67	103
AlH ₄ Na	966	0.0025	74	87
F ₂ I ₂ Pb ₂	354	0.0025	24	35
F ₂ Lu ₂ Se ₂	168	0.0025	10	18
Ho ₂ I ₂ S ₂	978	0.0025	75	88
Cl ₄ Mn	786	0.0025	66	78
In ₂ Se ₂	730	0.0025	55	100
I ₂ Nd ₂ S ₂	654	0.0025	45	64
I ₂ Zn	630	0.0025	55	100

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CrS₂ (P3m1 (156))

Structural and electronic properties

	Formula	CrS ₂
	Spacegroup	P3m1 (156)
	Prototype	CdI2
	Parent 3D	CrTlS ₂
	Source DB	COD
	DB ID	1530653
DF2-C09	Binding energy [meV/ Å²]	52.96
RVV10	Binding energy [meV/ Å²]	59.06
	Band gap (PBE) [eV]	0.0

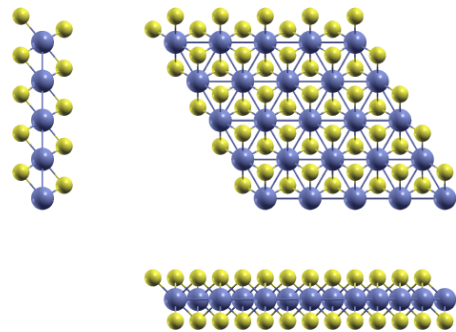


Band structure: Electronic band structure of CrS₂ (P3m1 (156)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CrS₂ (P3m1 (156)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.06329578	0.00000000	0.00000000
a₂		-1.53164789	2.65289197	0.00000000
a₃		0.00000000	0.00000000	22.80798788
		x [Å]	y [Å]	z [Å]
●	S	0.00000000	1.76859465	9.92994637
●	Cr	1.53164789	0.88429732	11.40369529
●	S	1.53164789	2.65289197	12.87746468



Orthographic projections: views of CrS₂ (P3m1 (156)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Nd	4	0.2555	1	1
Sm	4	1.5317	1	1
Cl ₂ Zn	6	3.0443	1	1
MoTe ₂	6	2.9818	1	1
ReSe ₂	6	0.4796	1	1
S ₂ Ta	6	0.4518	1	1
Te ₂ V	6	3.0075	1	1
Br ₂ Cu	6	5.0231	1	1
ReS ₂	6	0.0061	1	1
CrO ₂	6	0.2655	1	1
Cl ₂ Zn	6	0.3228	1	1
MnO ₂	6	0.2687	1	1
S ₂ Ti	6	0.4642	1	1
NbS ₂	6	0.4507	1	1
N ₂ W	6	0.0067	1	1
Br ₂ Mn	6	3.0281	1	1
Cl ₂ Ni	6	0.4819	1	1
Cl ₂ Co	6	0.4633	1	1
CrTe ₂	6	0.498	1	1
PtS ₂	6	2.9655	1	1
Br ₂ V	6	0.4775	1	1
ClN ₂ Zr	6	0.4721	1	1
Cl ₂ Fe	6	0.4615	1	1
CdClO	6	3.001	1	1
Se ₂ Ti	6	2.9307	1	1
Br ₂ Ti	6	0.4964	1	1
Te ₂ W	6	2.984	1	1
AsSe ₂	6	0.4857	1	1
OTl ₂	6	3.0035	1	1
CdO ₂	6	0.4629	1	1
BrN ₂ Zr	6	2.8392	1	1
NbSe ₂	6	0.483	1	1
O ₂ Zn	6	0.0033	1	1
Br ₂ Cr	6	0.4972	1	1
Cl ₂ Zr	6	0.4624	1	1
FeSe ₂	6	0.1501	1	1
Se ₂ Ta	6	0.4833	1	1
NbSe ₂	6	0.4864	1	1
F ₂ Ni	6	0.3146	1	1
Se ₂ Ta	6	0.4944	1	1
Cl ₂ Hf ₂	7	0.4548	1	1
Fe ₂ Se ₂	7	0.3135	1	1
Cu ₂ Te ₂	7	0.3282	1	1
Cl ₂ Zr ₂	7	0.4755	1	1
Br ₂ Zr ₂	7	2.9257	1	1
LiMnSe ₂	7	13.6157	1	1
KS ₂ Ti	7	3.0334	1	1
Cu ₂ Se ₂	7	0.3157	1	1
LiNbS ₂	7	0.452	1	1
Ho ₂ S ₂	7	1.2003	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

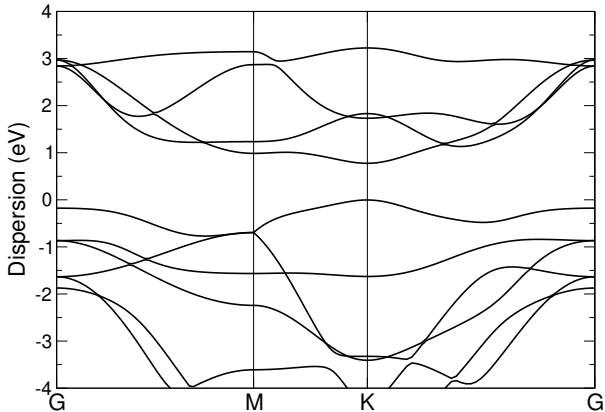
Formula	N° atoms	strain	cell size 1	cell size 2
Nd	244	0.0	57	73
Se ₂ Ta	390	0.0	73	57
NbSe ₂	390	0.0001	73	57
Br ₂ Ca	222	0.0001	49	25
Cl ₂ Fe	543	0.0001	100	81
Cl ₂ H ₂ Sc ₂	486	0.0002	64	49
PSn ₂	183	0.0002	36	25
LiMnSe ₂	439	0.0002	81	49
Cl ₂ Zr ₂	499	0.0002	81	64
I ₂ Y ₂	331	0.0002	61	37
Au ₂ K ₂ Se ₂	249	0.0002	63	10
Ga ₂ I ₂ Tb ₂	297	0.0003	49	25
Cl ₂ Tb ₂	331	0.0003	61	37
S ₂ Sn	183	0.0003	36	25
F ₂ Se ₂ Tm ₂	537	0.0003	81	49
CdClO	255	0.0003	49	36
GdI ₂	354	0.0004	79	39
As ₂ Ir ₂	197	0.0004	39	20
Se ₂ Ta	339	0.0004	64	49
Br ₂ Ti	339	0.0004	64	49
AlLiTe ₂	496	0.0004	100	49
F ₂ Lu ₂ Se ₂	102	0.0005	16	9
Br ₂ O ₂ Sc ₂	135	0.0005	21	12
Cl ₂ Ni	390	0.0005	73	57
OTl ₂	255	0.0005	49	36
Cl ₂ Zr	543	0.0005	100	81
Cl ₂ Hf ₂ N ₂	363	0.0005	49	36
CdH ₂ O ₂	327	0.0005	49	36
Ca ₂ O ₂	387	0.0005	65	48
Ga ₂ Gd ₂ I ₂	297	0.0005	49	25
S ₂ Zr	183	0.0006	36	25
Br ₂ H ₂ Zr ₂	486	0.0006	64	49
Br ₂ V	435	0.0006	81	64
CCL ₂ Sc ₂	563	0.0006	81	64
Br ₂ Cr	339	0.0007	64	49
Ca ₂ H ₂ I ₂	237	0.0007	39	20
CdO ₂	543	0.0007	100	81
Dy ₂ I ₂ S ₂	114	0.0008	22	8
NbTe ₂	183	0.0008	36	25
MnO ₂	543	0.0008	81	100
PbS ₂	123	0.0008	25	16
Te ₂ V	255	0.0008	49	36
CrO ₂	492	0.0008	73	91
Bi ₂ Pd	339	0.0008	65	48
LiMnSe ₂	331	0.0008	61	37
Br ₂ Ho ₂ S ₂	42	0.0008	8	3
Cl ₂ Co	543	0.0008	100	81
Br ₂ Zr ₂	343	0.0009	57	43
Gd	13	0.0009	3	4
I ₂ Pr	222	0.0009	49	25

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CrSe₂ (P3m1 (156))

Structural and electronic properties

	Formula	CrSe ₂
	Spacegroup	P3m1 (156)
	Prototype	MoS2
	Parent 3D	CrTlSe ₂
	Source DB	ICSD
	DB ID	626736
DF2-C09	Binding energy [meV/ Å²]	N/A
RVV10	Binding energy [meV/ Å²]	43.8
	Band gap (PBE) [eV]	0.78

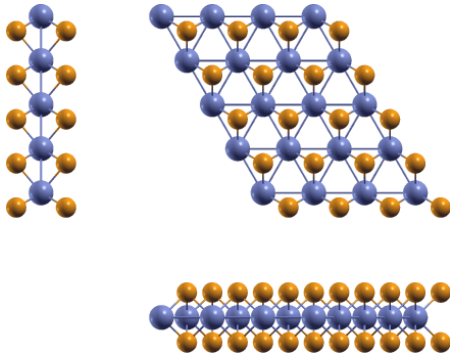


Band structure: Electronic band structure of CrSe₂ (P3m1 (156)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CrSe₂ (P3m1 (156)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.20635193	0.00000000	0.00000000
a₂	-1.60317597	2.77678223	0.00000000
a₃	0.00000000	0.00000000	23.08460666
	x [Å]	y [Å]	z [Å]
● Se	1.60317597	0.92559408	13.11186504
● Se	1.60317597	0.92559408	9.96857046
● Cr	0.00000000	1.85118815	11.54011009



Orthographic projections: views of CrSe₂ (P3m1 (156)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Sn	4	0.1369	1	1
Na	4	0.4565	1	1
In	4	0.1405	1	1
In	4	0.0067	1	1
As ₂	5	0.4765	1	1
LiO	5	0.0037	1	1
Mg ₂	5	0.1511	1	1
Cl ₂ Zn	6	0.4738	1	1
S ₂ V	6	0.0036	1	1
MoS ₂	6	0.0029	1	1
MoTe ₂	6	0.4621	1	1
PSn ₂	6	0.4999	1	1
Br ₂ Zn	6	3.0317	1	1
HfS ₂	6	0.4836	1	1
Te ₂ V	6	0.4669	1	1
I ₂ Pr	6	0.328	1	1
CuTe ₂	6	0.4826	1	1
S ₂ Zr	6	0.4978	1	1
Br ₂ Cu	6	1.365	1	1
NSr ₂	6	3.1958	1	1
NiO ₂	6	0.2534	1	1
Br ₂ Co	6	0.4754	1	1
Ca ₂ N	6	0.4779	1	1
Te ₂ Ti	6	3.0358	1	1
Te ₂ Zn	6	0.4617	1	1
RhTe ₂	6	2.9772	1	1
S ₂ W	6	0.0028	1	1
Br ₂ Mn	6	0.4708	1	1
PtS ₂	6	0.459	1	1
CoTe ₂	6	0.4844	1	1
CdClO	6	0.4657	1	1
Se ₂ Ti	6	0.4525	1	1
Te ₂ W	6	0.4625	1	1
I ₂ Nd	6	0.33	1	1
S ₂ Sn	6	0.4985	1	1
Cl ₂ V	6	0.0012	1	1
OTl ₂	6	0.4662	1	1
Br ₂ Fe	6	0.4756	1	1
Br ₂ Ni	6	2.8372	1	1
CeI ₂	6	0.3264	1	1
FeSe ₂	6	0.1318	1	1
NbTe ₂	6	0.4973	1	1
MoS ₂	6	0.0027	1	1
Cl ₂ Mg	6	2.8379	1	1
CrSe ₂	6	0.0025	1	1
O ₂ Pt	6	0.0082	1	1
N ₂ Re	6	0.2617	1	1
Se ₂ Sn	6	3.1924	1	1
F ₂ Zn	6	0.3198	1	1
CoO ₂	6	1.6378	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

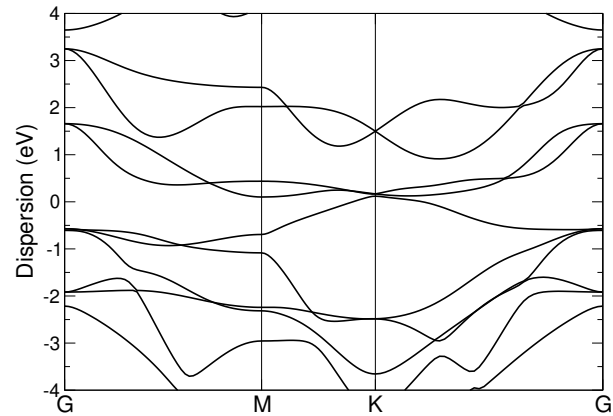
Formula	N° atoms	strain	cell size 1	cell size 2
Te ₂ V	492	0.0	91	73
CrO ₂	255	0.0	36	49
CoI ₂	183	0.0	36	25
SnTe ₂	294	0.0001	61	37
Br ₂ Cd	123	0.0001	25	16
CCl ₂ Lu ₂	563	0.0001	81	64
HfLiS ₂	624	0.0001	100	81
I ₂ La ₂ Sb	545	0.0001	100	49
FHOZn	7	0.0001	1	1
CaI ₂	222	0.0001	49	25
HfS ₂	390	0.0001	73	57
Br ₂ La ₂ P	93	0.0002	16	9
CdI ₂	75	0.0002	16	9
Br ₂ Fe	435	0.0002	81	64
Te ₂ Zn	543	0.0002	100	81
As ₂	371	0.0002	81	64
CuTe ₂	390	0.0002	73	57
Br ₂ Co	435	0.0002	81	64
Cu ₂ Rb ₂ Te ₂	714	0.0002	130	54
Br ₂ PY ₂	155	0.0002	25	16
Gd ₂ GeI ₂	93	0.0003	16	9
CdI ₂	75	0.0003	16	9
Cl ₂ Hf ₂ N ₂	711	0.0003	91	73
I ₂ Ti	183	0.0003	36	25
Pb ₂ Se ₂	822	0.0003	170	78
OTl ₂	492	0.0003	91	73
BH ₄ Li	537	0.0003	81	49
BH ₄ Li	405	0.0003	61	37
I ₂ N ₂ Zr ₂	363	0.0004	49	36
CeLi ₂ P ₂	488	0.0004	81	49
MoTe ₂	543	0.0004	100	81
C ₄ Ca ₂	738	0.0004	120	63
I ₂ N ₂ Ti ₂	750	0.0004	110	70
CoTe ₂	390	0.0005	73	57
K	349	0.0005	100	49
CdClO	492	0.0005	91	73
AsSb	158	0.0005	36	25
C ₂ Br ₂ Tb ₂	459	0.0005	67	43
BiClTe	75	0.0005	16	9
Bi ₂ In ₂	606	0.0005	130	54
CBr ₂ Lu ₂	437	0.0005	64	49
Te ₂ W	543	0.0005	100	81
C ₂ Br ₂ Gd ₂	459	0.0006	67	43
Au ₂ I ₂	398	0.0006	82	38
Br ₂ N ₂ Zr ₂	486	0.0006	64	49
I ₂ Pr	75	0.0006	16	9
Ga ₂ S ₂	447	0.0006	73	57
Ga ₂ Se ₂	291	0.0006	49	36
CaCl	516	0.0007	118	81
CaH ₂ O ₂	504	0.0007	73	57

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CrTe₂ (P-3m1 (164))

Structural and electronic properties

	Formula	CrTe ₂
	Spacegroup	P-3m1 (164)
	Prototype	CdI ₂
	Parent 3D	CrTiTe ₂
	Source DB	ICSD
	DB ID	79007
DF2-C09	Binding energy [meV/ Å²]	41.14
RVV10	Binding energy [meV/ Å²]	45.34
	Band gap (PBE) [eV]	0.0

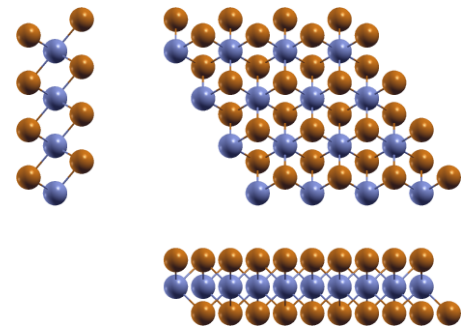


Band structure: Electronic band structure of CrTe₂ (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CrTe₂ (P-3m1 (164)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.50811365	0.00000000	0.00000000
a₂	-1.75405683	3.03811554	0.00000000
a₃	0.00000000	0.00000000	23.33511011
	x [Å]	y [Å]	z [Å]
● Cr	0.00000000	0.00000000	11.66755506
● Te	0.00000000	2.02541036	9.95985086
● Te	1.75405683	1.01270518	13.37525926



Orthographic projections: views of CrTe₂ (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	4	0.1293	1	1
Sn	4	0.1121	1	1
Na	4	0.0054	1	1
In	4	0.1138	1	1
In	4	0.2682	1	1
Gd	4	0.1126	1	1
HgO	5	0.1386	1	1
GeTe	5	0.4598	1	1
S ₂	5	0.4637	1	1
Mg ₂	5	0.1193	1	1
Sb ₂	5	3.0139	1	1
IrTe ₂	6	0.4621	1	1
CrS ₂	6	0.248	1	1
S ₂ V	6	0.2729	1	1
MoS ₂	6	0.274	1	1
CdCl ₂	6	0.4571	1	1
MoTe ₂	6	0.0078	1	1
AgTe ₂	6	0.1314	1	1
ReSe ₂	6	0.0069	1	1
InSe ₂	6	0.4581	1	1
GeTe ₂	6	0.4547	1	1
HfTe ₂	6	0.4833	1	1
I ₂ Mn	6	0.4574	1	1
NSr ₂	6	0.4489	1	1
ReS ₂	6	0.256	1	1
AuTe ₂	6	2.91	1	1
PdTe ₂	6	0.4973	1	1
FeI ₂	6	0.452	1	1
I ₂ Ni	6	0.4551	1	1
Mg ₃	6	0.1253	1	1
CrI ₂	6	0.4509	1	1
I ₂ Zn	6	2.9702	1	1
Te ₂ Zn	6	0.0076	1	1
S ₂ W	6	0.2741	1	1
Bi ₂ Pd	6	0.1469	1	1
N ₂ W	6	1.561	1	1
Cl ₂ Ni	6	0.006	1	1
PtS ₂	6	0.0065	1	1
Br ₂ V	6	0.0077	1	1
CdClO	6	0.0092	1	1
Ba ₂ N	6	0.4873	1	1
Se ₂ Ti	6	0.0038	1	1
Br ₂ Ti	6	0.0006	1	1
Te ₂ Zr	6	0.4846	1	1
Te ₂ W	6	0.0079	1	1
AsSe ₂	6	0.0046	1	1
STl ₂	6	3.1946	1	1
OTl ₂	6	0.0094	1	1
BrNZr	6	0.0033	1	1
NbSe ₂	6	0.0056	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

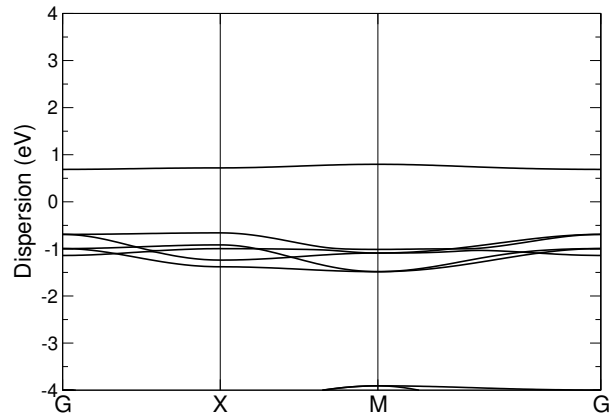
Formula	N° atoms	strain	cell size 1	cell size 2
HfTe ₂	390	0.0	73	57
S ₂ Zn ₂	565	0.0	91	73
In ₂ Se ₃	504	0.0001	73	57
Cl ₂ Sc ₂	7	0.0001	1	1
BaF ₂	183	0.0001	36	25
Ga ₂ I ₂ Y ₂	258	0.0001	36	25
Br ₂ O ₂ Yb ₂	483	0.0002	65	48
F ₂ Se ₂ Yb ₂	711	0.0002	91	73
Er ₂ F ₂ Se ₂	561	0.0002	73	57
C ₂	275	0.0002	39	79
Br ₂ Cd	339	0.0002	64	49
Br ₂ Er ₂	343	0.0002	57	43
Dy ₂ I ₂ S ₂	537	0.0002	81	49
NS ₂ Ta	304	0.0003	36	49
Br ₂ Cr	6	0.0003	1	1
P ₂ Sn ₂	565	0.0003	91	73
AuTe ₂	300	0.0003	57	43
In ₂ S ₃	705	0.0003	100	81
IrTe ₂	543	0.0004	100	81
ReS ₂	390	0.0004	57	73
Br ₂ H ₂ Zr ₂	9	0.0004	1	1
Dy ₂ I ₂ S ₂	405	0.0004	61	37
Br ₂ PY ₂	437	0.0004	64	49
Fe ₂ Te ₂	387	0.0004	65	48
DyI ₂	390	0.0005	81	49
In	343	0.0005	81	100
F ₂ Lu ₂ Se ₂	363	0.0005	49	36
BrKO ₃	17	0.0005	4	1
Te ₂ Zr	390	0.0005	73	57
Bi ₂ Te ₃	155	0.0005	25	16
AlLiTe ₂	139	0.0005	25	16
Ga ₂ Se ₂	624	0.0005	100	81
GeTe	462	0.0006	100	81
Br ₂ Ti	6	0.0006	1	1
BiTe	123	0.0006	25	16
Ce ₂ I ₂ S ₂	102	0.0006	16	9
Ca ₂ Si	75	0.0006	16	9
I ₂ O ₂ Y ₂	840	0.0006	118	81
CoH ₂ O ₂	536	0.0006	57	73
Br ₂ Nd ₂ O ₂	840	0.0006	118	81
F ₂ Se ₂ Tm ₂	627	0.0007	81	64
BN	173	0.0007	25	49
Pt ₂ Te ₂	447	0.0007	73	57
I ₄ Zr ₂	627	0.0007	115	47
PdTe ₂	339	0.0007	64	49
H ₂ MnO ₂	255	0.0007	25	36
PtTe ₂	300	0.0007	57	43
Br ₂ Gd ₂	343	0.0008	57	43
LiMnSe ₂	499	0.0008	81	64
O ₂ Zn	300	0.0008	43	57

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CsBr₂F (P4/mmm (123))

Structural and electronic properties

	Formula	CsBr ₂ F
	Spacegroup	P4/mmm (123)
	Prototype	Br2CsF
	Parent 3D	CsBr ₂ F
	Source DB	ICSD
	DB ID	84019
DF2-C09	Binding energy [meV/ Å²]	101.83
RVV10	Binding energy [meV/ Å²]	104.28
	Band gap (PBE) [eV]	1.35

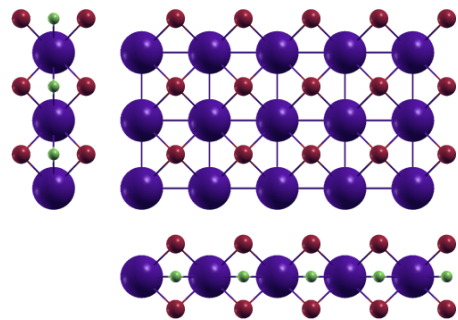


Band structure: Electronic band structure of CsBr₂F (P4/mmm (123)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CsBr₂F (P4/mmm (123)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		4.61485594	0.00000000	0.00000000
a₂		0.00000000	4.61485594	0.00000000
a₃		0.00000000	0.00000000	24.92221844
		x [Å]	y [Å]	z [Å]
●	Br	2.30742797	2.30742797	14.67277735
●	Cs	0.00000000	0.00000000	12.46110922
●	Br	2.30742797	2.30742797	10.24944109
●	F	2.30742797	2.30742797	12.46110922



Orthographic projections: views of CsBr₂F (P4/mmm (123)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
AsSb	6	0.1091	1	1
Sm	6	0.1441	1	2
Br ₂ Zn	7	0.1113	1	1
SiTe ₂	7	0.1104	1	1
Br ₂ Cu	7	0.1009	1	1
NSr ₂	7	0.1087	1	1
Te ₂ Ti	7	0.1112	1	1
CNRb	7	0.0418	1	1
CKN	7	0.0497	1	1
NiTe ₂	7	0.1105	1	1
I ₂ V	7	0.1101	1	1
Se ₂ Zr	7	0.1103	1	1
BiTe	7	0.109	1	1
CoI ₂	7	0.109	1	1
I ₂ La	7	0.5654	1	1
Se ₂ Sn	7	0.1088	1	1
HfSe ₂	7	0.1112	1	1
Li ₂ Tl ₂	8	0.1487	1	1
Bi ₂ In ₂	8	0.002	1	1
Cu ₂ I ₂	8	0.2115	1	1
Ag ₂ Br ₂	8	0.5669	1	1
S ₂ Sn ₂	8	0.2143	1	1
K	8	2.3263	1	4
AlLiTe ₂	8	0.1087	1	1
N ₃ Na	8	0.025	1	1
O ₂ Pb ₂	8	0.2079	1	1
Ga ₂ Se ₂	8	0.1097	1	1
CaClHO	8	0.1106	1	1
Au ₂ I ₂	8	0.0271	1	1
Ag ₂ Te ₂	8	0.5358	1	1
Bi ₂ O ₂	8	0.2093	1	1
PbS ₂ Sn	8	0.2239	1	1
As ₂ Rh ₂	8	0.5662	1	1
Sn ₂ Te ₂	8	0.0058	1	1
As ₂ O ₃	9	0.1865	1	1
Bi ₂ Te ₃	9	0.109	1	1
PTe ₂ Zr ₂	9	0.1092	1	1
F ₄ Nb	9	0.2156	1	1
NaO ₄	9	0.1582	1	1
AgNO ₃	9	0.159	1	1
Cl ₄ Mn	9	0.0077	1	1
Ba ₂ H ₂ I ₂	10	0.0019	1	1
Br ₂ Ho ₂ S ₂	10	0.0641	1	1
Br ₂ F ₂ Sr ₂	10	0.2137	1	1
Au ₂ K ₂ S ₂	10	2.5371	1	1
Ho ₂ I ₂ S ₂	10	0.3699	1	1
Eu ₂ F ₂ I ₂	10	0.2087	1	1
Cl ₂ F ₂ Pb ₂	10	0.5911	1	1
F ₂ I ₂ Sm ₂	10	0.2077	1	1
Ba ₂ Ge ₂ Mn ₂	10	0.5868	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

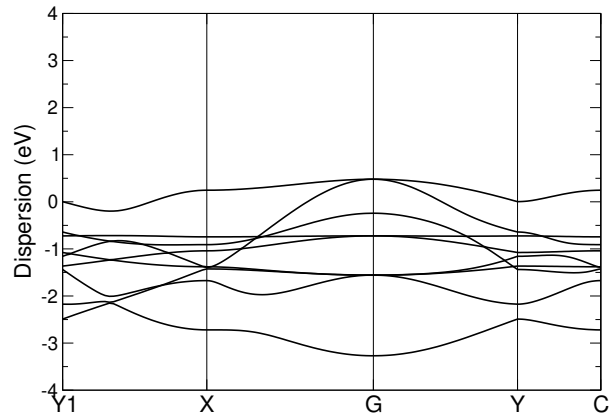
Formula	N° atoms	strain	cell size 1	cell size 2
I ₂ O ₂ Yb ₂	754	0.0	61	85
As ₂ Rh ₂	340	0.0	36	49
Br ₂ F ₂ Sr ₂	752	0.0001	65	82
Cu ₂ Te ₂	900	0.0001	89	136
Br ₂ Dy ₂ O ₂	316	0.0001	25	36
I ₃ Sn	164	0.0001	25	16
Br ₂ O ₂ Y ₂	316	0.0001	25	36
H ₂ NiO ₂	866	0.0002	54	130
As ₂ CeLi ₂	517	0.0002	48	65
Ga ₂ S ₃	275	0.0002	20	39
NS ₂ Zr	236	0.0002	20	39
PbTe	322	0.0002	48	65
Br ₂ F ₂ Pb ₂	752	0.0002	65	82
Cu ₂ S ₂	244	0.0002	25	36
I ₂ La	291	0.0002	36	49
H ₂ Li ₂ O ₂	814	0.0002	58	97
GeI ₂	387	0.0003	48	65
IKO ₃	515	0.0003	80	39
Ag ₂ Br ₂	340	0.0003	36	49
Bi ₂ Se ₂	852	0.0003	97	116
I ₂ La ₂ O ₂	934	0.0003	82	101
F ₂ Tl ₂	244	0.0003	25	36
Ir ₂ P ₂	584	0.0003	61	85
I ₂ Nd ₂ O ₂	580	0.0004	49	64
I ₂ Pr	499	0.0004	61	85
Na	119	0.0004	20	39
P ₂ Rh ₂	244	0.0004	25	36
Cl ₂ Rb ₂	296	0.0004	49	25
Br ₂ O ₂ Sm ₂	754	0.0005	61	85
LiMnTe ₂	452	0.0005	48	65
I ₂ Nd	499	0.0006	61	85
I ₂ O ₂ Pr ₂	590	0.0006	50	65
Br ₂ F ₂ Pb ₂	742	0.0006	64	81
Br ₂ Lu ₂ S ₂	486	0.0006	48	49
Li ₂ P ₂ Pr	914	0.0006	81	118
Fe ₂ S ₂	520	0.0007	49	81
Br ₂ S ₂ Yb ₂	560	0.0007	56	56
Br ₂ Lu ₂ S ₂	486	0.0007	48	49
PtS ₂	197	0.0007	20	39
H ₄ Ti	61	0.0007	4	9
Br ₂ O ₂ Pr ₂	438	0.0007	36	49
Br ₂ H ₂ Sr ₂	742	0.0008	64	81
O ₂ Sn ₂	244	0.0008	25	36
Cl ₂ Rh ₂ Te ₂	370	0.0008	40	35
Sb ₂	560	0.0008	81	118
Bi ₂ STe ₂	517	0.0008	48	65
Br ₂ F ₂ Sr ₂	742	0.0008	64	81
I ₂ La ₂ O ₂	924	0.0009	81	100
Cu ₂ Se ₂	164	0.0009	16	25
H ₂ I ₂ Yb ₂	438	0.0009	36	49

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CsBr₃ (P-6m2)

Structural and electronic properties

	Formula	CsBr ₃
	Spacegroup	P-6m2
	Prototype	Br3Cs
	Parent 3D	Br ₁₈ Cs ₆ In ₄
	Source DB	MPDS
	DB ID	S1712349
DF2-C09	Binding energy [meV/ Å²]	76.52
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

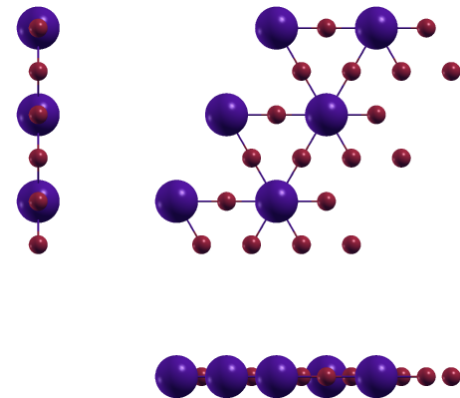


Band structure: Electronic band structure of CsBr₃ (P-6m2) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CsBr₃ (P-6m2) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.38772729	-5.86771579	0.00000000
a₂		6.77545458	0.00000000	0.00000000
a₃		0.00000000	0.00000000	12.00000000
		x [Å]	y [Å]	z [Å]
●	Cs	-0.00000000	-0.00000000	0.00000000
●	Br	-1.69367842	-2.93396483	0.00000000
●	Br	-3.38772729	0.00021388	0.00000000
●	Br	-5.08177616	-2.93396483	0.00000000



Orthographic projections: views of CsBr₃ (P-6m2) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Cl ₂ Rb ₂	8	0.151	1	1
AgNO ₂	8	0.1759	1	1
Tl	8	0.0092	1	4
Sn	8	0.04	1	4
SbSe ₂ Tl	8	0.1232	1	1
I ₃ Sn	8	0.1142	1	1
K ₂ PdS ₂	9	0.5376	1	1
IO ₃ Tl	9	0.0038	1	1
ClKO ₃	9	0.0034	1	1
K ₂ PdSe ₂	9	0.5492	1	1
Hg ₃ S ₂	9	0.461	1	1
K ₂ PtS ₂	9	0.5341	1	1
Ho ₂ I ₂ S ₂	10	0.1156	1	1
Cl ₄ Cu ₂	10	0.1341	1	1
H ₂ Na ₂ O ₂	10	0.1624	1	1
Gd ₂ I ₂ S ₂	10	0.1145	1	1
I ₂ S ₂ Tb ₂	10	0.115	1	1
I ₂ S ₂ Yb ₂	10	0.1167	1	1
Cl ₂ Ga ₂ Te ₂	10	0.1201	1	1
Ca ₄ Cu ₂	10	0.1181	1	1
Ag ₂ F ₄	10	0.1109	1	1
Dy ₂ I ₂ S ₂	10	0.1153	1	1
Br ₂ Ca ₃ Si	10	0.1126	1	1
Er ₂ I ₂ S ₂	10	0.116	1	1
I ₂ S ₂ Tm ₂	10	0.1165	1	1
HfTe ₂	11	0.1635	2	1
K	11	0.1437	2	3
CKN	11	0.1547	2	1
Ba ₂ N	11	0.1636	2	1
Te ₂ Zr	11	0.1635	2	1
NaPSn	11	0.1634	2	1
Bi ₂ Te ₂	12	0.2232	1	2
Bi ₂ In ₂	12	0.1548	2	1
Pb ₂ Se ₂	12	0.136	1	2
LiMnSe ₂	12	0.1632	2	1
Ho ₂ S ₂	12	0.1883	1	2
SbSe ₂ Tl	12	0.0424	1	2
Pt ₂ Te ₂	12	0.1634	2	1
Br ₂ CsF	12	0.1549	2	1
I ₂ Y ₂	12	0.1632	2	1
Sn ₂ Te ₂	12	0.1551	2	1
In ₂ Se ₃	13	0.1635	2	1
Bi ₂ Pd	13	0.1131	1	3
Ba ₂ H ₂ I ₂	14	0.1549	2	1
FKO ₂ Se	14	0.2894	1	2
GeNi ₃ Te ₂	14	0.1634	2	1
Cu ₂ Rb ₂ Te ₂	14	0.1548	2	1
F ₂ Se ₂ Tm ₂	14	0.1632	2	1
Cu ₃ Se ₃	14	0.1636	2	1
F ₂ Ho ₂ Se ₂	14	0.1637	2	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

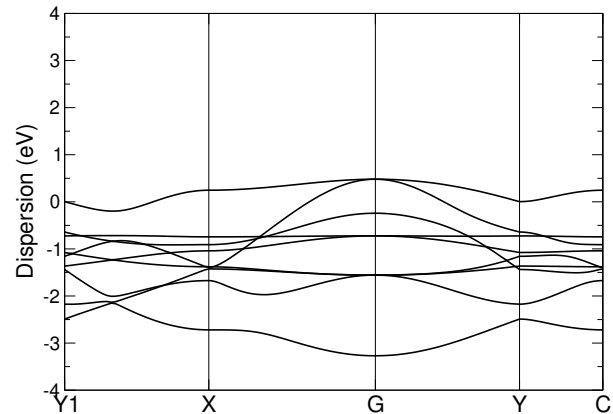
Formula	N° atoms	strain	cell size 1	cell size 2
HfSe ₂	343	0.0	25	81
Te ₂ Ti	343	0.0	25	81
In ₂ Se ₂	136	0.0001	9	25
I ₂ S ₂ Tb ₂	70	0.0002	4	9
Bi ₂ Se ₂ Te	420	0.0002	25	64
DyI ₂	43	0.0002	4	9
GeI ₂ Y ₂	420	0.0003	25	64
CNRb	414	0.0003	45	78
I ₄ Sr ₂	496	0.0003	49	50
Br ₂ Zn	343	0.0003	25	81
Cl ₂ Hf ₂	20	0.0004	1	4
CCl ₂ Gd ₂	505	0.0005	25	81
As ₂ Li ₂ Nd	420	0.0005	25	64
Br ₂ Lu ₂ S ₂	972	0.0005	63	120
F ₄ Pb	556	0.0005	39	80
FeI ₂	211	0.0005	16	49
Br ₂ Lu ₂ S ₂	972	0.0005	63	120
Sb ₂ SeTe ₂	420	0.0006	25	64
GeTe ₂	211	0.0006	16	49
Nd	41	0.0006	4	25
ClH ₃ O	551	0.0006	39	79
In ₂ Te ₃	420	0.0006	25	64
Br ₂ Mg	211	0.0007	16	49
I ₂ Ni	211	0.0008	16	49
I ₂ Lu ₂ S ₂	886	0.0008	58	109
As ₂ O ₃	189	0.0008	16	25
Te ₄ TiZr	422	0.0008	32	49
Br ₂ Pr ₂	424	0.0008	25	81
CrI ₂	211	0.0009	16	49
Dy ₂ I ₂ S ₂	70	0.0009	4	9
NS ₂ Ta	388	0.0009	16	81
Br ₂ CsF	804	0.001	70	131
CBr ₂ Y ₂	505	0.001	25	81
Ba ₂ H ₂ I ₂	642	0.001	42	79
I ₂ La ₂ Si ₂	484	0.0011	25	64
Cl ₂ La ₂	136	0.0011	9	25
As ₂ Li ₂ Pr	420	0.0011	25	64
CuO ₂	198	0.0011	12	50
InSe	228	0.0012	25	64
F ₂ Se ₂ Y ₂	394	0.0012	25	49
I ₂ Zn	111	0.0012	9	25
La ₂ S ₂	188	0.0012	15	32
Cl ₄ Mg ₂	932	0.0013	65	112
N ₂ W	307	0.0013	16	81
Ni ₂ Te ₂	260	0.0014	16	49
Br ₂ Hg ₃	56	0.0014	9	4
HgI ₂	807	0.0014	81	161
SbSe ₂ Tl	892	0.0014	80	143
SbSe ₂ Tl	780	0.0014	70	125
AsLi ₃	356	0.0015	25	64

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CsBr₃ (P-6m2)

Structural and electronic properties

	Formula	CsBr ₃
	Spacegroup	P-6m2
	Prototype	Br3Cs
	Parent 3D	Br ₁₈ Cs ₆ In ₄
	Source DB	MPDS
	DB ID	S1712349
DF2-C09	Binding energy [meV/ Å²]	76.52
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

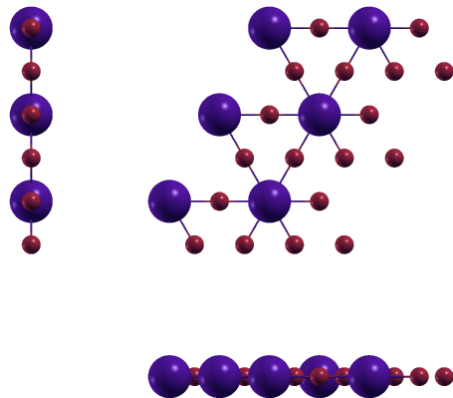


Band structure: Electronic band structure of CsBr₃ (P-6m2) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CsBr₃ (P-6m2) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.38772729	-5.86771579	0.00000000
a₂		6.77545458	0.00000000	0.00000000
a₃		0.00000000	0.00000000	12.00000000
		x [Å]	y [Å]	z [Å]
●	Cs	-0.00000000	-0.00000000	0.00000000
●	Br	-1.69367842	-2.93396483	0.00000000
●	Br	-3.38772729	0.00021388	0.00000000
●	Br	-5.08177616	-2.93396483	0.00000000



Orthographic projections: views of CsBr₃ (P-6m2) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Cl ₂ Rb ₂	8	0.151	1	1
AgNO ₂	8	0.1759	1	1
Tl	8	0.0092	1	4
Sn	8	0.04	1	4
SbSe ₂ Tl	8	0.1232	1	1
I ₃ Sn	8	0.1142	1	1
K ₂ PdS ₂	9	0.5376	1	1
IO ₃ Tl	9	0.0038	1	1
ClKO ₃	9	0.0034	1	1
K ₂ PdSe ₂	9	0.5492	1	1
Hg ₃ S ₂	9	0.461	1	1
K ₂ PtS ₂	9	0.5341	1	1
Ho ₂ I ₂ S ₂	10	0.1156	1	1
Cl ₄ Cu ₂	10	0.1341	1	1
H ₂ Na ₂ O ₂	10	0.1624	1	1
Gd ₂ I ₂ S ₂	10	0.1145	1	1
I ₂ S ₂ Tb ₂	10	0.115	1	1
I ₂ S ₂ Yb ₂	10	0.1167	1	1
Cl ₂ Ga ₂ Te ₂	10	0.1201	1	1
Ca ₄ Cu ₂	10	0.1181	1	1
Ag ₂ F ₄	10	0.1109	1	1
Dy ₂ I ₂ S ₂	10	0.1153	1	1
Br ₂ Ca ₃ Si	10	0.1126	1	1
Er ₂ I ₂ S ₂	10	0.116	1	1
I ₂ S ₂ Tm ₂	10	0.1165	1	1
HfTe ₂	11	0.1635	2	1
K	11	0.1437	2	3
CKN	11	0.1547	2	1
Ba ₂ N	11	0.1636	2	1
Te ₂ Zr	11	0.1635	2	1
NaPSn	11	0.1634	2	1
Bi ₂ Te ₂	12	0.2232	1	2
Bi ₂ In ₂	12	0.1548	2	1
Pb ₂ Se ₂	12	0.136	1	2
LiMnSe ₂	12	0.1632	2	1
Ho ₂ S ₂	12	0.1883	1	2
SbSe ₂ Tl	12	0.0424	1	2
Pt ₂ Te ₂	12	0.1634	2	1
Br ₂ CsF	12	0.1549	2	1
I ₂ Y ₂	12	0.1632	2	1
Sn ₂ Te ₂	12	0.1551	2	1
In ₂ Se ₃	13	0.1635	2	1
Bi ₂ Pd	13	0.1131	1	3
Ba ₂ H ₂ I ₂	14	0.1549	2	1
FKO ₂ Se	14	0.2894	1	2
GeNi ₃ Te ₂	14	0.1634	2	1
Cu ₂ Rb ₂ Te ₂	14	0.1548	2	1
F ₂ Se ₂ Tm ₂	14	0.1632	2	1
Cu ₃ Se ₃	14	0.1636	2	1
F ₂ Ho ₂ Se ₂	14	0.1637	2	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

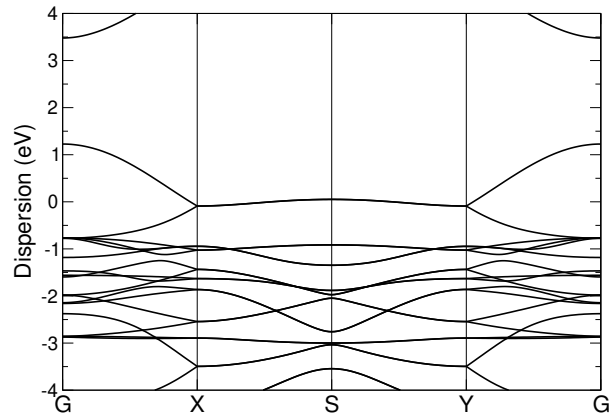
Formula	N° atoms	strain	cell size 1	cell size 2
HfSe ₂	343	0.0	25	81
Te ₂ Ti	343	0.0	25	81
In ₂ Se ₂	136	0.0001	9	25
I ₂ S ₂ Tb ₂	70	0.0002	4	9
Bi ₂ Se ₂ Te	420	0.0002	25	64
DyI ₂	43	0.0002	4	9
GeI ₂ Y ₂	420	0.0003	25	64
CNRb	414	0.0003	45	78
I ₄ Sr ₂	496	0.0003	49	50
Br ₂ Zn	343	0.0003	25	81
Cl ₂ Hf ₂	20	0.0004	1	4
CCl ₂ Gd ₂	505	0.0005	25	81
As ₂ Li ₂ Nd	420	0.0005	25	64
Br ₂ Lu ₂ S ₂	972	0.0005	63	120
F ₄ Pb	556	0.0005	39	80
FeI ₂	211	0.0005	16	49
Br ₂ Lu ₂ S ₂	972	0.0005	63	120
Sb ₂ SeTe ₂	420	0.0006	25	64
GeTe ₂	211	0.0006	16	49
Nd	41	0.0006	4	25
ClH ₃ O	551	0.0006	39	79
In ₂ Te ₃	420	0.0006	25	64
Br ₂ Mg	211	0.0007	16	49
I ₂ Ni	211	0.0008	16	49
I ₂ Lu ₂ S ₂	886	0.0008	58	109
As ₂ O ₃	189	0.0008	16	25
Te ₄ TiZr	422	0.0008	32	49
Br ₂ Pr ₂	424	0.0008	25	81
CrI ₂	211	0.0009	16	49
Dy ₂ I ₂ S ₂	70	0.0009	4	9
NS ₂ Ta	388	0.0009	16	81
Br ₂ CsF	804	0.001	70	131
CBr ₂ Y ₂	505	0.001	25	81
Ba ₂ H ₂ I ₂	642	0.001	42	79
I ₂ La ₂ Si ₂	484	0.0011	25	64
Cl ₂ La ₂	136	0.0011	9	25
As ₂ Li ₂ Pr	420	0.0011	25	64
CuO ₂	198	0.0011	12	50
InSe	228	0.0012	25	64
F ₂ Se ₂ Y ₂	394	0.0012	25	49
I ₂ Zn	111	0.0012	9	25
La ₂ S ₂	188	0.0012	15	32
Cl ₄ Mg ₂	932	0.0013	65	112
N ₂ W	307	0.0013	16	81
Ni ₂ Te ₂	260	0.0014	16	49
Br ₂ Hg ₃	56	0.0014	9	4
HgI ₂	807	0.0014	81	161
SbSe ₂ Tl	892	0.0014	80	143
SbSe ₂ Tl	780	0.0014	70	125
AsLi ₃	356	0.0015	25	64

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Cu₂Cl₄ (P2/m)

Structural and electronic properties

	Formula	Cu ₂ Cl ₄
	Spacegroup	P2/m
	Prototype	Cl ₂ Cu
	Parent 3D	Cl ₈ Cu ₂ N ₄
	Source DB	MPDS
	DB ID	S1812058
DF2-C09	Binding energy [meV/ Å²]	75.17
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

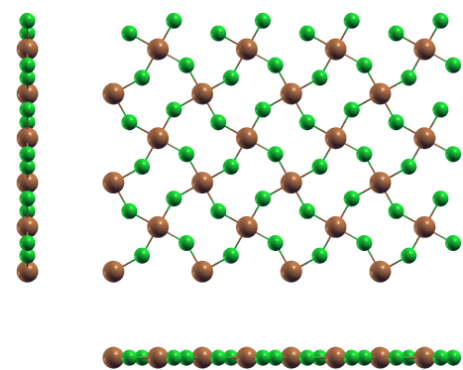


Band structure: Electronic band structure of Cu₂Cl₄ (P2/m) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Cu₂Cl₄ (P2/m) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		6.19580634	0.00000085	0.00000000
a₂		0.00000084	6.19296931	0.00000000
a₃		0.00000000	0.00000000	12.00000000
		x [Å]	y [Å]	z [Å]
●	Cu	3.09790275	-3.09648423	-6.00000000
●	Cl	1.98741767	-5.08256282	-6.00000000
●	Cl	1.11047734	-1.98607095	-6.00000000
●	Cl	4.20838782	-1.11040564	-6.00000000
●	Cu	0.00000000	0.00000000	-6.00000000
●	Cl	5.08532815	-4.20689752	-6.00000000



Orthographic projections: views of Cu₂Cl₄ (P2/m) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Na	8	0.1458	1	2
Li ₂ Tl ₂	10	0.1113	1	1
N ₃ Na	10	0.4021	1	1
Br ₃ Cs	10	0.1484	1	1
As ₂	10	0.1486	1	2
IO ₃ Tl	11	0.1449	1	1
Hg ₃ N ₂	11	0.161	1	1
ClKO ₃	11	0.1516	1	1
NaO ₄	11	0.1092	1	1
AgNO ₃	11	0.109	1	1
IKO ₃	11	0.172	1	1
BrKO ₃	11	0.1658	1	1
KNO ₃	11	0.1359	1	1
Cl ₂ Zn	12	0.1482	1	2
MoTe ₂	12	0.1465	1	2
Au ₂ K ₂ S ₂	12	1.339	1	1
Te ₂ V	12	0.1472	1	2
Br ₂ Co	12	0.1485	1	2
Ca ₂ N	12	0.1488	1	2
K ₂ O ₂ Tl ₂	12	0.1511	1	1
Br ₂ Mn	12	0.1478	1	2
Pd ₂ S ₄	12	0.211	1	1
CrTe ₂	12	0.1441	1	2
PtS ₂	12	0.1461	1	2
CNRb	12	0.297	1	2
CdClO	12	0.147	1	2
Cl ₄ Mg ₂	12	0.1469	1	1
Se ₂ Ti	12	0.1453	1	2
Br ₂ Ti	12	0.144	1	2
Te ₂ W	12	0.1466	1	2
Cl ₂ Cu	12	0.1003	1	2
S ₂	12	0.1478	1	3
OTl ₂	12	0.1471	1	2
Br ₂ Fe	12	0.1485	1	2
Br ₂ Cr	12	0.144	1	2
Br ₂ Ni	12	0.1506	1	2
Cu ₂ F ₄	12	0.5652	1	1
Ag ₂ F ₄	12	0.2035	1	1
NbTe ₂	12	0.152	1	2
Cl ₂ Mg	12	0.1506	1	2
Te ₄ W ₂	12	0.149	1	1
Se ₂ Ta	12	0.1437	1	2
NS ₂ Zr	14	0.1459	1	2
Cu ₂ O ₂	14	0.2118	1	2
Pb ₂ Se ₂	14	0.0025	1	2
AgBrO ₂	14	0.1723	1	2
Br ₂ Zr ₂	14	0.1451	1	2
KS ₂ Ti	14	0.1479	1	2
Mg ₂	14	0.0063	1	4
Cl ₂ Sc ₂	14	0.1441	1	2

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

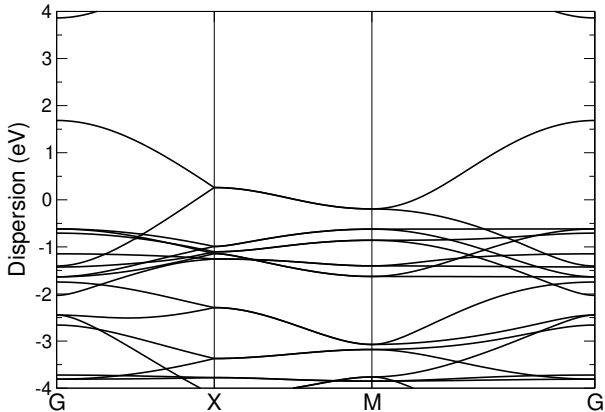
Formula	N° atoms	strain	cell size 1	cell size 2
ClH ₃ O	315	0.0001	20	39
N ₂ Re	267	0.0001	12	65
Br ₂ Ca ₂ H ₂	738	0.0001	34	89
Br ₂ Ca ₂ F ₂	534	0.0002	25	64
K	427	0.0002	53	109
Cu ₂ F ₄	510	0.0003	36	49
F ₂ Zn	342	0.0003	25	64
Br ₂ Ca	714	0.0003	54	130
Ca ₂ Mn ₂ Si ₂	738	0.0003	34	89
Ho ₂ S ₂	516	0.0004	32	81
I ₂ S ₂ Yb ₂	198	0.0005	12	21
Br ₂ Ho ₂ O ₂	738	0.0005	34	89
As ₂ Mg ₂ Na ₂	972	0.0005	53	109
Br ₂ Gd ₂ O ₂	534	0.0005	25	64
Br ₂ F ₂ Yb ₂	534	0.0006	25	64
F ₄ Nb	69	0.0006	4	9
Cl ₂ Zn	129	0.0006	9	25
Cu ₂ O ₂	516	0.0007	32	81
Br ₂ Er ₂ O ₂	738	0.0008	34	89
Br ₂ Er ₂ Se ₂	288	0.0008	18	30
Bi ₂	584	0.0008	54	130
I ₂ Pr	714	0.001	54	130
Br ₂ OV	584	0.0011	32	98
Ca ₂ Cl ₂ H ₂	204	0.0011	9	25
Bi ₂ SeTe ₂	863	0.0011	48	115
Br ₂ Cu ₂	406	0.0011	25	64
Bi ₂	518	0.0011	48	115
BiClTe	714	0.0011	54	130
Cl ₂ O ₂ V ₂	126	0.0011	5	16
Bi ₂ In ₂	118	0.0011	9	16
I ₂ Lu ₂ O ₂	534	0.0012	25	64
Br ₂ F ₂ Tm ₂	534	0.0012	25	64
Se ₂ Sn ₂	694	0.0013	49	100
Ba ₂ N	633	0.0013	44	123
Se ₂ Si ₂ Zr ₂	390	0.0013	16	49
Ca ₂ Ge ₂ Mn ₂	534	0.0014	25	64
Cu ₂ Rb ₂ Te ₂	150	0.0015	9	16
CdI ₂	714	0.0015	54	130
I ₂ S ₂ Tm ₂	198	0.0015	12	21
Te ₂ Zr	633	0.0015	44	123
Br ₂ O ₂ Tb ₂	534	0.0015	25	64
Cu ₂ Na ₂ Te ₂	894	0.0015	49	100
Hf ₃ Te ₂	179	0.0016	9	25
Cl ₂ N ₂ Zr ₂	174	0.0017	8	21
P ₂ Rh ₂	560	0.0017	34	89
CrI ₂	507	0.0017	34	101
Br ₂ Mg	507	0.0017	34	101
NSr ₂	507	0.0017	34	101
Br ₂ Ca	633	0.0017	48	115
FeI ₂	507	0.0018	34	101

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Cu₂F₄ (Pbam)

Structural and electronic properties

	Formula	Cu ₂ F ₄
	Spacegroup	Pbam
	Prototype	F2Zn
	Parent 3D	Cu ₂ F ₈ N ₄
	Source DB	ICSD
	DB ID	39721
DF2-C09	Binding energy [meV/ Å²]	76.3
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

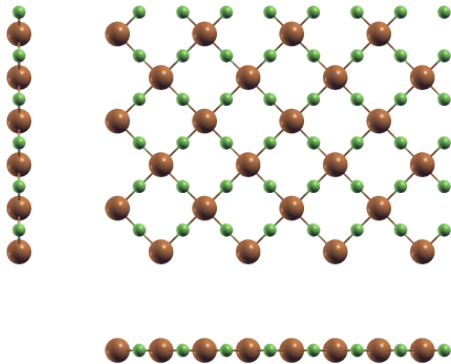


Band structure: Electronic band structure of Cu₂F₄ (Pbam) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Cu₂F₄ (Pbam) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		5.30689627	0.00000000	0.00000000
a₂		0.00000000	5.30689627	0.00000000
a₃		0.00000000	0.00000000	12.00000000
		x [Å]	y [Å]	z [Å]
●	Cu	0.00000000	-2.65344814	0.00000000
●	Cu	2.65344814	0.00000000	0.00000000
●	F	3.98239725	1.32449903	0.00000000
●	F	3.97794716	-1.32894911	0.00000000
●	F	1.32449903	-1.32449903	0.00000000
●	F	1.32894911	1.32894911	0.00000000



Orthographic projections: views of Cu₂F₄ (Pbam) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Gd	8	0.146	1	2
BiBrTe	9	0.1112	1	1
CNRb	9	0.1778	1	1
CKN	9	0.1836	1	1
BiTe	9	0.1097	1	1
GdI ₂	9	0.1105	1	1
Li ₂ Tl ₂	10	0.109	1	1
Bi ₂ In ₂	10	0.5922	1	1
Cu ₂ Sr ₂	10	0.1109	1	1
AlLiTe ₂	10	0.11	1	1
Br ₂ CsF	10	0.5861	1	1
Sn ₂ Te ₂	10	0.5737	1	1
Bi ₂ Te ₃	11	0.1097	1	1
I ₂ La ₂ P	11	0.1107	1	1
Cd ₂ I ₃	11	0.1091	1	1
Cl ₄ Mn	11	0.2097	1	1
CrS ₂	12	0.147	1	2
Br ₂ Ho ₂ S ₂	12	0.1833	1	1
Ho ₂ I ₂ S ₂	12	0.1909	1	1
Cu ₄ Te ₂	12	0.1115	1	1
AlH ₄ Na	12	0.2126	1	1
ReS ₂	12	0.1492	1	2
Cl ₄ Cu ₂	12	1.1634	1	1
Br ₂ S ₂ Y ₂	12	0.1831	1	1
I ₂ S ₂ Tb ₂	12	0.5232	1	1
I ₂ S ₂ Yb ₂	12	0.1868	1	1
Cu ₂ Rb ₂ Te ₂	12	0.5912	1	1
Br ₂ Dy ₂ S ₂	12	0.1852	1	1
Ag ₂ K ₂ Te ₂	12	0.2188	1	1
O ₄ PSn	12	0.5655	1	1
Br ₂ S ₂ Yb ₂	12	0.4756	1	1
Br ₂ Er ₂ S ₂	12	0.1822	1	1
Na	12	0.7952	1	6
O ₄ PTl	12	0.5588	1	1
Ag ₂ F ₄	12	0.0388	1	1
Dy ₂ I ₂ S ₂	12	0.1925	1	1
As ₂ Cd ₂ K ₂	12	0.5638	1	1
Ge ₂ I ₂ La ₂	12	0.1088	1	1
Er ₂ I ₂ S ₂	12	0.1892	1	1
I ₂ S ₂ Tm ₂	12	0.1875	1	1
Bi ₂ Se ₂	14	0.3942	1	2
NS ₂ Ta	14	0.1441	1	2
ReSe ₂	15	0.1632	1	3
CuTe ₂	15	0.1903	1	3
Te ₂ Zn	15	0.1799	1	3
Cl ₂ Ni	15	0.1641	1	3
Br ₂ V	15	0.1623	1	3
ClNZr	15	0.16	1	3
NbSe ₂	15	0.1646	1	3
TaTe ₂	15	0.768	1	3

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

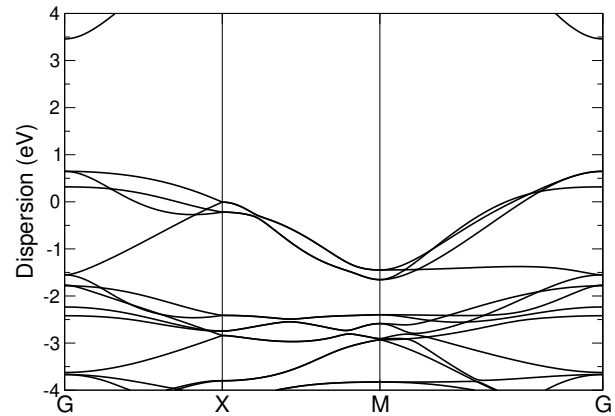
Formula	N° atoms	strain	cell size 1	cell size 2
Cu ₂ Na ₂ Te ₂	612	0.0001	41	61
AgTe ₂	129	0.0001	9	25
In	376	0.0002	41	130
AlH ₄ Na	870	0.0002	64	81
I ₂ La ₂ Si ₂	606	0.0002	36	65
Cl ₄ Cu ₂	510	0.0003	49	36
As ₂ Ir ₂	118	0.0003	9	16
S ₂ Sn	714	0.0003	54	130
PSn ₂	714	0.0003	54	130
F ₄ Nb	699	0.0003	49	81
Cl ₂ Zn	594	0.0004	49	100
O ₄ PSn	510	0.0004	36	49
Bi ₂ Se ₂	998	0.0004	81	128
Br ₂ F ₂ Pb ₂	930	0.0004	58	97
Hf ₃ Te ₂	863	0.0004	53	109
S ₂ Zr	714	0.0005	54	130
I ₂ S ₂ Yb ₂	96	0.0005	7	9
F ₂ Lu ₂ Se ₂	354	0.0006	20	39
Bi ₂ Se ₂	506	0.0006	41	65
Ca ₂ O ₂	406	0.0006	25	64
I ₂ Sb ₂ Te ₂	828	0.0006	73	65
Br ₂ F ₂ Sr ₂	930	0.0007	58	97
NbTe ₂	714	0.0007	54	130
Bi ₂ Pd	342	0.0007	25	64
Ca ₂ H ₂ I ₂	150	0.0007	9	16
GeI ₂ Y ₂	541	0.0008	36	65
As ₂ Cd ₂ K ₂	510	0.0008	36	49
Ca ₂ Cl ₂ H ₂	894	0.0009	49	100
Sn	231	0.0009	25	81
Ag ₂ I ₂	706	0.0009	61	85
Bi ₂ In ₂	550	0.0009	49	64
Br ₂ H ₂ Sr ₂	930	0.0009	58	97
I ₂ Zn	237	0.001	20	39
Br ₂ O ₂ Yb ₂	444	0.001	25	49
I ₂ N ₂ Ti ₂	108	0.0011	6	12
Ge ₂ Mn ₂ Sr ₂	150	0.0011	9	16
Ge ₂ S ₂	558	0.0012	43	75
Cu ₂ Rb ₂ Te ₂	678	0.0012	49	64
Br ₂ CsF	962	0.0012	85	113
H ₂ Li ₂ Pt	715	0.0013	35	101
PSn ₂	633	0.0013	48	115
Cl ₂ Co	633	0.0013	44	123
S ₂ Ti	633	0.0013	44	123
Br ₂ Ca ₃ Si	804	0.0013	65	69
Cl ₂ Er ₂ S ₂	42	0.0013	3	4
Cu ₂ I ₂	736	0.0013	58	97
Cl ₂ Zr	633	0.0014	44	123
Au ₂ I ₂	284	0.0014	24	35
Hf ₃ Te ₂	794	0.0014	49	100
Fe ₂ Te ₂	346	0.0014	25	49

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CuS (P4/nmm (129))

Structural and electronic properties

	Formula	CuS
	Spacegroup	P4/nmm (129)
	Prototype	FeSe
	Parent 3D	Cu ₂ TlS ₂
	Source DB	COD
	DB ID	9012392
DF2-C09	Binding energy [meV/ Å²]	93.63
RVV10	Binding energy [meV/ Å²]	93.31
	Band gap (PBE) [eV]	0.0

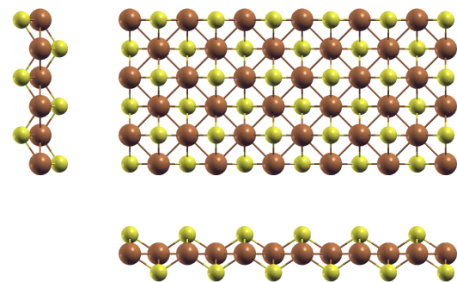


Band structure: Electronic band structure of CuS (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CuS (P4/nmm (129)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.84743924	0.00000000	0.00000000
a₂		0.00000000	3.84743924	0.00000000
a₃		0.00000000	0.00000000	22.85429126
		x [Å]	y [Å]	z [Å]
●	S	3.84743924	0.00000000	10.15811222
●	Cu	0.00000000	1.92371962	11.42714563
●	Cu	1.92371962	0.00000000	11.42714563
●	S	1.92371962	1.92371962	12.69617905



Orthographic projections: views of CuS (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.3925	1	1
K	5	0.1932	1	1
In	5	0.1105	1	1
InSe	6	0.1523	1	1
Bi ₂	6	0.1582	1	1
PbTe	6	0.1541	1	1
Sb ₂	6	0.138	1	1
I ₂ Mg	7	0.1428	1	1
S ₂ V	7	0.1098	1	1
MoS ₂	7	0.1096	1	1
CdI ₂	7	0.1558	1	1
Nd	7	0.7834	1	3
Br ₂ Ca	7	0.1571	1	1
CaI ₂	7	0.1815	1	1
I ₂ Pr	7	0.0072	1	1
Br ₂ La	7	0.1431	1	1
Br ₂ Cu	7	0.109	1	1
Ca ₂ Si	7	0.7767	1	1
I ₂ Yb	7	0.1784	1	1
BiClTe	7	0.1562	1	1
AuTe ₂	7	0.1318	1	1
BrCdI	7	0.1456	1	1
PdTe ₂	7	0.1301	1	1
HgI ₂	7	1.1559	1	1
I ₂ Zn	7	0.1353	1	1
BaF ₂	7	0.1487	1	1
BiBrTe	7	0.162	1	1
S ₂ W	7	0.1096	1	1
GeI ₂	7	0.1412	1	1
AsKSn	7	0.1473	1	1
PbTe ₂	7	0.1447	1	1
I ₂ Nd	7	0.0082	1	1
Cl ₂ Cu	7	0.1003	1	1
I ₂ Tm	7	0.18	1	1
SnTe ₂	7	0.1392	1	1
Cl ₂ V	7	0.1088	1	1
GeI ₂	7	0.1543	1	1
I ₂ Pb	7	0.7663	1	1
STl ₂	7	0.1496	1	1
BiTe	7	0.1692	1	1
DyI ₂	7	0.185	1	1
Br ₂ Ni	7	0.1085	1	1
CeI ₂	7	0.0065	1	1
Se ₂ Yb	7	0.1414	1	1
MoS ₂	7	0.1096	1	1
Cl ₂ Mg	7	0.1085	1	1
BiTe ₂	7	0.1416	1	1
GdI ₂	7	0.1651	1	1
CrSe ₂	7	0.109	1	1
PtTe ₂	7	0.1315	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

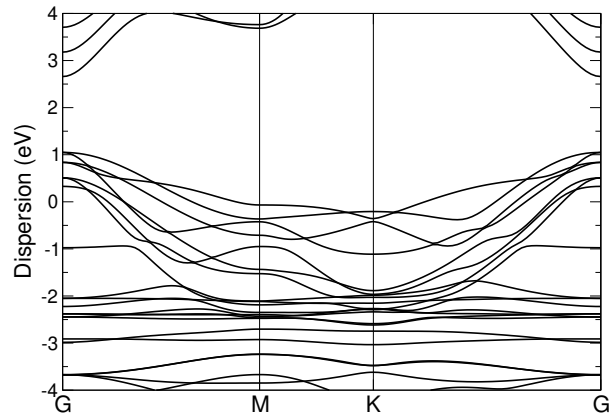
Formula	N° atoms	strain	cell size 1	cell size 2
Cl ₂ S ₂ Tl ₂	736	0.0	97	58
As ₂ Cd ₂ K ₂	706	0.0001	85	61
Br ₂ O ₂ Y ₂	10	0.0001	1	1
I ₃ Sn	52	0.0001	9	4
Br ₂ Dy ₂ O ₂	10	0.0001	1	1
Pb ₂ Se ₂	628	0.0001	89	68
Ag ₂ I ₂	340	0.0002	49	36
Br ₂ CsF	244	0.0002	36	25
NS ₂ Zr	452	0.0002	48	65
Ga ₂ S ₃	517	0.0003	48	65
Cu ₂ O ₂	396	0.0003	50	49
La ₂ S ₂	640	0.0004	89	71
K	393	0.0004	82	65
PtS ₂	387	0.0005	48	65
Ho ₂ S ₂	396	0.0005	50	49
F ₂ Tl ₂	8	0.0005	1	1
Mg ₆	316	0.0005	25	36
O ₂ Sn ₂	8	0.0006	1	1
Na	257	0.0006	48	65
P ₂ Rh ₂	8	0.0007	1	1
As ₂ Mg ₂ Na ₂	718	0.0007	82	65
P ₄	284	0.0008	36	35
O ₄ PSn	706	0.0009	85	61
H ₄ Ti	189	0.0009	16	25
In	329	0.001	58	97
CNRb	891	0.001	150	97
F ₄ Pb	501	0.0011	64	49
K	388	0.0012	81	64
HgI ₂	304	0.0012	49	36
Se ₂ Sn ₂	580	0.0012	81	64
HfLiS ₂	452	0.0012	48	65
Sn	485	0.0013	85	145
Se ₂ Sn ₂	572	0.0013	80	63
Se ₂ Ta ₄	590	0.0014	50	65
Bi ₂ Se ₂	852	0.0014	116	97
C ₂ I ₂ La ₂	982	0.0014	103	95
Bi ₂ Se ₂	716	0.0014	98	81
Br ₂ O ₂ Tb ₂	10	0.0014	1	1
C ₂ I ₂ La ₂	114	0.0014	12	11
CNb ₂ S ₂	946	0.0015	79	126
Cu ₂ Rb ₂ Te ₂	294	0.0015	36	25
As ₂ Mg ₂ Na ₂	708	0.0015	81	64
H ₂ Li ₂ Pd	189	0.0015	16	25
ClNZr	678	0.0015	81	118
C ₄ Ca ₂	636	0.0015	69	60
Te ₂ Zn	387	0.0015	48	65
AuI ₄ Li	612	0.0015	90	42
PtSe ₂	479	0.0016	62	77
Au ₂ I ₂	532	0.0016	75	58
AsSn ₂	479	0.0016	62	77

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CuSe (P-6m2 (187))

Structural and electronic properties

	Formula	CuSe
	Spacegroup	P-6m2 (187)
	Prototype	CuSe
	Parent 3D	Cu ₆ Se ₆
	Source DB	COD
	DB ID	9000063
DF2-C09	Binding energy [meV/ Å²]	96.78
RVV10	Binding energy [meV/ Å²]	94.91
	Band gap (PBE) [eV]	0.0

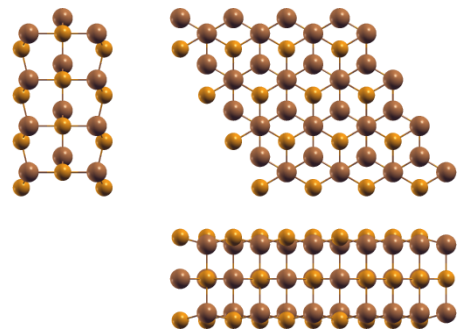


Band structure: Electronic band structure of CuSe (P-6m2 (187)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CuSe (P-6m2 (187)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.98103264	0.00000000	0.00000000
a₂	-1.99051632	3.44767540	0.00000000
a₃	0.00000000	0.00000000	26.21631886
	x [Å]	y [Å]	z [Å]
● Cu	0.00000000	2.29845026	13.10815943
● Cu	1.99051632	1.14922513	15.65936214
● Cu	1.99051632	1.14922513	10.55695672
● Se	1.99051632	1.14922513	13.10815943
● Se	0.00000000	0.00000000	16.20136018
● Se	0.00000000	0.00000000	10.01495868



Orthographic projections: views of CuSe (P-6m2 (187)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	7	2.9043	1	1
Na	7	0.2611	1	1
As ₂	8	0.2725	1	1
S ₂	8	0.0088	1	1
CaCl	8	0.1302	1	1
Cl ₂ Zn	9	0.271	1	1
MoTe ₂	9	0.2643	1	1
ReSe ₂	9	1.591	1	1
CaI ₂	9	0.4785	1	1
HfTe ₂	9	0.0013	1	1
Te ₂ V	9	0.267	1	1
Ca ₂ Si	9	3.0332	1	1
I ₂ Yb	9	0.472	1	1
Br ₂ Co	9	0.2719	1	1
Ca ₂ N	9	0.2733	1	1
AuTe ₂	9	0.0066	1	1
Cl ₂ Zn	9	0.1417	1	1
PdTe ₂	9	0.0041	1	1
S ₂ Ti	9	1.5469	1	1
Te ₂ Zn	9	0.264	1	1
Ba ₂ Hg	9	0.2061	1	1
Br ₂ Mn	9	0.2692	1	1
Cl ₂ Ni	9	1.5977	1	1
Cl ₂ Co	9	1.5444	1	1
CrTe ₂	9	0.2537	1	1
PtS ₂	9	0.2625	1	1
Br ₂ V	9	1.585	1	1
Cl ₂ Fe	9	1.5392	1	1
CdClO	9	0.2663	1	1
Ba ₂ N	9	0.0003	1	1
Se ₂ Ti	9	0.2589	1	1
Br ₂ Ti	9	1.6391	1	1
Te ₂ Zr	9	0.0008	1	1
Te ₂ W	9	0.2645	1	1
AsSe ₂	9	0.2475	1	1
I ₂ Tm	9	0.4754	1	1
I ₂ Pb	9	2.9972	1	1
OTl ₂	9	0.2666	1	1
BiTe	9	0.4525	1	1
BrNZr	9	0.2493	1	1
NbSe ₂	9	0.2462	1	1
Br ₂ Fe	9	0.272	1	1
GeS ₂	9	0.1224	1	1
MnSe ₂	9	0.1302	1	1
Br ₂ Cr	9	0.2533	1	1
DyI ₂	9	0.4858	1	1
Cl ₂ Zr	9	1.542	1	1
Se ₂ Ta	9	0.2463	1	1
NbSe ₂	9	0.2479	1	1
F ₂ Ni	9	0.1383	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

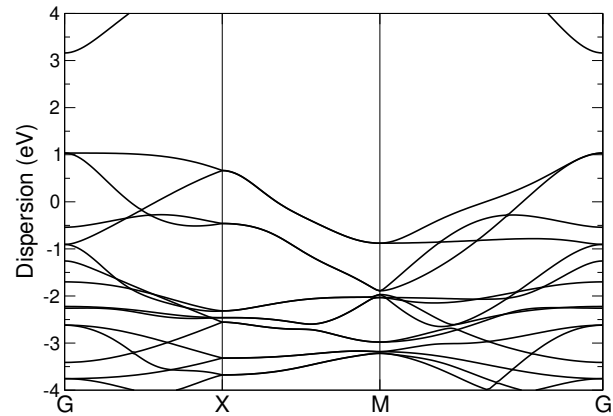
Formula	N° atoms	strain	cell size 1	cell size 2
S ₂ Ti	363	0.0	36	49
BrNZr	486	0.0	49	64
I ₂ Pb	402	0.0	49	36
MoTe ₂	711	0.0	73	91
Se ₂ W	258	0.0001	25	36
CoH ₂ O ₂	699	0.0001	49	81
Te ₂ W	711	0.0001	73	91
ReSe ₂	429	0.0002	43	57
Te ₂ Zn	711	0.0002	73	91
I ₂ Tm	678	0.0002	81	64
MoSe ₂	258	0.0002	25	36
Ba ₂ N	9	0.0003	1	1
MoS ₂	171	0.0003	16	25
ReS ₂	405	0.0003	37	61
I ₂ La ₂ Te	629	0.0003	64	49
Dy ₂ I ₂ S ₂	780	0.0003	73	57
Se ₂ Ti	627	0.0003	64	81
S ₂ W	171	0.0003	16	25
Cl ₂ Co	363	0.0004	36	49
Te ₂ V	786	0.0004	81	100
Br ₂ Hf ₂	550	0.0004	49	64
I ₂ La ₂ Sb	557	0.0004	57	43
As ₂ Mg ₂ Na ₂	678	0.0004	65	48
S ₂ V	171	0.0004	16	25
Br ₂ Ca ₃ Si	678	0.0005	64	49
GeI ₂ La ₂	806	0.0005	81	64
HfLiS ₂	802	0.0005	73	91
CdO ₂	363	0.0005	36	49
MoS ₂	171	0.0005	16	25
Tl	186	0.0005	25	36
Se ₂ Sn ₂	902	0.0005	101	74
CdH ₂ O ₂	893	0.0006	73	91
Hg ₃ N ₂	374	0.0006	49	16
Cl ₂ Zr	363	0.0007	36	49
OTl ₂	786	0.0007	81	100
Br ₂ Zr ₂	708	0.0007	64	81
Cl ₂ Ni	429	0.0007	43	57
CoH ₂ O ₂	527	0.0007	37	61
K	438	0.0007	65	48
K	385	0.0008	57	43
Te ₂ Zr	9	0.0008	1	1
I ₂ Pr ₂ S ₂	510	0.0008	49	36
HgI ₂	951	0.0009	118	81
CdClO	786	0.0009	81	100
CaI ₂	678	0.001	81	64
AgNO ₂	728	0.001	78	65
Br ₂ V	429	0.001	43	57
DyI ₂	609	0.001	73	57
Cl ₂ N ₂ Zr ₂	558	0.001	48	45
Br ₂ Ca ₃ Si	678	0.001	64	49

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CuSe (P4mm (99))

Structural and electronic properties

	Formula	CuSe
	Spacegroup	P4mm (99)
	Prototype	FeSe
	Parent 3D	Cu ₂ TlSe ₂
	Source DB	ICSD
	DB ID	629124
DF2-C09	Binding energy [meV/ Å²]	84.13
RVV10	Binding energy [meV/ Å²]	102.58
	Band gap (PBE) [eV]	0.0

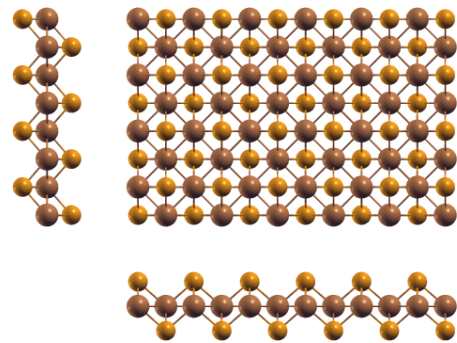


Band structure: Electronic band structure of CuSe (P4mm (99)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CuSe (P4mm (99)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.68495422	0.00000000	0.00000000
a₂	0.00000000	3.68495422	0.00000000
a₃	0.00000000	0.00000000	23.11290713
	x [Å]	y [Å]	z [Å]
● Se	0.00000000	0.00000000	9.94450744
● Cu	1.84247711	0.00000000	11.55644684
● Cu	0.00000000	1.84247711	11.55644684
● Se	1.84247711	1.84247711	13.16841315



Orthographic projections: views of CuSe (P4mm (99)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	1.1739	1	1
Tl	5	0.5681	1	1
InSe	6	0.1744	1	1
HgO	6	0.2079	1	1
AsSb	6	0.1299	1	1
Bi ₂	6	0.1814	1	1
GeTe	6	0.1344	1	1
AgTl	6	0.3847	1	1
S ₂	6	0.1356	1	1
PbTe	6	0.1765	1	1
Sb ₂	6	0.1568	1	1
IrTe ₂	7	0.1351	1	1
CrS ₂	7	0.1092	1	1
I ₂ Mg	7	0.1627	1	1
CdCl ₂	7	0.1336	1	1
CdI ₂	7	0.1785	1	1
Br ₂ Ca	7	0.18	1	1
CaI ₂	7	0.7823	1	1
InSe ₂	7	0.1338	1	1
GeTe ₂	7	0.1328	1	1
HfTe ₂	7	0.142	1	1
I ₂ Mn	7	0.1337	1	1
Br ₂ La	7	0.1631	1	1
Br ₂ Cu	7	0.1221	1	1
NSr ₂	7	0.1311	1	1
I ₂ Yb	7	0.7725	1	1
BiClTe	7	0.179	1	1
AuTe ₂	7	0.149	1	1
BrCdI	7	0.1662	1	1
Cl ₂ Zn	7	0.0035	1	1
PdTe ₂	7	0.1467	1	1
FeI ₂	7	0.132	1	1
I ₂ Ni	7	0.1329	1	1
CrI ₂	7	0.1316	1	1
I ₂ Zn	7	0.1535	1	1
BaF ₂	7	0.1699	1	1
BiBrTe	7	0.1859	1	1
Bi ₂ Pd	7	0.2186	1	1
GeI ₂	7	0.1607	1	1
Ba ₂ Hg	7	0.4045	1	1
N ₂ W	7	0.1107	1	1
CrTe ₂	7	0.1091	1	1
Ba ₂ N	7	0.1433	1	1
Br ₂ Ti	7	0.1089	1	1
AsKSn	7	0.1683	1	1
Te ₂ Zr	7	0.1424	1	1
PbTe ₂	7	0.1651	1	1
Cl ₂ Cu	7	0.1084	1	1
I ₂ Tm	7	0.7777	1	1
SnTe ₂	7	0.1584	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

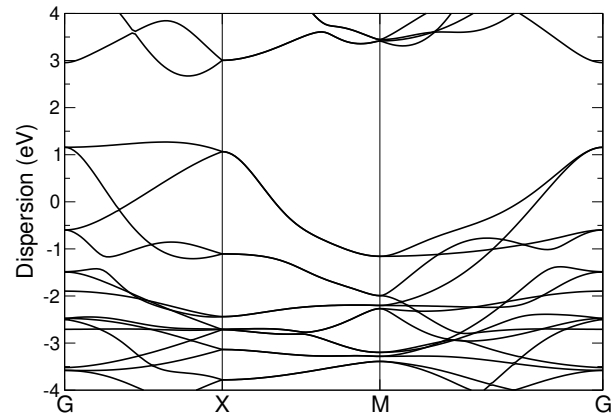
Formula	N° atoms	strain	cell size 1	cell size 2
Cu ₂ Na ₂ Te ₂	706	0.0	85	61
In	492	0.0001	89	136
AgCuTe ₂	448	0.0001	56	56
Ca ₂ O ₂	732	0.0001	82	101
Br ₂ H ₂ Sr ₂	886	0.0001	100	81
H ₄ Ti	280	0.0002	25	36
FeSe ₂	995	0.0002	113	181
I ₂ S ₂ Tl ₂	10	0.0002	1	1
Cu ₂ I ₂	724	0.0003	100	81
Cl ₂ Fe	387	0.0003	48	65
Mg ₃	499	0.0003	61	85
Mg ₄	340	0.0004	36	49
H ₂ Li ₂ Pd	280	0.0004	25	36
Cl ₂ Rb ₂	260	0.0004	49	16
F ₂ I ₂ Pb ₂	550	0.0004	64	49
Bi ₂ Se ₂	628	0.0005	89	68
Ag ₂ K ₂ Te ₂	736	0.0005	97	58
Ba ₂ Cd	410	0.0005	65	50
F ₂ Ni	7	0.0006	1	1
Si ₂ Te ₂ Zr ₂	10	0.0006	1	1
Ba ₂ Cd	403	0.0006	64	49
Cu ₂ Se ₂ Tl ₂	896	0.0006	101	82
CNb ₂ S ₂	914	0.0006	81	118
Ca ₂ O ₂	724	0.0006	81	100
Cl ₂ Zr	387	0.0007	48	65
Bi ₂ Pd	624	0.0007	81	100
Tl	193	0.0007	36	49
H ₂ I ₂ Sr ₂	412	0.0008	49	36
P ₂	560	0.0008	81	118
I ₂ S ₂ Tb ₂	770	0.0008	101	61
C ₄ Ca ₂	494	0.0008	56	45
Br ₂ Dy ₂ S ₂	982	0.0008	127	79
CdO ₂	387	0.0008	48	65
Br ₂ CsF	164	0.0009	25	16
Sn	89	0.0009	16	25
Cl ₂ Ti	678	0.0009	81	118
S ₂ Sn ₂	556	0.001	78	61
CS ₂ Ta ₂	914	0.001	81	118
C ₂ Br ₂ Y ₂	686	0.001	68	69
AlH ₄ Na	814	0.001	106	65
Cl ₂ Co	387	0.001	48	65
Ba ₂ Hg	919	0.001	145	113
C ₂ Br ₂ Y ₂	596	0.001	59	60
Cl ₂ Cu	334	0.001	46	50
Ba ₂ H ₂ I ₂	196	0.001	25	16
As ₂ O ₃	526	0.001	79	42
HgO	742	0.0011	113	145
Fe ₂ Se ₂	8	0.0011	1	1
C ₂ Br ₂ Y ₂	586	0.0011	58	59
Cl ₄ KTI	766	0.0011	130	41

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CuTe (P4/nmm (129))

Structural and electronic properties

	Formula	CuTe
	Spacegroup	P4/nmm (129)
	Prototype	FeSe
	Parent 3D	Cu ₂ Bi ₂ Te ₂ O ₂
	Source DB	ICSD
	DB ID	187824
DF2-C09	Binding energy [meV/ Å²]	107.87
RVV10	Binding energy [meV/ Å²]	102.13
	Band gap (PBE) [eV]	0.0

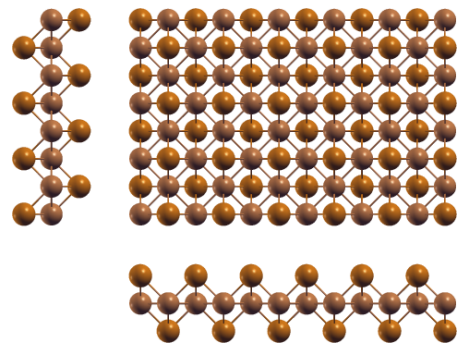


Band structure: Electronic band structure of CuTe (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CuTe (P4/nmm (129)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.73247743	0.00000000	0.00000000
a₂	0.00000000	3.73247743	0.00000000
a₃	0.00000000	0.00000000	23.53380988
	x [Å]	y [Å]	z [Å]
● Cu	0.00000000	0.00000000	11.76690494
● Cu	1.86623871	1.86623871	11.76690494
● Te	1.86623871	0.00000000	13.62719107
● Te	0.00000000	1.86623871	9.90661881



Orthographic projections: views of CuTe (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Na	5	0.1089	1	1
InSe	6	0.1674	1	1
HgO	6	0.5857	1	1
Bi ₂	6	0.1741	1	1
GeTe	6	0.1299	1	1
AgTl	6	0.3719	1	1
S ₂	6	0.131	1	1
PbTe	6	0.1694	1	1
Sb ₂	6	0.1507	1	1
IrTe ₂	7	0.1305	1	1
CrS ₂	7	0.1105	1	1
I ₂ Mg	7	0.1564	1	1
CdI ₂	7	0.1714	1	1
AgTe ₂	7	0.5593	1	1
Br ₂ Ca	7	0.1728	1	1
InSe ₂	7	0.1294	1	1
HfTe ₂	7	0.1369	1	1
Br ₂ La	7	0.1567	1	1
Br ₂ Cu	7	0.1177	1	1
I ₂ Yb	7	0.1967	1	1
BiClTe	7	0.1718	1	1
ReS ₂	7	0.1093	1	1
AuTe ₂	7	0.1435	1	1
BrCdI	7	0.1596	1	1
Cl ₂ Zn	7	0.0026	1	1
PdTe ₂	7	0.1413	1	1
I ₂ Zn	7	0.1476	1	1
BaF ₂	7	0.1632	1	1
BiBrTe	7	0.1784	1	1
Bi ₂ Pd	7	0.2118	1	1
GeI ₂	7	0.1545	1	1
Ba ₂ Hg	7	0.3911	1	1
Ba ₂ N	7	0.1381	1	1
Se ₂ Ti	7	0.1085	1	1
AsKSn	7	0.1616	1	1
Te ₂ Zr	7	0.1373	1	1
PbTe ₂	7	0.1586	1	1
Cl ₂ Cu	7	0.1055	1	1
I ₂ Tm	7	0.7545	1	1
SnTe ₂	7	0.1523	1	1
GeI ₂	7	0.1697	1	1
STl ₂	7	0.1642	1	1
BiTe	7	0.1865	1	1
DyI ₂	7	0.7698	1	1
Se ₂ Yb	7	0.1547	1	1
BiTe ₂	7	0.155	1	1
GdI ₂	7	0.1819	1	1
CNNa	7	0.4636	1	1
F ₂ Ni	7	0.0065	1	1
PtTe ₂	7	0.1431	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

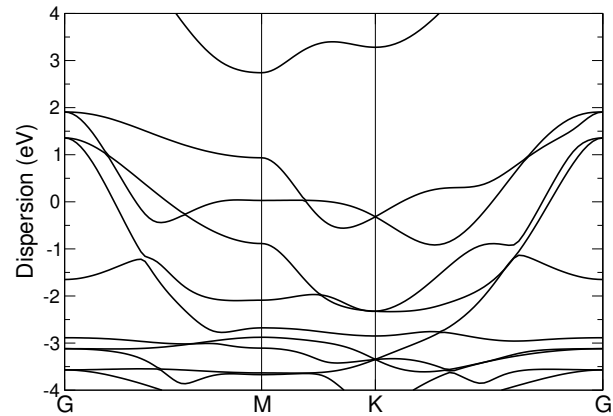
Formula	N° atoms	strain	cell size 1	cell size 2
Cl ₂ S ₂ Tl ₂	118	0.0001	16	9
Br ₂ CsF	900	0.0001	136	89
F ₄ Pb	645	0.0001	85	61
Mg ₄	584	0.0001	61	85
HgI ₂	219	0.0002	36	25
Tl	329	0.0002	61	85
Ho ₂ I ₂ Se ₂	180	0.0003	24	14
Ca ₂ O ₂	588	0.0003	65	82
Cl ₂ Zr ₂	452	0.0003	48	65
As ₂ Co ₂ Li ₂	10	0.0004	1	1
Ag ₂ K ₂ Te ₂	814	0.0004	106	65
Pb ₂ Se ₂	172	0.0004	25	18
Ca ₂ O ₂	580	0.0004	64	81
Mg ₆	438	0.0005	36	49
Bi ₂ Se ₂	228	0.0005	32	25
Cu ₂ Na ₂ Te ₂	412	0.0005	49	36
Br ₂ V	387	0.0005	48	65
N ₃ Na	272	0.0006	40	28
AgNO ₃	757	0.0006	108	65
CCl ₂ Sc ₂	517	0.0007	48	65
Tl	442	0.0007	81	118
Sn	633	0.0007	113	181
In	89	0.0007	16	25
Gd ₂ I ₂ S ₂	614	0.0008	80	49
Br ₂ Ca ₃ Si	718	0.0008	82	65
Ba ₂ Cd	516	0.0008	81	64
Se ₂ V	678	0.0008	81	118
Bi ₂ Pd	499	0.0009	64	81
Ag ₂ I ₂	244	0.0009	36	25
Dy ₂ I ₂ S ₂	672	0.0009	87	54
CKN	613	0.0009	103	67
F ₂ I ₂ Pb ₂	708	0.0009	81	64
Ge ₂ Hf ₂ Te ₂	10	0.001	1	1
H ₂ MgO ₂	946	0.001	79	126
Br ₂ H ₂ Zr ₂	582	0.001	48	65
Ba ₂ Hg	523	0.001	82	65
Se ₂ W	678	0.0011	81	118
Cu ₂ O ₄	264	0.0012	24	28
C	113	0.0012	12	65
MoSe ₂	678	0.0012	81	118
F ₂ Se ₂ Y ₂	958	0.0012	118	81
HgO	566	0.0012	85	113
As ₂ Mg ₂ Na ₂	962	0.0012	113	85
H ₂ I ₂ Sr ₂	962	0.0012	113	85
Er ₂ I ₂ Se ₂	180	0.0013	24	14
I ₂ S ₂ Tb ₂	672	0.0013	87	54
ReSe ₂	387	0.0013	48	65
S ₂ V	694	0.0014	79	126
Sb ₂ Te ₃	857	0.0014	103	89
NaO ₄	757	0.0014	108	65

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

CuTe₂ (P-3m1)

Structural and electronic properties

	Formula	CuTe ₂
	Spacegroup	P-3m1
	Prototype	CdI ₂
	Parent 3D	CuTe ₂
	Source DB	MPDS
	DB ID	S1404528
DF2-C09	Binding energy [meV/ Å²]	77.85
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

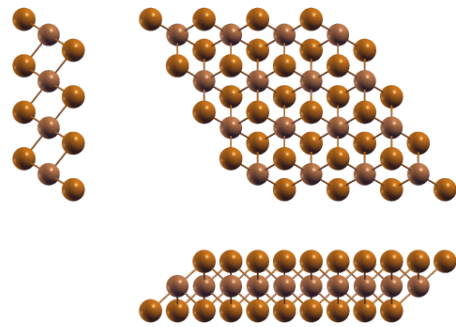


Band structure: Electronic band structure of CuTe₂ (P-3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of CuTe₂ (P-3m1) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		1.81341970	−3.14093505	0.00000000
a₂		1.81341970	3.14093505	0.00000000
a₃		0.00000000	0.00000000	17.58807502
		x [Å]	y [Å]	z [Å]
●	Te	0.00000000	1.04697835	−1.66889757
●	Cu	−1.81341970	0.00000000	0.00000000
●	Te	0.00000000	−1.04697835	1.66889757



Orthographic projections: views of CuTe₂ (P-3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	4	0.1196	1	1
In	4	0.427	1	1
In	4	0.2467	1	1
HgO	5	0.1268	1	1
As ₂	5	0.0024	1	1
LiO	5	0.2609	1	1
P ₂	5	0.2718	1	1
Mg ₂	5	0.1123	1	1
Sb ₂	5	0.4831	1	1
Cl ₂ Zn	6	0.0034	1	1
I ₂ Mg	6	0.498	1	1
MoTe ₂	6	0.0079	1	1
AgTe ₂	6	0.1212	1	1
PSn ₂	6	0.0066	1	1
HfS ₂	6	0.0004	1	1
FeO ₂	6	4.8596	1	1
Te ₂ V	6	0.0061	1	1
S ₂ Zr	6	0.0058	1	1
Br ₂ La	6	0.4989	1	1
Br ₂ Co	6	0.0028	1	1
Ca ₂ N	6	0.0018	1	1
Cl ₂ Ti	6	0.272	1	1
AuTe ₂	6	0.463	1	1
PdTe ₂	6	0.4569	1	1
Mg ₃	6	0.1166	1	1
I ₂ Zn	6	0.4746	1	1
Te ₂ Zn	6	0.0081	1	1
Bi ₂ Pd	6	0.1336	1	1
GeI ₂	6	0.4931	1	1
Br ₂ Mn	6	0.0046	1	1
PtS ₂	6	0.0091	1	1
CoTe ₂	6	0.0007	1	1
CdClO	6	0.0065	1	1
Ba ₂ N	6	0.4476	1	1
Te ₂ W	6	0.0078	1	1
PbTe ₂	6	2.9097	1	1
S ₂ Sn	6	0.0061	1	1
SnTe ₂	6	0.4871	1	1
Cl ₂ V	6	0.2574	1	1
OTl ₂	6	0.0063	1	1
Br ₂ Fe	6	0.0027	1	1
Br ₂ Ni	6	0.0024	1	1
CuO ₂	6	2.6298	1	1
NbTe ₂	6	0.0056	1	1
Se ₂ Yb	6	0.4937	1	1
Cl ₂ Mg	6	0.0024	1	1
BiTe ₂	6	0.4944	1	1
CrSe ₂	6	0.2558	1	1
PtTe ₂	6	0.462	1	1
Br ₂ Cd	6	0.4546	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

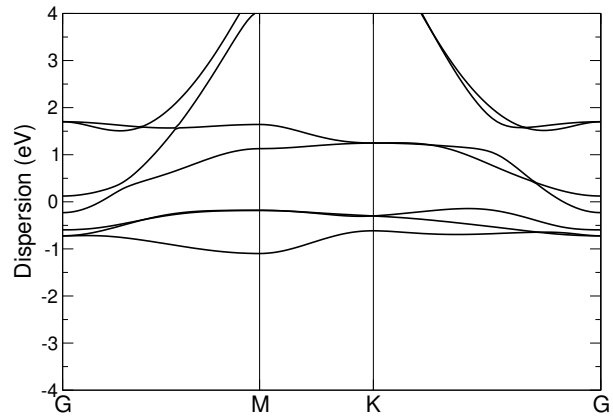
Formula	N° atoms	strain	cell size 1	cell size 2
O ₂ Pt	300	0.0	43	57
CoO ₂	390	0.0	49	81
Sb ₂ Se ₂ Te	437	0.0	64	49
Sb ₂	333	0.0001	73	57
NiO ₂	294	0.0001	37	61
CrSe ₂	435	0.0001	64	81
AgNO ₃	432	0.0001	79	39
Sb ₂ Te ₂	331	0.0002	61	37
Bi ₂ Se ₂ Te	327	0.0002	49	36
Sb ₂ SeTe ₂	327	0.0002	49	36
Br ₂ Eu ₂ F ₂	483	0.0002	65	48
CrSe ₂	390	0.0002	57	73
MnNaTe ₂	343	0.0002	57	43
Er ₂ I ₂ O ₂	483	0.0002	65	48
I ₂ Se ₂ Tm ₂	660	0.0002	112	54
In ₂ Te ₃	327	0.0002	49	36
Br ₂ La ₂	447	0.0003	73	57
AlH ₄ Na	237	0.0003	39	20
FHOZn	463	0.0003	57	73
PtTe ₂	543	0.0003	100	81
As ₂ Sn ₂	565	0.0004	91	73
H ₂ MgO ₂	467	0.0004	49	64
PbTe ₂	300	0.0004	57	43
HfS ₂	6	0.0004	1	1
BiTe ₂	339	0.0004	64	49
Sb ₂ Se ₂ Te	437	0.0004	64	49
Gd ₂ I ₂ S ₂	171	0.0004	25	16
Gd	253	0.0004	52	97
Al ₂ Cl ₂ O ₂	435	0.0004	49	48
CaH ₂ O ₂	8	0.0004	1	1
I ₂ La ₂ P	233	0.0004	36	25
Br ₂ Gd ₂	565	0.0004	91	73
N ₂ W	183	0.0005	25	36
GdI ₂	183	0.0005	36	25
Li ₂ P ₂ Pr	504	0.0005	73	57
I ₂ Zn	435	0.0005	81	64
SSb ₂ Te ₂	386	0.0006	57	43
Bi ₂ Br ₂ O ₂	483	0.0006	65	48
I ₂ O ₂ Tm ₂	483	0.0006	65	48
CoO ₂	294	0.0006	37	61
Ga ₂ Ge ₂ Te ₂	561	0.0006	73	57
Br ₂ Ho ₂	624	0.0006	100	81
BrCdI	300	0.0006	57	43
GeI ₂ Y ₂	327	0.0006	49	36
As ₂ Cd ₂ K ₂	411	0.0006	65	36
Se ₂ Yb	339	0.0006	64	49
Br ₂ Ca ₃ Si	171	0.0007	25	16
Cl ₂ N ₂ Zr ₂	9	0.0007	1	1
CoTe ₂	6	0.0007	1	1
NaO ₄	432	0.0007	79	39

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Fe(OH)₂ (P-3m1)

Structural and electronic properties

	Formula	Fe(OH) ₂
	Spacegroup	P-3m1
	Prototype	Mn(OH) ₂
	Parent 3D	FeH ₂ O ₂
	Source DB	MPDS
	DB ID	S1020258
DF2-C09	Binding energy [meV/ Å²]	30.83
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

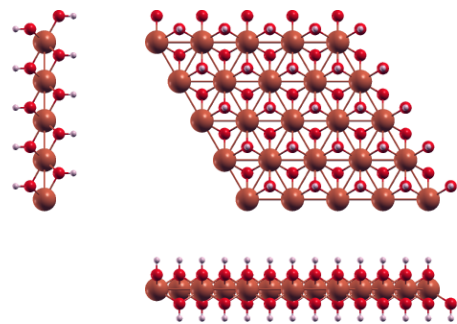


Band structure: Electronic band structure of Fe(OH)₂ (P-3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Fe(OH)₂ (P-3m1) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		1.51359427	-2.62162217	0.00000000
a₂		1.51359427	2.62162217	0.00000000
a₃		0.00000000	0.00000000	19.62220813
		x [Å]	y [Å]	z [Å]
•	H	1.51359427	-0.87387406	1.93918516
•	O	1.51359427	-0.87387406	0.96344603
•	Fe	0.00000000	0.00000000	0.00000000
•	H	1.51359427	0.87387406	-1.93918516
•	O	1.51359427	0.87387406	-0.96344603



Orthographic projections: views of Fe(OH)₂ (P-3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Nd	6	0.2632	1	1
CrS ₂	8	0.0057	1	1
Cl ₂ Mn	8	0.4605	1	1
ReSe ₂	8	0.4942	1	1
S ₂ Ta	8	0.4657	1	1
CrO ₂	8	0.2736	1	1
S ₂ Ti	8	0.4784	1	1
NbS ₂	8	0.4646	1	1
N ₂ W	8	0.0012	1	1
Cl ₂ Ni	8	0.4966	1	1
Cl ₂ Co	8	0.4775	1	1
NbS ₂	8	0.4538	1	1
CNRb	8	1.6772	1	1
ClNZr	8	0.4865	1	1
Cl ₂ Fe	8	0.4756	1	1
S ₂ Ta	8	0.4518	1	1
Se ₂ V	8	0.4485	1	1
AsSe ₂	8	0.5005	1	1
CdO ₂	8	0.4771	1	1
NbSe ₂	8	0.4978	1	1
O ₂ Zn	8	0.0023	1	1
Cl ₂ Zr	8	0.4766	1	1
Se ₂ Ta	8	0.498	1	1
NbSe ₂	8	0.5012	1	1
HNiO ₂	9	0.0085	1	1
Cl ₂ Hf ₂	9	0.4688	1	1
Br ₂ Hf ₂	9	2.9057	1	1
C ₂ F ₂	9	1.561	1	1
LiNbS ₂	9	0.4659	1	1
NS ₂ Ta	9	0.0034	1	1
Cl ₂ NSc ₂	10	0.4617	1	1
LiOS ₂ Ti	10	0.4567	1	1
Ga ₂ S ₃	10	3.0313	1	1
Cl ₂ H ₂ Zr ₂	11	0.4545	1	1
Br ₂ H ₂ Zr ₂	11	2.8336	1	1
Sn	11	0.229	2	1
I ₂ Sb ₂ Te ₂	11	3.1495	1	1
Bi ₂	12	0.2246	2	1
PbTe	12	0.2194	2	1
CdI ₂	13	0.2216	2	1
Br ₂ Ca	13	0.2232	2	1
BiClTe	13	0.222	2	1
Cl ₂ Cu	13	0.1065	2	1
GeI ₂	13	0.2197	2	1
CNNa	13	0.5747	2	1
CdI ₂	13	0.221	2	1
I ₂ Pr	13	0.2221	2	1
In ₂ Se ₂	14	0.8406	2	1
LiMnTe ₂	14	0.2201	2	1
Pb ₂ Se ₂	14	0.3494	2	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

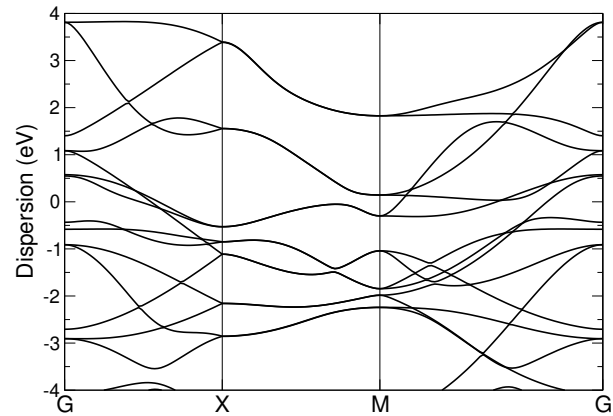
Formula	N° atoms	strain	cell size 1	cell size 2
AuTe ₂	107	0.0	16	9
Cl ₂ O ₂ Tm ₂	221	0.0	25	16
Cl ₂ Er ₂ H ₂	527	0.0001	61	37
CoTe ₂	255	0.0001	36	25
Ga ₂ S ₂	280	0.0001	36	25
InSe ₂	416	0.0001	61	37
CaClHO	189	0.0001	25	16
As ₂ Li ₂ Nd	370	0.0001	49	25
GeI ₂ Y ₂	370	0.0001	49	25
Br ₂ Ca ₃ Si	69	0.0001	9	4
Cl ₂ Fe	597	0.0001	81	64
GeTe	503	0.0002	81	49
I ₂ Mn	416	0.0002	61	37
Cl ₂ NSc ₂	905	0.0002	100	81
Br ₂ Zr ₂	389	0.0002	49	36
H ₂ Si ₂	601	0.0002	81	49
Cl ₂ Zr	597	0.0002	81	64
BrNZr	414	0.0003	57	43
Cl ₂ Mn	743	0.0003	100	81
Bi ₂ Br ₂ O ₂	315	0.0003	39	20
CdCl ₂	416	0.0003	61	37
Gd ₂ I ₂ S ₂	69	0.0003	9	4
In ₂ S ₃	650	0.0004	81	49
HfS ₂	255	0.0004	36	25
LiNbS ₂	747	0.0004	91	73
H ₂ Si ₂	453	0.0004	61	37
PtTe ₂	107	0.0004	16	9
CdO ₂	597	0.0004	81	64
ReSe ₂	467	0.0004	64	49
Cl ₂ Ni	467	0.0005	64	49
S ₂ Ta	674	0.0005	91	73
Ni ₂ Te ₂	453	0.0005	61	37
Sb ₂ Te ₃	590	0.0005	79	39
Br ₂ Er ₂	116	0.0005	16	9
Li ₂ Tl ₂	161	0.0005	25	9
Bi ₂ Se ₂ Te	370	0.0006	49	25
Cl ₂ Co	597	0.0006	81	64
Se ₂ Ti	353	0.0006	49	36
Er ₂ I ₂ O ₂	315	0.0006	39	20
Sn ₂ Te ₂	137	0.0006	21	8
BiBrTe	647	0.0006	100	49
Bi ₂ SeTe ₂	590	0.0006	79	39
Br ₂ Eu ₂ F ₂	315	0.0006	39	20
Br ₂ Ca ₃ Si	408	0.0007	60	18
Cu ₄ Te ₂	794	0.0007	100	49
Br ₂ Hf ₂	457	0.0007	57	43
NiTe ₂	173	0.0007	25	16
I ₂ La ₂ Si ₂	395	0.0007	49	25
Cl ₂ Hf ₂	747	0.0007	91	73
I ₂ O ₂ Y ₂	315	0.0007	39	20

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

FeAs (P4mm (99))

Structural and electronic properties

	Formula	FeAs
	Spacegroup	P4mm (99)
	Prototype	FeSe
	Parent 3D	KFe ₂ As ₂
	Source DB	ICSD
	DB ID	189036
DF2-C09	Binding energy [meV/ Å²]	105.05
RVV10	Binding energy [meV/ Å²]	99.59
	Band gap (PBE) [eV]	0.0

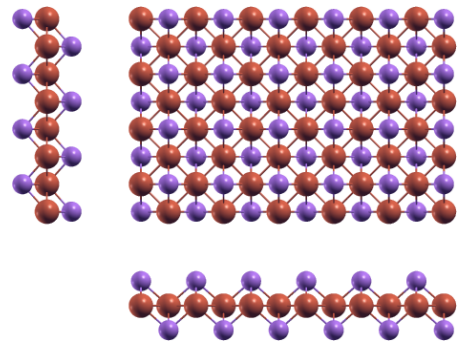


Band structure: Electronic band structure of FeAs (P4mm (99)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of FeAs (P4mm (99)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.51524556	0.00000000	0.00000000
a₂		0.00000000	3.51524556	0.00000000
a₃		0.00000000	0.00000000	22.83061078
		x [Å]	y [Å]	z [Å]
●	As	0.00000000	0.00000000	9.84997387
●	Fe	1.75762278	0.00000000	11.41529227
●	Fe	0.00000000	1.75762278	11.41529227
●	As	1.75762278	1.75762278	12.98066315



Orthographic projections: views of FeAs (P4mm (99)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	5	0.2193	1	1
InSe	6	0.7669	1	1
AsSb	6	0.1482	1	1
Bi ₂	6	0.7894	1	1
K	6	1.6812	1	2
GeTe	6	0.1541	1	1
S ₂	6	0.1557	1	1
PbTe	6	0.7737	1	1
Mg ₂	6	0.5857	1	1
Sb ₂	6	0.182	1	1
IrTe ₂	7	0.155	1	1
I ₂ Mg	7	0.1892	1	1
CdCl ₂	7	0.1531	1	1
CdI ₂	7	0.7804	1	1
PSn ₂	7	0.1309	1	1
Br ₂ Zn	7	0.1392	1	1
Br ₂ Ca	7	0.7851	1	1
InSe ₂	7	0.1534	1	1
AsSn ₂	7	0.1337	1	1
GeTe ₂	7	0.1521	1	1
SiTe ₂	7	0.1427	1	1
HfTe ₂	7	0.1638	1	1
I ₂ Pr	7	0.3824	1	1
I ₂ Mn	7	0.1532	1	1
S ₂ Zr	7	0.1303	1	1
Br ₂ La	7	0.1896	1	1
NSr ₂	7	0.1498	1	1
PbS ₂	7	0.1459	1	1
BiClTe	7	0.7818	1	1
AuTe ₂	7	0.1725	1	1
BrCdI	7	0.1933	1	1
PdTe ₂	7	0.1697	1	1
FeI ₂	7	0.151	1	1
I ₂ Ni	7	0.1523	1	1
Mg ₃	7	0.2126	1	1
Te ₂ Ti	7	0.1394	1	1
CrI ₂	7	0.1506	1	1
I ₂ Zn	7	0.178	1	1
BaF ₂	7	0.7523	1	1
RhTe ₂	7	0.1359	1	1
GeI ₂	7	0.1868	1	1
NbS ₂	7	0.1089	1	1
S ₂ Ta	7	0.1087	1	1
Ba ₂ N	7	0.1655	1	1
Se ₂ V	7	0.1084	1	1
AsKSn	7	0.1958	1	1
Te ₂ Zr	7	0.1643	1	1
PbTe ₂	7	0.192	1	1
I ₂ Nd	7	0.3844	1	1
NiTe ₂	7	0.1422	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

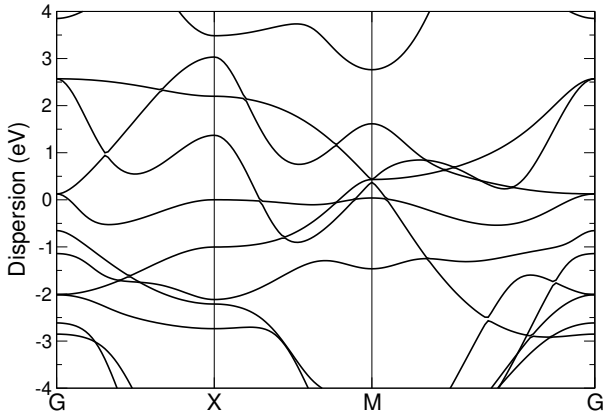
Formula	N° atoms	strain	cell size 1	cell size 2
H ₂ I ₂ Yb ₂	718	0.0	82	65
I ₂ Pr	643	0.0	100	81
Tl	424	0.0001	81	100
I ₂ O ₂ Pr ₂	962	0.0001	113	85
Br ₂ Eu ₂ O ₂	896	0.0001	101	82
Mg ₃	499	0.0001	64	81
I ₂ La	516	0.0001	81	64
Eu ₂ H ₂ I ₂	560	0.0001	65	50
As ₂ Rh ₂	580	0.0001	81	64
CeI ₂	650	0.0002	101	82
Ag ₂ I ₂	684	0.0002	106	65
I ₂ O ₂ Sm ₂	560	0.0002	65	50
Ba ₂ F ₂ I ₂	618	0.0002	81	49
Ho ₂ S ₂	472	0.0003	65	53
Ba ₂ Ge ₂ Mn ₂	550	0.0003	64	49
Cl ₄ Mn	109	0.0003	16	9
Nd	119	0.0004	20	39
Ag ₂ Br ₂	580	0.0004	81	64
Mg ₄	724	0.0004	81	100
I ₂ O ₂ Yb ₂	886	0.0004	100	81
Ni ₂ Se ₂	732	0.0004	101	82
Hf ₂ Se ₂ Si ₂	10	0.0005	1	1
As ₂ Cd ₂ K ₂	736	0.0005	97	58
F ₂ I ₂ Yb ₂	560	0.0005	65	50
O ₄ PTl	618	0.0005	81	49
O ₄ PSn	736	0.0005	97	58
In	329	0.0005	61	85
F ₂ I ₂ Yb ₂	550	0.0006	64	49
H ₄ Ti	516	0.0006	49	64
Br ₂ H ₂ Sr ₂	412	0.0006	49	36
Br ₂ Eu ₂ O ₂	886	0.0006	100	81
Br ₂ F ₂ Pb ₂	412	0.0007	49	36
PbS ₂ Sn	488	0.0007	72	50
Br ₂ Ca ₃ Si	958	0.0007	118	81
Br ₂ Lu ₂ S ₂	204	0.0007	27	16
CeI ₂	643	0.0007	100	81
S ₂ Sn ₂	568	0.0008	83	59
Br ₂ Lu ₂ S ₂	204	0.0008	27	16
H ₂ I ₂ Yb ₂	708	0.0008	81	64
Ir ₂ P ₂	724	0.0008	100	81
Br ₂ Nd ₂ O ₂	718	0.0008	82	65
GeS ₂	7	0.0009	1	1
Br ₂ O ₂ Pr ₂	708	0.0009	81	64
AgNO ₃	874	0.0009	131	70
I ₂ La ₂ Te	877	0.0009	118	81
FeO ₂	339	0.0009	36	65
Br ₂ O ₂ Sm ₂	886	0.0009	100	81
Br ₂ F ₂ Sr ₂	412	0.001	49	36
F ₂ I ₂ Tm ₂	550	0.001	64	49
Ni ₂ Se ₂	724	0.001	100	81

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

FeSe₂ (P4/mmm)

Structural and electronic properties

	Formula	FeSe ₂
	Spacegroup	P4/mmm
	Prototype	Zr ₂ Cu
	Parent 3D	FeSe ₂ Tl ₂
	Source DB	MPDS
	DB ID	S538916
DF2-C09	Binding energy [meV/ Å²]	48.42
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

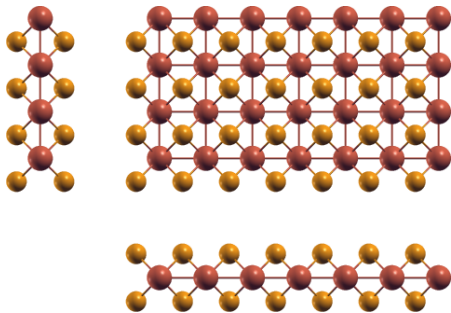


Band structure: Electronic band structure of FeSe₂ (P4/mmm) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of FeSe₂ (P4/mmm) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		2.91300790	0.00000000	0.00000000
a₂		0.00000000	2.91300790	0.00000000
a₃		0.00000000	0.00000000	16.94247621
		x [Å]	y [Å]	z [Å]
●	Se	2.91300790	0.00000000	-1.49010062
●	Fe	1.45650395	-1.45650395	0.00000000
●	Se	0.00000000	0.00000000	1.49010062



Orthographic projections: views of FeSe₂ (P4/mmm) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	4	0.1687	1	1
Sn	4	0.0066	1	1
Na	4	0.7827	1	1
In	4	0.1449	1	1
Gd	4	0.4909	1	1
HgO	5	0.3849	1	1
LiO	5	0.1549	1	1
P ₂	5	0.1629	1	1
CrS ₂	6	0.1327	1	1
S ₂ V	6	0.1478	1	1
MoS ₂	6	0.1485	1	1
Cl ₂ Mn	6	0.1754	1	1
MoSe ₂	6	0.1678	1	1
ReSe ₂	6	0.1918	1	1
S ₂ Ta	6	0.1779	1	1
ReS ₂	6	0.1374	1	1
Cl ₂ Ti	6	0.163	1	1
S ₂ Ti	6	0.184	1	1
NbS ₂	6	0.1773	1	1
S ₂ W	6	0.1485	1	1
Bi ₂ Pd	6	0.4061	1	1
Cl ₂ Ni	6	0.1929	1	1
Cl ₂ Co	6	0.1835	1	1
PtS ₂	6	0.7867	1	1
NbS ₂	6	0.1722	1	1
Br ₂ V	6	0.1907	1	1
ClNZr	6	0.188	1	1
Cl ₂ Fe	6	0.1826	1	1
S ₂ Ta	6	0.1712	1	1
Se ₂ V	6	0.1697	1	1
Se ₂ Ti	6	0.7764	1	1
AsSe ₂	6	0.1949	1	1
Cl ₂ V	6	0.1524	1	1
CdO ₂	6	0.1834	1	1
BrNZr	6	0.1967	1	1
NbSe ₂	6	0.1935	1	1
O ₂ Zn	6	0.1302	1	1
Cl ₂ Zr	6	0.1831	1	1
Se ₂ Ta	6	0.1936	1	1
NbSe ₂	6	0.1952	1	1
MoS ₂	6	0.1487	1	1
CrSe ₂	6	0.1512	1	1
CrSe ₂	6	0.1536	1	1
O ₂ Pt	6	0.1435	1	1
Se ₂ W	6	0.168	1	1
NS ₂ Zr	7	0.7843	1	1
Cl ₂ Hf ₂	7	0.1793	1	1
Bi ₂ Mn ₂	7	0.5997	1	1
Bi ₂	7	2.2061	1	2
Ca ₂ O ₂	7	1.1035	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

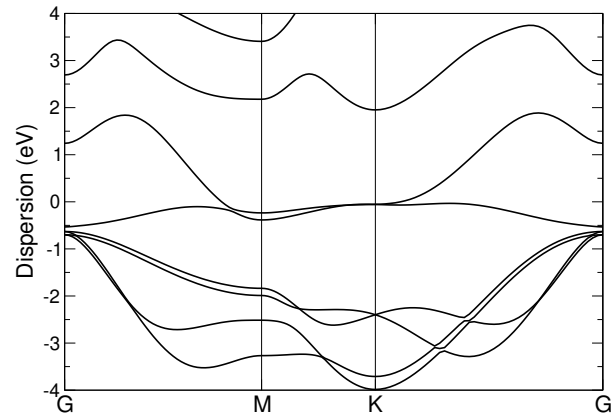
Formula	N° atoms	strain	cell size 1	cell size 2
Ca ₂ O ₂	395	0.0001	65	50
I ₂ La ₂ O ₂	594	0.0001	100	49
Ca ₂ Cl ₂	775	0.0001	145	85
CaCl	586	0.0001	136	89
Ca ₂ Ge ₂ Mn ₂	102	0.0001	16	9
F ₄ Sn	592	0.0002	109	53
MnSe ₂	675	0.0002	136	89
AuTe ₂	519	0.0002	108	65
Cu ₂ Se ₂	995	0.0002	181	113
Ge ₂ Te ₂ Zr ₂	639	0.0002	97	58
AlH ₄ Na	471	0.0003	89	34
Br ₂ F ₂ Tm ₂	102	0.0003	16	9
PtTe ₂	519	0.0003	108	65
As ₂ Ru ₂	775	0.0003	145	85
Fe ₂ Te ₂	775	0.0003	145	85
I ₂ Lu ₂ O ₂	102	0.0004	16	9
As ₂ Co ₂	139	0.0004	25	16
Bi ₂ O ₂	247	0.0004	49	25
Bi ₂ Cl ₂ O ₂	102	0.0004	16	9
Br ₂ Lu ₂ O ₂	639	0.0005	97	58
Br ₂ O ₂ V ₂	282	0.0005	40	27
CaI ₂	357	0.0005	80	39
Co ₂ S ₂	764	0.0005	136	89
Br ₂ O ₂ Ti ₂	327	0.0005	49	30
Br ₂ O ₂ Tm ₂	945	0.0005	145	85
Ge ₂ Hf ₂ Te ₂	537	0.0006	81	49
Ba ₂ Hg	486	0.0006	109	53
F ₂ Na	597	0.0006	118	81
Cl ₂ O ₂ Yb ₂	840	0.0007	118	81
Br ₂ Hf ₂ N ₂	594	0.0007	92	53
Cu ₂ Se ₂ Tl ₂	297	0.0007	49	25
I ₂ Tm	357	0.0007	80	39
Br ₂ Er ₂	584	0.0007	108	65
Br ₂ O ₂ Yb ₂	945	0.0007	145	85
F ₂ Ni	882	0.0008	181	113
I ₂ Pr	603	0.0008	131	70
BiClTe	603	0.0009	131	70
Br ₂ Ca ₃ Si	645	0.0009	109	53
Br ₂ La ₂ O ₂	297	0.0009	49	25
Cl ₂ O ₂ Tm ₂	840	0.0009	118	81
Gd ₂ GeI ₂	743	0.0009	131	70
Eu ₂ F ₂ I ₂	297	0.001	49	25
GeI ₂ La ₂	435	0.001	80	39
Co ₂ Se ₂	139	0.001	25	16
H ₂ Na ₂ Pd	233	0.001	36	25
F ₄ Nb	817	0.001	149	74
Cl ₂ Zn	513	0.001	106	65
Br ₂ Gd ₂ O ₂	102	0.001	16	9
Br ₂ Ca	603	0.001	131	70
CdI ₂	603	0.001	131	70

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

GaSe (P-3m1 (164))

Structural and electronic properties

	Formula	GaSe
	Spacegroup	P-3m1 (164)
	Prototype	PtTe
	Parent 3D	Ga ₄ Se ₄
	Source DB	ICSD
	DB ID	20237
DF2-C09	Binding energy [meV/ Å²]	40.95
RVV10	Binding energy [meV/ Å²]	42.43
	Band gap (PBE) [eV]	0.0

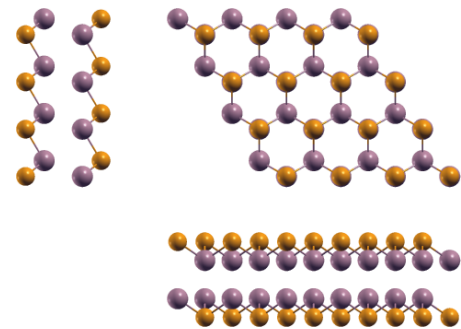


Band structure: Electronic band structure of GaSe (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of GaSe (P-3m1 (164)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.74587822	0.00000000	0.00000000
a₂	-1.87293911	3.24402570	0.00000000
a₃	0.00000000	0.00000000	25.18549233
	x [Å]	y [Å]	z [Å]
● Ga	0.00000000	2.16268380	13.90927091
● Se	1.87293911	1.08134190	15.19025083
● Ga	1.87293911	1.08134190	11.27622141
● Se	0.00000000	2.16268380	9.99524150



Orthographic projections: views of GaSe (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	5	0.1127	1	1
Tl	5	0.2576	1	1
InSe	6	0.4849	1	1
HgO	6	0.118	1	1
Bi ₂	6	0.5002	1	1
P ₂	6	0.2505	1	1
PbTe	6	2.841	1	1
I ₂ Mg	7	0.4588	1	1
MoS ₂	7	1.5216	1	1
Cl ₂ Mn	7	0.2657	1	1
CdI ₂	7	0.4941	1	1
AgTe ₂	7	0.1138	1	1
PSn ₂	7	0.0085	1	1
MoSe ₂	7	0.2566	1	1
S ₂ Ta	7	0.2687	1	1
Br ₂ Zn	7	0.002	1	1
Br ₂ Ca	7	0.4974	1	1
AsSn ₂	7	0.0049	1	1
SiTe ₂	7	0.0061	1	1
Br ₂ La	7	0.4596	1	1
Br ₂ Cu	7	0.961	1	1
BiClTe	7	0.4951	1	1
Cl ₂ Ti	7	1.6266	1	1
BrCdI	7	0.4666	1	1
S ₂ Ti	7	0.276	1	1
Mg ₃	7	0.4426	1	1
Te ₂ Ti	7	0.0023	1	1
NbS ₂	7	0.268	1	1
BaF ₂	7	0.475	1	1
RhTe ₂	7	0.0021	1	1
S ₂ W	7	1.5221	1	1
Bi ₂ Pd	7	0.1232	1	1
GeI ₂	7	0.4542	1	1
Cl ₂ Co	7	0.2754	1	1
NbS ₂	7	0.2618	1	1
Cl ₂ Fe	7	0.2744	1	1
S ₂ Ta	7	0.2607	1	1
Se ₂ V	7	0.2588	1	1
AsKSn	7	0.4714	1	1
PbTe ₂	7	0.4641	1	1
NiTe ₂	7	0.0055	1	1
S ₂ Sn	7	0.009	1	1
SnTe ₂	7	0.4486	1	1
I ₂ V	7	0.0075	1	1
Cl ₂ V	7	1.5509	1	1
GeI ₂	7	2.844	1	1
Se ₂ Zr	7	0.0066	1	1
STl ₂	7	0.4775	1	1
PtSe ₂	7	0.0042	1	1
BiTe	7	3.0264	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

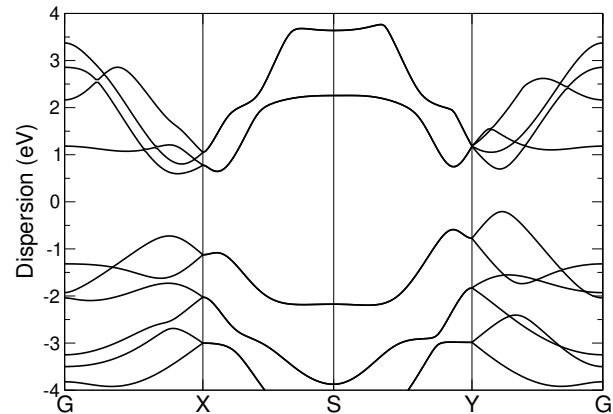
Formula	N° atoms	strain	cell size 1	cell size 2
As ₂ Li ₂ Nd	577	0.0	73	57
Br ₂ Gd ₂ Ge	805	0.0	100	81
Cu ₂ I ₂	724	0.0	100	81
Sb ₂ Te ₃	443	0.0	57	43
I ₂ Pr	403	0.0	64	49
N ₃ W ₂	601	0.0001	49	81
BrCdI	583	0.0001	91	73
BiClTe	403	0.0001	64	49
SSb ₂ Te ₂	729	0.0002	91	73
GeI ₂ Y ₂	577	0.0002	73	57
NbS ₂	624	0.0003	81	100
Gd ₂ I ₂	724	0.0003	100	81
Se ₂ V	499	0.0004	64	81
Gd ₂ GeI ₂	501	0.0004	64	49
BaF ₂	516	0.0004	81	64
CNb ₂ S ₂	516	0.0004	49	64
CdI ₂	403	0.0005	64	49
MnNaTe ₂	656	0.0005	91	73
I ₂ O ₂ Pr ₂	548	0.0005	65	48
FHOZn	340	0.0005	36	49
Cl ₂ V	291	0.0006	36	49
Bi ₂ Se ₃	805	0.0006	100	81
STl ₂	516	0.0006	81	64
LiOS ₂ Ti	747	0.0006	73	91
I ₂ La ₂ Si ₂	634	0.0006	73	57
Ga ₂ I ₂ Y ₂	708	0.0006	81	64
Cu ₄ Te ₂	486	0.0006	57	43
F ₂ I ₂ Pb ₂	958	0.0006	118	81
Br ₂ La	643	0.0006	100	81
F ₂ I ₂ Sm ₂	548	0.0006	65	48
Ba ₂ Cd	715	0.0006	118	81
As ₂ Li ₂ Pr	577	0.0006	73	57
CrSe ₂	291	0.0006	36	49
Br ₂ OV	496	0.0006	63	61
Er ₂ I ₂ S ₂	650	0.0007	89	49
InSe	406	0.0007	73	57
N ₃ W ₂	453	0.0007	37	61
Bi ₂ Se ₂ Te	577	0.0007	73	57
Cl ₂ Y ₂	8	0.0007	1	1
Br ₂ Ca	403	0.0007	64	49
S ₂ Ta	624	0.0007	81	100
CaI ₂	219	0.0008	36	25
PbS ₂ Sn	848	0.0008	126	86
Br ₂ La ₂ P	501	0.0008	64	49
LiNbS ₂	724	0.0008	81	100
O ₂ Pb ₂	452	0.0008	65	48
MoSe ₂	447	0.0008	57	73
Cl ₂ NSc ₂	824	0.0009	81	100
Cl ₂ OV	568	0.0009	70	72
Al ₂ Cl ₂ O ₂	748	0.0009	73	76

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Ge₂Te₂ (P1)

Structural and electronic properties

	Formula	Ge ₂ Te ₂
	Spacegroup	P1
	Prototype	FeSe
	Parent 3D	Ge ₄ Te ₄
	Source DB	ICSD
	DB ID	638005
DF2-C09	Binding energy [meV/ Å²]	35.05
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.8

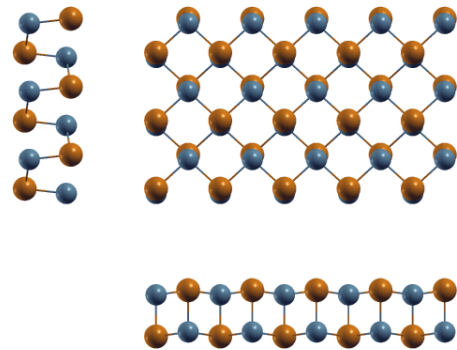


Band structure: Electronic band structure of Ge₂Te₂ (P1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ge₂Te₂ (P1) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	-4.20367737	0.00002201	0.00000000
a₂	-0.00002274	-4.44319338	0.00000000
a₃	0.00000000	0.00000000	17.88104871
	x [Å]	y [Å]	z [Å]
● Ge	-1.09626016	-1.83490829	-1.21091713
● Ge	-3.19789804	-4.05658236	1.21084644
● Te	-1.09608064	-2.14496985	1.51088710
● Te	-3.19807731	-4.36643411	-1.51081641



Orthographic projections: views of Ge₂Te₂ (P1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.136	1	1
Sm	6	0.1483	1	2
Nd	7	0.1458	1	3
CaI ₂	7	0.1292	1	1
I ₂ Pr	7	0.2306	1	1
I ₂ Yb	7	0.1275	1	1
HgI ₂	7	0.0226	1	1
Ba ₂ Hg	7	0.019	1	1
CNRb	7	0.2981	1	1
CKN	7	0.0555	1	1
I ₂ Nd	7	0.2318	1	1
I ₂ Tm	7	0.1284	1	1
DyI ₂	7	0.1312	1	1
CeI ₂	7	0.2297	1	1
I ₂ La	7	0.2378	1	1
Ba ₂ Cd	7	0.0173	1	1
Ir ₂ P ₂	8	0.2315	1	1
Ag ₂ Br ₂	8	0.2385	1	1
O ₂ Sn ₂	8	0.646	1	1
Cu ₂ S ₂	8	0.222	1	1
Au ₂ Br ₂	8	0.0154	1	1
Br ₂ Cu ₂	8	0.2242	1	1
N ₃ Na	8	0.3263	1	1
As ₂ Ir ₂	8	0.2416	1	1
Ge ₂ S ₂	8	0.0394	1	1
As ₄	8	0.223	1	1
P ₄	8	0.1848	1	1
O ₂ Sn ₂	8	0.2227	1	1
P ₂ Rh ₂	8	0.2213	1	1
F ₂ Tl ₂	8	0.2214	1	1
O ₂ Sn ₂	8	0.2126	1	1
Ag ₂ Te ₂	8	0.1985	1	1
AgClO ₂	8	0.12	1	1
La ₂ S ₂	8	0.0048	1	1
Ni ₂ Se ₂	8	0.2294	1	1
Ba ₂ Cu ₂	8	0.1274	1	1
As ₂ Rh ₂	8	0.2381	1	1
Ag ₂ I ₂	8	0.0235	1	1
Se ₂ Sn ₂	8	0.0078	1	1
O ₂ Sn ₂	8	0.2121	1	1
F ₄ Pb	9	0.0167	1	1
F ₄ Sn	9	0.0196	1	1
AsI ₂ La ₂	9	0.1244	1	1
GeI ₂ La ₂	9	0.1283	1	1
Cd ₂ I ₃	9	0.1244	1	1
NaO ₄	9	0.1961	1	1
AgNO ₃	9	0.1972	1	1
ClH ₃ O	9	0.1531	1	1
I ₂ La ₂ Sb	9	0.1363	1	1
Cl ₄ Mn	9	0.3473	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

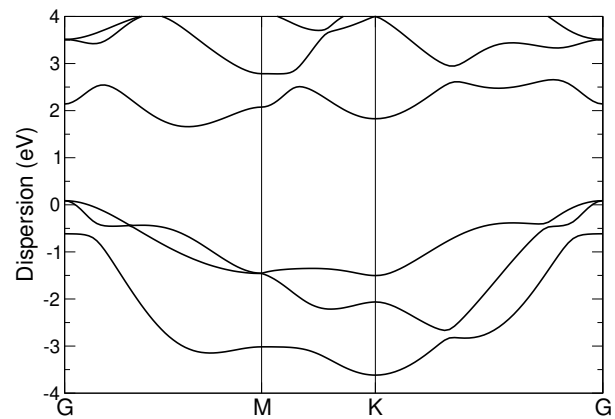
Formula	N° atoms	strain	cell size 1	cell size 2
Cl ₂ N ₂ Ti ₂	710	0.0005	56	81
Ce ₂ I ₂ S ₂	994	0.0005	100	99
Br ₂ Er ₂ O ₂	712	0.0006	61	78
Au ₂ Se ₂	996	0.0006	139	110
Fe ₂ SeTe	872	0.0007	94	124
I ₂ Yb	442	0.0007	61	66
Br ₂ N ₂ Ti ₂	398	0.0007	32	45
Ba ₂ Cu ₂	508	0.0007	61	66
I ₂ Tm	839	0.0007	116	125
Co ₂ Se ₂	568	0.0008	59	83
AgClO ₂	656	0.0008	70	94
KS ₂ Ti	448	0.0008	42	70
As ₂ Co ₂	568	0.0008	59	83
Cl ₂ Zn	378	0.0009	42	70
I ₂ Nd ₂ S ₂	526	0.0009	52	53
Sb ₂ Te ₂	796	0.001	100	99
K ₂ O ₂ Tl ₂	552	0.001	63	50
Te ₄ W ₂	452	0.0011	50	42
Br ₂ Mn	378	0.0011	42	70
Br ₂ Ca ₂ H ₂	712	0.0011	61	78
Dy ₂ I ₂ S ₂	54	0.0011	6	5
Se ₄ TiZr	616	0.0012	70	56
GeI ₂ La ₂	574	0.0012	61	66
Ca ₄ Cu ₂	34	0.0013	4	3
I ₂ La ₂ Te	956	0.0013	104	108
Ca ₂ Mn ₂ Si ₂	712	0.0013	61	78
I ₂ S ₂ Sm ₂	978	0.0013	96	99
Br ₂ O ₂ V ₂	868	0.0013	67	100
Br ₂ Co	378	0.0013	42	70
Hf ₂ Si ₂ Te ₂	734	0.0013	59	83
K	483	0.0013	96	99
Br ₂ Fe	378	0.0014	42	70
Cl ₂ Fe ₂ O ₂	204	0.0014	15	24
I ₂ Tm	442	0.0014	61	66
Br ₂ Ho ₂ O ₂	712	0.0015	61	78
I ₂ La ₂ Sb	879	0.0015	96	99
Ca ₂ Cl ₂	568	0.0015	59	83
Ge ₂ Se ₂ Zr ₂	734	0.0015	59	83
ClN ₂ Zr	342	0.0015	36	66
I ₂ Tm	390	0.0015	54	58
Tl	88	0.0016	15	28
CCL ₂ Lu ₂	518	0.0016	42	70
Sn	86	0.0016	14	30
Mg ₄	172	0.0016	15	28
AuI ₄ Li	536	0.0016	71	42
Br ₂ O ₂ Yb ₂	636	0.0016	54	70
GeI ₂ La ₂	506	0.0016	54	58
CaI ₂	390	0.0016	54	58
Cl ₂ O ₂ Ti ₂	838	0.0016	67	95
S ₂ W	508	0.0017	49	104

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

GeTe (P3m1 (156))

Structural and electronic properties

	Formula	GeTe
	Spacegroup	P3m1 (156)
	Prototype	GeTe
	Parent 3D	Ge ₂ Sb ₂ Te ₅
	Source DB	ICSD
	DB ID	637823
DF2-C09	Binding energy [meV/ Å²]	34.45
RVV10	Binding energy [meV/ Å²]	35.27
	Band gap (PBE) [eV]	1.57

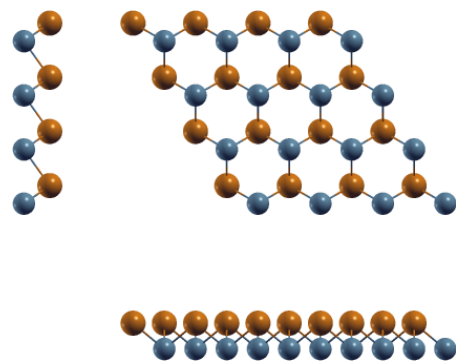


Band structure: Electronic band structure of GeTe (P3m1 (156)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of GeTe (P3m1 (156)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.89334753	0.00000000	0.00000000
a₂	-1.94667376	3.37173786	0.00000000
a₃	0.00000000	0.00000000	21.40892393
	x [Å]	y [Å]	z [Å]
● Ge	0.00000000	2.24782524	11.50804343
● Te	1.94667376	3.37173786	9.90088050



Orthographic projections: views of GeTe (P3m1 (156)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	3	3.0438	1	1
Tl	3	1.5306	1	1
AsSb	4	0.006	1	1
Bi ₂	4	0.4534	1	1
S ₂	4	0.0016	1	1
CaCl	4	0.1383	1	1
IrTe ₂	5	0.0009	1	1
CdCl ₂	5	0.0011	1	1
CdI ₂	5	0.4478	1	1
AgTe ₂	5	0.4213	1	1
MoSe ₂	5	1.5253	1	1
ReSe ₂	5	0.2585	1	1
S ₂ Ta	5	1.5872	1	1
Br ₂ Ca	5	0.4508	1	1
CaI ₂	5	2.9215	1	1
InSe ₂	5	0.0007	1	1
GeTe ₂	5	0.0021	1	1
HfTe ₂	5	0.0094	1	1
I ₂ Mn	5	0.0009	1	1
NSr ₂	5	0.0044	1	1
I ₂ Yb	5	0.4994	1	1
PbS ₂	5	0.0085	1	1
BiClTe	5	0.4487	1	1
LiO ₂	5	0.0674	1	1
Cl ₂ Zn	5	0.1513	1	1
FeI ₂	5	0.0031	1	1
I ₂ Ni	5	0.0019	1	1
S ₂ Ti	5	0.2503	1	1
NbS ₂	5	1.5838	1	1
CrI ₂	5	0.0035	1	1
BiBrTe	5	0.4623	1	1
Bi ₂ Pd	5	0.114	1	1
N ₂ W	5	4.8464	1	1
Cl ₂ Ni	5	0.2597	1	1
Cl ₂ Co	5	0.2498	1	1
CrTe ₂	5	0.2684	1	1
Br ₂ V	5	0.2574	1	1
ClNZr	5	0.2545	1	1
Cl ₂ Fe	5	0.2489	1	1
S ₂ Ta	5	1.5463	1	1
Se ₂ V	5	1.5367	1	1
Se ₂ Ti	5	0.2739	1	1
Br ₂ Ti	5	0.2675	1	1
AsSe ₂	5	0.2618	1	1
I ₂ Tm	5	2.9063	1	1
BiTe	5	0.479	1	1
CdO ₂	5	0.2496	1	1
BrNZr	5	0.2636	1	1
NbSe ₂	5	0.2603	1	1
CoI ₂	5	0.0056	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

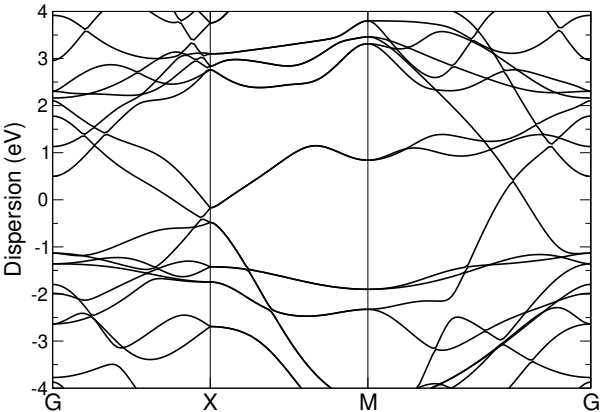
Formula	N° atoms	strain	cell size 1	cell size 2
AlLiTe ₂	418	0.0	81	64
Br ₂ Ti	462	0.0	81	100
Ce ₂ I ₂ S ₂	222	0.0001	36	25
Ca ₂ Si	147	0.0001	36	25
S ₂ Ta	219	0.0001	36	49
Cl ₂ Zr	290	0.0001	49	64
I ₂ La ₂ P	547	0.0001	91	73
FeH ₂ O ₂	503	0.0002	49	81
Br ₂ H ₂ Zr ₂	762	0.0002	81	100
Br ₂ H ₂ Zr ₂	552	0.0002	57	73
In ₂ S ₃	7	0.0002	1	1
CCl ₂ Sc ₂	479	0.0002	57	73
Br ₂ Cr	462	0.0003	81	100
Br ₂ Ca ₃ Si	314	0.0003	49	36
CdO ₂	290	0.0003	49	64
Cl ₂ Fe	290	0.0003	49	64
Cl ₂ Ni	371	0.0003	64	81
H ₂ Si ₂	6	0.0004	1	1
Cl ₂ Co	290	0.0004	49	64
I ₂ N ₂ Ti ₂	732	0.0004	96	90
Cl ₂ Sc ₂	562	0.0005	81	100
BiBrTe	443	0.0005	100	81
CNNa	334	0.0005	77	60
Gd ₂ I ₂ S ₂	314	0.0005	49	36
BrNZr	419	0.0005	73	91
Cl ₂ Hf ₂	314	0.0005	43	57
CaI ₂	243	0.0005	57	43
CrTe ₂	462	0.0006	81	100
Cl ₂ H ₂ Sc ₂	762	0.0006	81	100
Cl ₂ Zr ₂	406	0.0006	57	73
ReSe ₂	371	0.0006	64	81
I ₂ Tm	243	0.0006	57	43
LiNbS ₂	314	0.0006	43	57
InSe ₂	5	0.0007	1	1
S ₂ Ta	257	0.0007	43	57
ClNZr	333	0.0007	57	73
NbSe ₂	371	0.0007	64	81
ClKO ₃	178	0.0007	49	16
NbS ₂	219	0.0008	36	49
S ₂ Ti	290	0.0008	49	64
FeH ₂ O ₂	379	0.0008	37	61
Cu ₂ Sr ₂	474	0.0008	91	73
Se ₂ Ta	462	0.0008	81	100
Cu ₄ Te ₂	686	0.0008	100	81
Se ₂ Ta	371	0.0008	64	81
Cl ₂ Er ₂ H ₂	8	0.0008	1	1
GeI ₂ La ₂	329	0.0009	57	43
IrTe ₂	5	0.0009	1	1
Br ₂ Hf ₂	510	0.0009	73	91
Br ₂ Cr ₂ O ₂	602	0.0009	73	76

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

HfGeTe (P4/nmm (129))

Structural and electronic properties

	Formula	HfGeTe
	Spacegroup	P4/nmm (129)
	Prototype	PbClF
	Parent 3D	Hf ₂ Ge ₂ Te ₂
	Source DB	ICSD
	DB ID	25743
DF2-C09	Binding energy [meV/ Å²]	62.4
RVV10	Binding energy [meV/ Å²]	51.26
	Band gap (PBE) [eV]	0.0

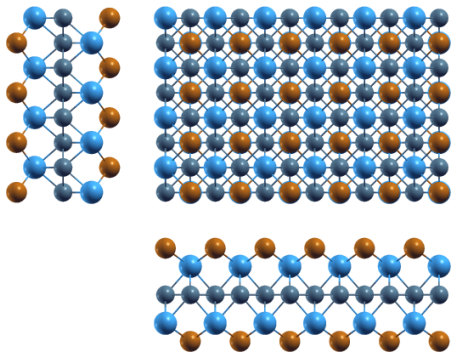


Band structure: Electronic band structure of HfGeTe (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of HfGeTe (P4/nmm (129)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.74044907	0.00000000	0.00000000
a₂		0.00000000	3.74044907	0.00000000
a₃		0.00000000	0.00000000	26.51804152
		x [Å]	y [Å]	z [Å]
●	Hf	0.00000000	1.87022454	15.39704250
●	Te	1.87022454	0.00000000	16.75636986
●	Hf	1.87022454	0.00000000	11.12099903
●	Ge	1.87022454	1.87022454	13.25902076
●	Ge	0.00000000	0.00000000	13.25902076
●	Te	0.00000000	1.87022454	9.76167166



Orthographic projections: views of HfGeTe (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Na	7	0.1086	1	1
InSe	8	0.1663	1	1
HgO	8	0.5827	1	1
Bi ₂	8	0.1729	1	1
AgTl	8	0.3698	1	1
S ₂	8	0.1303	1	1
PbTe	8	0.1683	1	1
Sb ₂	8	0.1498	1	1
IrTe ₂	9	0.1298	1	1
CrS ₂	9	0.1108	1	1
I ₂ Mg	9	0.1554	1	1
CdI ₂	9	0.1702	1	1
Br ₂ Ca	9	0.1716	1	1
CaI ₂	9	0.7552	1	1
HfTe ₂	9	0.1361	1	1
Br ₂ La	9	0.1557	1	1
Br ₂ Cu	9	0.117	1	1
I ₂ Yb	9	0.1954	1	1
BiClTe	9	0.1706	1	1
ReS ₂	9	0.1095	1	1
AuTe ₂	9	0.1426	1	1
BrCdI	9	0.1586	1	1
Cl ₂ Zn	9	0.0036	1	1
PdTe ₂	9	0.1405	1	1
I ₂ Zn	9	0.1467	1	1
BaF ₂	9	0.1621	1	1
BiBrTe	9	0.1771	1	1
Bi ₂ Pd	9	0.2107	1	1
GeI ₂	9	0.1535	1	1
Ba ₂ Hg	9	0.3889	1	1
PtS ₂	9	0.1089	1	1
Ba ₂ N	9	0.1373	1	1
AsKSn	9	0.1606	1	1
Te ₂ Zr	9	0.1365	1	1
PbTe ₂	9	0.1576	1	1
Cl ₂ Cu	9	0.1051	1	1
I ₂ Tm	9	0.1972	1	1
SnTe ₂	9	0.1513	1	1
GeI ₂	9	0.1685	1	1
STl ₂	9	0.1631	1	1
BiTe	9	0.1852	1	1
Se ₂ Yb	9	0.1537	1	1
BiTe ₂	9	0.154	1	1
GdI ₂	9	0.1806	1	1
CNNa	9	1.29	1	1
F ₂ Ni	9	0.0075	1	1
PtTe ₂	9	0.1422	1	1
Br ₂ Cd	9	0.1397	1	1
CdI ₂	9	0.1697	1	1
Ba ₂ Cd	9	0.3946	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

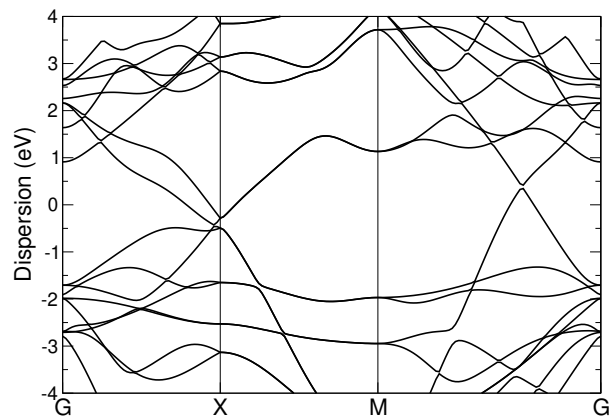
Formula	N° atoms	strain	cell size 1	cell size 2
F ₂ I ₂ Pb ₂	870	0.0001	81	64
Ag ₂ I ₂	316	0.0001	36	25
Ba ₂ Cd	678	0.0002	81	64
Sn	859	0.0003	113	181
HgO	736	0.0003	85	113
ReSe ₂	483	0.0004	48	65
Br ₂ V	483	0.0005	48	65
Mg ₆	510	0.0005	36	49
K	763	0.0005	113	85
Ca ₂ O ₂	708	0.0006	64	81
Pb ₂ Se ₂	222	0.0006	25	18
As ₂ Co ₂ Li ₂	12	0.0006	1	1
FeSe ₂	537	0.0006	49	81
AgClO ₄	930	0.0007	97	58
Se ₂ V	840	0.0008	81	118
Tl	451	0.0008	61	85
PbS ₂ Sn	732	0.0008	80	63
F ₄ Pb	815	0.0009	85	61
Cu ₂ Te ₂	10	0.001	1	1
S ₂ V	852	0.001	79	126
Mg ₃	258	0.001	25	36
Cl ₂ S ₂ Tl ₂	150	0.0011	16	9
S ₂ Ta	840	0.0011	81	118
I ₂ S ₂ Tb ₂	846	0.0011	87	54
Cl ₄ Mg ₂	942	0.0011	120	37
Mg ₄	706	0.0011	61	85
HgI ₂	291	0.0012	36	25
Ho ₂ I ₂ Se ₂	228	0.0012	24	14
N ₃ Na	352	0.0012	40	28
MoS ₂	852	0.0012	79	126
S ₂ W	852	0.0012	79	126
Cl ₂ Ni	483	0.0012	48	65
Cl ₂ Zr ₂	548	0.0013	48	65
MoS ₂	852	0.0013	79	126
Bi ₂ Se ₂	292	0.0014	32	25
Tl	604	0.0014	81	118
Cl ₄ Mn	230	0.0014	25	16
I ₂ N ₂ Zr ₂	114	0.0015	10	9
Cu ₂ Na ₂ Te ₂	510	0.0015	49	36
Se ₂ Sn ₂	504	0.0015	56	42
AgClO ₂	854	0.0015	85	86
CKN	819	0.0015	103	67
Gd ₂ I ₂ S ₂	774	0.0016	80	49
ClH ₃ O	698	0.0016	73	52
Cu ₄ Te ₂	996	0.0016	89	77
BiBrTe	885	0.0016	103	89
Br ₂ Fe	603	0.0016	62	77
CCL ₂ Lu ₂	757	0.0016	62	77
Br ₂ Co	603	0.0016	62	77
As ₂	526	0.0016	62	77

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

HfSiSe (P4/nmm (129))

Structural and electronic properties

	Formula	HfSiSe
	Spacegroup	P4/nmm (129)
	Prototype	PbClF
	Parent 3D	Hf ₂ Si ₂ Se ₂
	Source DB	ICSD
	DB ID	25736
DF2-C09	Binding energy [meV/ Å²]	59.23
RVV10	Binding energy [meV/ Å²]	42.55
	Band gap (PBE) [eV]	0.0

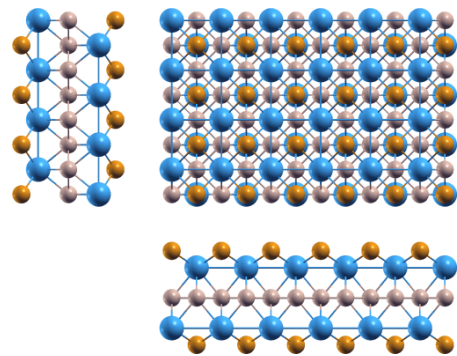


Band structure: Electronic band structure of HfSiSe (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of HfSiSe (P4/nmm (129)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.51894855	0.00000000	0.00000000
a₂		0.00000000	3.51894855	0.00000000
a₃		0.00000000	0.00000000	26.25921354
		x [Å]	y [Å]	z [Å]
●	Hf	1.75947427	0.00000000	10.98816739
●	Se	0.00000000	1.75947427	9.80067509
●	Hf	0.00000000	1.75947427	15.27104615
●	Si	1.75947427	1.75947427	13.12960677
●	Si	0.00000000	0.00000000	13.12960677
●	Se	1.75947427	0.00000000	16.45853845



Orthographic projections: views of HfSiSe (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	7	0.2187	1	1
AsSb	8	0.1478	1	1
Bi ₂	8	0.7874	1	1
K	8	1.6773	1	2
GeTe	8	0.1536	1	1
S ₂	8	0.1552	1	1
PbTe	8	0.7717	1	1
Mg ₂	8	0.5842	1	1
Sb ₂	8	0.1814	1	1
IrTe ₂	9	0.1545	1	1
I ₂ Mg	9	0.1885	1	1
CdCl ₂	9	0.1526	1	1
CdI ₂	9	0.7784	1	1
PSn ₂	9	0.1305	1	1
Br ₂ Zn	9	0.1388	1	1
Br ₂ Ca	9	0.7832	1	1
InSe ₂	9	0.1529	1	1
AsSn ₂	9	0.1333	1	1
GeTe ₂	9	0.1516	1	1
SiTe ₂	9	0.1423	1	1
HfTe ₂	9	0.1632	1	1
I ₂ Pr	9	0.3813	1	1
I ₂ Mn	9	0.1527	1	1
S ₂ Zr	9	0.13	1	1
Br ₂ La	9	0.189	1	1
NSr ₂	9	0.1493	1	1
PbS ₂	9	0.1454	1	1
BiClTe	9	0.7798	1	1
AuTe ₂	9	0.172	1	1
BrCdI	9	0.1926	1	1
PdTe ₂	9	0.1691	1	1
FeI ₂	9	0.1505	1	1
I ₂ Ni	9	0.1518	1	1
Mg ₃	9	0.2121	1	1
Te ₂ Ti	9	0.139	1	1
CrI ₂	9	0.1501	1	1
I ₂ Zn	9	0.1774	1	1
BaF ₂	9	0.1971	1	1
RhTe ₂	9	0.1355	1	1
GeI ₂	9	0.1862	1	1
NbS ₂	9	0.1088	1	1
S ₂ Ta	9	0.1086	1	1
Ba ₂ N	9	0.1649	1	1
AsKSn	9	0.1951	1	1
Te ₂ Zr	9	0.1638	1	1
PbTe ₂	9	0.1913	1	1
I ₂ Nd	9	0.3834	1	1
NiTe ₂	9	0.1418	1	1
S ₂ Sn	9	0.1302	1	1
SnTe ₂	9	0.1833	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

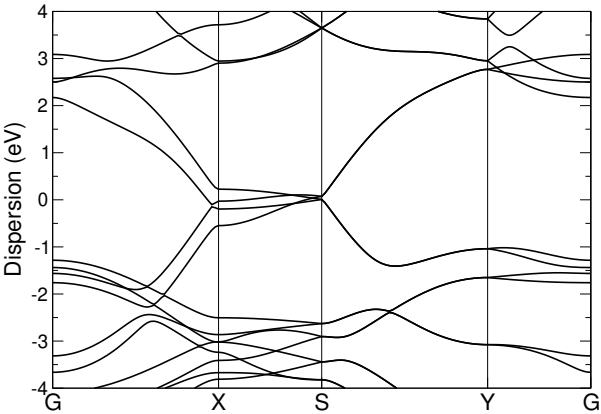
Formula	N° atoms	strain	cell size 1	cell size 2
H ₂ I ₂ Sr ₂	612	0.0	61	41
F ₂ I ₂ Yb ₂	690	0.0	65	50
In	451	0.0001	61	85
I ₂ Pr	852	0.0001	101	82
Ag ₂ Br ₂	742	0.0001	81	64
I ₂ La	687	0.0001	82	65
Br ₂ F ₂ Pb ₂	510	0.0002	49	36
Cl ₄ Mn	141	0.0002	16	9
Nd	159	0.0002	20	39
Ba ₂ F ₂ I ₂	780	0.0002	81	49
Ir ₂ P ₂	924	0.0003	100	81
Br ₂ Lu ₂ S ₂	258	0.0003	27	16
Ba ₂ Ge ₂ Mn ₂	690	0.0003	65	50
O ₄ PSn	930	0.0003	97	58
As ₂ Rh ₂	742	0.0004	81	64
Eu ₂ H ₂ I ₂	690	0.0004	65	50
Br ₂ O ₂ Pr ₂	870	0.0004	81	64
Br ₂ Lu ₂ S ₂	258	0.0004	27	16
S ₂ Sn ₂	734	0.0004	83	59
FeO ₂	411	0.0004	36	65
Br ₂ F ₂ Sr ₂	510	0.0005	49	36
F ₂ I ₂ Tm ₂	678	0.0005	64	49
I ₂ Pr	843	0.0005	100	81
I ₂ Nd	843	0.0005	100	81
As ₂ Fe ₂	10	0.0005	1	1
H ₂ I ₂ Yb ₂	882	0.0005	82	65
Tl	586	0.0006	81	100
Bi ₂ Mn ₂	354	0.0006	35	36
Cu ₂ Na ₂ Se ₂	678	0.0006	64	49
Bi ₂ I ₂ O ₂	678	0.0006	64	49
Mg ₂	736	0.0006	85	113
Mg ₃	627	0.0006	64	81
I ₂ La	678	0.0006	81	64
Cl ₂ F ₂ Pb ₂	678	0.0007	64	49
Ge ₂ Se ₂	938	0.0007	105	77
CeI ₂	852	0.0007	101	82
Ag ₂ I ₂	896	0.0007	106	65
O ₄ PTl	780	0.0007	81	49
I ₂ O ₂ Sm ₂	690	0.0007	65	50
PbS ₂ Sn	632	0.0007	72	50
Ho ₂ S ₂	602	0.0008	65	53
Ba ₂ Ge ₂ Mn ₂	678	0.0008	64	49
I ₂ La ₂ O ₂	876	0.0008	85	61
F ₄ Pb	230	0.0009	25	16
Mg ₄	886	0.0009	81	100
Ni ₂ Se ₂	934	0.0009	101	82
As ₂ Cd ₂ K ₂	930	0.001	97	58
Br ₂ S ₂ Yb ₂	228	0.001	24	14
CS ₃ Tl ₂	834	0.0011	112	27
F ₂ I ₂ Yb ₂	678	0.0011	64	49

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Hg₂N₂Cl₂ (Pmma)

Structural and electronic properties







Formula	Hg ₂ N ₂ Cl ₂
Spacegroup	Pmma
Prototype	ClHgN
Parent 3D	Cl ₂ Hg ₂ N ₂
Source DB	MPDS
DB ID	S1500374
DF2-C09 Binding energy [meV/ Å²]	31.77
RVV10 Binding energy [meV/ Å²]	N/A
Band gap (PBE) [eV]	0.0

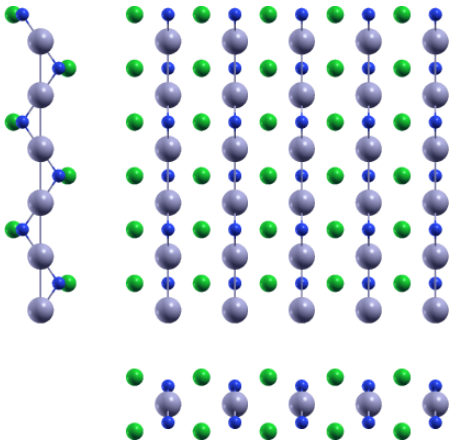


Band structure: Electronic band structure of Hg₂N₂Cl₂ (Pmma) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Hg₂N₂Cl₂ (Pmma) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		0.00000000	−4.26219108	0.00000000
a₂		6.85594376	0.00000000	0.00000000
a₃		0.00000000	0.00000000	18.99617758
		x [Å]	y [Å]	z [Å]
	N	5.14195782	2.13109554	1.16090144
	Cl	5.14195782	0.00000000	1.72697641
	Hg	3.42797188	2.13109554	0.00000000
	Hg	0.00000000	2.13109554	0.00000000
	N	1.71398594	2.13109554	−1.16090144
	Cl	1.71398594	0.00000000	−1.72697641



Orthographic projections: views of Hg₂N₂Cl₂ (Pmma) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
InSe	8	0.4591	1	1
Bi ₂	8	0.4731	1	1
PbTe	8	0.4633	1	1
Sb ₂	8	0.4227	1	1
I ₂ Mg	9	0.4353	1	1
CdI ₂	9	0.4675	1	1
Br ₂ Zn	9	1.7004	1	1
Br ₂ Ca	9	0.4704	1	1
HfS ₂	9	1.5731	1	1
Br ₂ La	9	0.4361	1	1
BiClTe	9	0.4684	1	1
AuTe ₂	9	0.4058	1	1
BrCdI	9	0.4424	1	1
Te ₂ Ti	9	1.7028	1	1
I ₂ Zn	9	0.4156	1	1
BaF ₂	9	0.4501	1	1
RhTe ₂	9	1.6688	1	1
GeI ₂	9	0.4311	1	1
AsKSn	9	0.4468	1	1
GeI ₂	9	0.4639	1	1
STl ₂	9	0.4523	1	1
Se ₂ Yb	9	0.4317	1	1
BiTe ₂	9	0.4323	1	1
PtTe ₂	9	0.405	1	1
CdI ₂	9	0.4664	1	1
I ₂ Pr	9	0.4686	1	1
HfSe ₂	9	1.7029	1	1
Li ₂ Tl ₂	10	0.1447	1	1
LiMnTe ₂	10	0.4646	1	1
CdClHO	10	1.663	1	1
AsLi ₃	10	0.4598	1	1
Cl ₂ Y ₂	10	1.6907	1	1
Cl ₂ La ₂	10	0.4106	1	1
MnNaTe ₂	10	0.4415	1	1
AsCuLi ₂	10	0.4301	1	1
Cu ₂ I ₂	10	0.4375	1	1
In ₂ Se ₂	10	0.4132	1	1
Ga ₂ Te ₂	10	0.4307	1	1
As ₂ Sn ₂	10	0.4083	1	1
CaCl	10	0.1311	1	2
Ga ₂ Se ₂	10	1.6852	1	1
Br ₂ HLa	10	0.4291	1	1
CeLi ₂ P ₂	11	0.4282	1	1
As ₂ Li ₂ Nd	11	0.4576	1	1
Nd	11	0.0965	1	5
Ba ₂ Ni ₃	11	0.4307	1	1
Sb ₂ Se ₂ Te	11	0.433	1	1
Bi ₂ STe ₂	11	0.4614	1	1
Li ₂ P ₂ Pr	11	0.4239	1	1
As ₂ CeLi ₂	11	0.4634	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

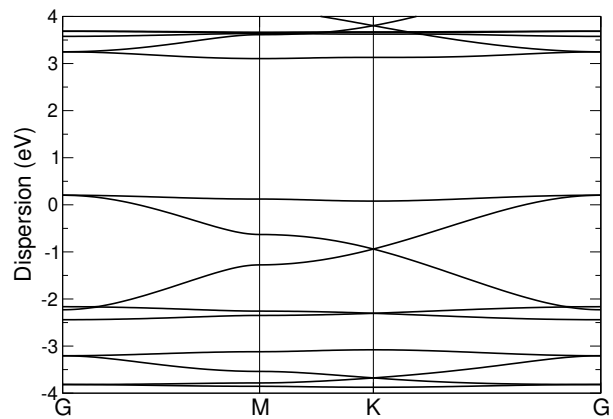
Formula	N° atoms	strain	cell size 1	cell size 2
STl ₂	561	0.0001	48	91
K ₂ PtSe ₂	240	0.0001	25	18
Cl ₂ Er ₂ O ₂	882	0.0003	44	103
Se ₂ Zr	573	0.0004	44	103
SiTe ₂	573	0.0004	44	103
CoI ₂	732	0.0005	57	130
AsSb	602	0.0006	57	130
Au ₂ Br ₂	472	0.0006	38	61
Bi ₂ Te ₃	960	0.0006	65	114
Au ₂ Br ₂	448	0.0006	36	58
BiITe	732	0.0007	65	114
CS ₂ Ta ₂	519	0.0007	24	75
Cl ₂ Ti	369	0.0007	24	75
Li ₂ P ₂ Pr	240	0.0007	15	30
P ₂	294	0.0007	24	75
As ₂ Li ₂ Nd	385	0.0008	25	47
Ga ₂ Ge ₂ Te ₂	270	0.0008	15	30
Bi ₂ Se ₂ Te	385	0.0008	25	47
AlLiTe ₂	846	0.0008	65	114
Sb ₂	150	0.0008	15	30
CdClHO	334	0.0008	21	52
Hf ₂ I ₂ N ₂	438	0.0009	21	52
Au ₂ Br ₂	410	0.0009	33	53
BaF ₂	561	0.0009	48	91
C ₂ I ₂ Y ₂	546	0.0009	30	61
NiTe ₂	573	0.0009	44	103
Br ₂ La ₂	210	0.0009	15	30
I ₂ Lu ₂ Se ₂	390	0.001	30	35
CNb ₂ S ₂	519	0.001	24	75
Sb ₂ SeTe ₂	385	0.001	25	47
In ₂ Te ₃	385	0.0011	25	47
Ga ₂ I ₂ Y ₂	834	0.0011	48	91
I ₂ V	573	0.0011	44	103
PTe ₂ Zr ₂	992	0.0011	57	130
Se ₂ Sn	732	0.0012	57	130
HN ₃ OZn	594	0.0012	24	75
ClNZr	102	0.0012	7	20
Bi ₂	338	0.0012	35	64
Ga ₂ Gd ₂ I ₂	594	0.0012	35	64
C	122	0.0012	7	80
Cl ₂ Gd ₂	236	0.0012	16	35
Br ₂ H ₂ Zr ₂	162	0.0012	7	20
Cl ₂ Tb ₂	236	0.0012	16	35
Br ₂ O ₂ Yb ₂	726	0.0013	40	81
C ₂ Br ₂ Y ₂	960	0.0013	50	110
Ga ₂ I ₂ Tb ₂	594	0.0013	35	64
Fe ₂ Te ₂	564	0.0013	40	81
SnTe ₂	180	0.0014	15	30
C ₂ Cl ₂ Y ₂	138	0.0014	7	16
Cu ₂ O ₂	248	0.0014	18	35

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Hg₃Br₂ (P-3m1 (164))

Structural and electronic properties

	Formula	Hg ₃ Br ₂
	Spacegroup	P-3m1 (164)
	Prototype	Br ₂ Hg ₃
	Parent 3D	Br ₄ Hg ₆ Se ₆ Zn ₂
	Source DB	ICSD
	DB ID	186941
DF2-C09	Binding energy [meV/ Å²]	65.99
RVV10	Binding energy [meV/ Å²]	42.69
	Band gap (PBE) [eV]	0.0

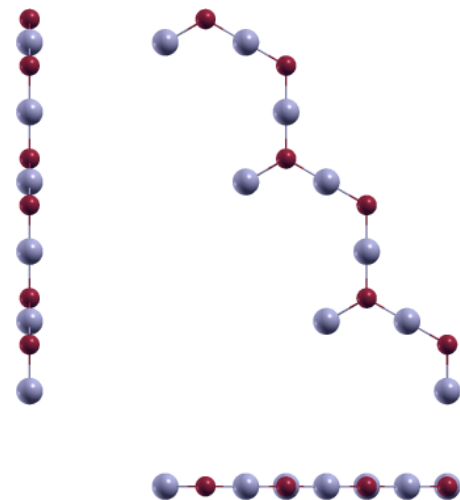


Band structure: Electronic band structure of Hg₃Br₂ (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Hg₃Br₂ (P-3m1 (164)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		10.13375145	0.00000000	0.00000000
a₂		-5.06687573	8.77608619	0.00000000
a₃		0.00000000	0.00000000	22.09269775
		x [Å]	y [Å]	z [Å]
●	Hg	-2.53343786	4.38804310	11.04634887
●	Hg	5.06687573	0.00000000	11.04634887
●	Hg	2.53343786	4.38804310	11.04634887
●	Br	5.06687573	2.92536206	11.05197091
●	Br	-0.00000000	5.85072413	11.04072683



Orthographic projections: views of Hg₃Br₂ (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
GeI ₃ Rb	10	0.0034	1	1
K	11	0.1291	1	6
Bi ₂ Se ₄	11	0.1459	1	1
Tl	14	0.0079	1	9
K ₂ O ₄	17	0.1181	1	2
HgI ₂	17	0.1231	1	4
I ₄ Zr ₂	17	0.5938	1	2
Li ₂ Tl ₂	21	0.0015	1	4
Au ₂ I ₂	21	0.0441	1	4
La ₂ S ₂	21	0.0505	1	4
Ag ₂ I ₂	21	0.1237	1	4
Se ₂ Sn ₂	21	0.0476	1	4
F ₄ Pb	25	0.0406	1	4
NaO ₄	25	0.0082	1	4
AgNO ₃	25	0.0091	1	4
BrKO ₃	25	0.1501	2	3
Au ₂ K ₂ S ₂	28	0.0513	2	3
Cu ₂ Na ₂ Te ₂	29	0.0439	1	4
Au ₂ Br ₂	29	0.118	1	6
N ₃ Na	29	0.3164	1	6
O ₄ PTl	29	0.1258	1	4
Cl ₂ Hg ₂ N ₂	29	0.2996	1	4
Cl ₂ Mn	32	0.0023	1	9
MoSe ₂	32	0.0086	1	9
S ₂ Ta	32	0.0002	1	9
S ₂ Ti	32	0.0048	1	9
NbS ₂	32	0.0006	1	9
Cl ₂ Co	32	0.0045	1	9
NbS ₂	32	0.0049	1	9
ClNZr	32	0.008	1	9
Cl ₂ Fe	32	0.0037	1	9
S ₂ Ta	32	0.0057	1	9
Se ₂ V	32	0.007	1	9
CdO ₂	32	0.0043	1	9
Cl ₂ Zr	32	0.0041	1	9
Se ₂ W	32	0.0084	1	9
Cl ₂ S ₂ Tl ₂	35	0.2375	1	5
BN	37	0.0045	1	16
K	38	0.0199	4	18
K	38	0.0343	4	18
Hg ₄ O ₂	39	0.0399	3	4
HgI ₂	40	0.0504	2	10
Te ₂ Zr	40	0.0907	2	10
Cl ₂ Hf ₂	41	0.001	1	9
Bi ₂ Mn ₂	41	0.1051	1	9
C	41	0.0085	1	36
Cl ₂ Zr ₂	41	0.0094	1	9
LiNbS ₂	41	0.0001	1	9
H ₂ I ₂ Sr ₂	41	0.1259	1	6
As ₂ Mg ₂ Na ₂	41	0.1288	1	6

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

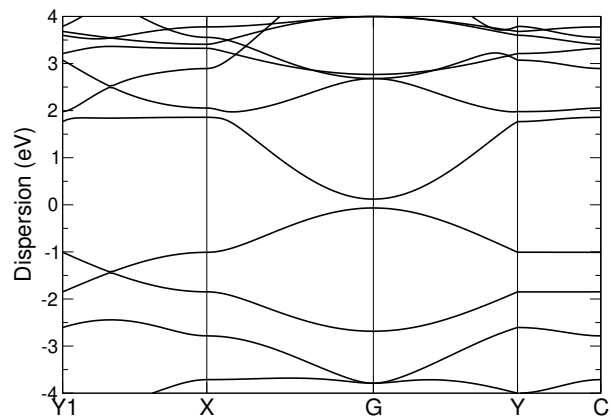
Formula	N° atoms	strain	cell size 1	cell size 2
LiNbS ₂	41	0.0001	1	9
S ₂ Ta	32	0.0002	1	9
Cl ₂ La ₂	120	0.0002	4	25
O ₂ Zn	345	0.0002	9	100
Se ₂ Zr	237	0.0003	9	64
Cu ₂ Sr ₂	241	0.0004	9	49
Dy ₂ I ₂ S ₂	566	0.0005	16	81
Cl ₂ Er ₂ O ₂	429	0.0005	9	64
SbSe ₂ Tl	126	0.0005	6	24
Au ₂ K ₂ S ₂	614	0.0005	40	69
Cl ₄ KTI	675	0.0005	39	80
I ₂ La ₂ P	290	0.0005	9	49
I ₂ V	237	0.0006	9	64
La ₂ S ₂	121	0.0006	5	24
NbS ₂	32	0.0006	1	9
SiTe ₂	237	0.0007	9	64
IKO ₃	745	0.0008	49	100
As ₂ Sn ₂	120	0.0008	4	25
Br ₂ Gd ₂	120	0.0009	4	25
IKO ₃	590	0.001	39	79
Cl ₂ Ho ₂ O ₂	429	0.001	9	64
Cl ₂ Hf ₂	41	0.001	1	9
DyI ₂	323	0.0011	16	81
NiTe ₂	237	0.0013	9	64
Br ₃ Cs	56	0.0014	4	9
BiBrTe	192	0.0014	9	49
In ₂ Se ₂	120	0.0014	4	25
CuO ₂	265	0.0014	8	75
Li ₂ Tl ₂	21	0.0015	1	4
Br ₂ Er ₂	120	0.0015	4	25
GdI ₂	192	0.0015	9	49
I ₂ S ₂ Tb ₂	566	0.0016	16	81
CaI ₂	323	0.0017	16	81
Cl ₂ O ₂ Y ₂	429	0.0017	9	64
Br ₂ Er ₂ S ₂	360	0.0018	12	50
Cl ₂ NSc ₂	50	0.0018	1	9
Br ₂ Lu ₂ S ₂	645	0.0019	21	90
Br ₂ Lu ₂ S ₂	645	0.0019	21	90
CaClHO	301	0.0019	9	64
Br ₂ S ₂ Yb ₂	360	0.002	12	50
FeH ₂ O ₂	545	0.002	9	100
AuTe ₂	95	0.002	4	25
Cl ₂ O ₂ Tm ₂	429	0.002	9	64
Ga ₂ Se ₂	301	0.0022	9	64
K ₂ O ₂ Tl ₂	411	0.0022	15	56
Cl ₂ Mn	32	0.0023	1	9
Cl ₄ Cu ₂	963	0.0023	51	118
IO ₃ Tl	65	0.0024	4	9
PtTe ₂	95	0.0024	4	25
Ca ₂ Cl ₂ F ₂	381	0.0025	9	56

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Hg₃N₂ (P321)

Structural and electronic properties

	Formula	Hg ₃ N ₂
	Spacegroup	P321
	Prototype	Hg ₃ N ₂
	Parent 3D	Br ₄ Hg ₄ N ₂
	Source DB	MPDS
	DB ID	S1711206
DF2-C09	Binding energy [meV/ Å²]	118.46
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.19

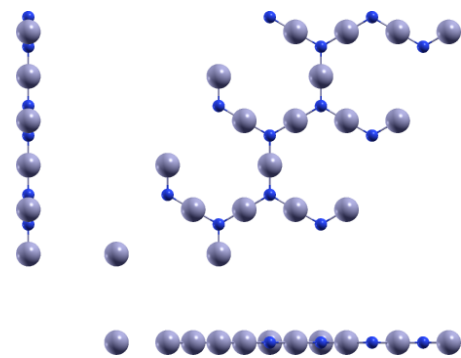


Band structure: Electronic band structure of Hg₃N₂ (P321) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Hg₃N₂ (P321) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.47897373	6.02575925	0.00000000
a₂		-3.47897373	6.02575925	0.00000000
a₃		0.00000000	0.00000000	12.00000000
		x [Å]	y [Å]	z [Å]
●	Hg	0.00000000	0.00000000	0.00000000
●	Hg	3.47897373	0.00000000	0.00000000
●	Hg	1.73948686	-3.01287963	0.00000000
●	N	1.73948686	-5.02146605	0.00000000
●	N	1.73948686	-1.00429321	0.00000000



Orthographic projections: views of Hg₃N₂ (P321) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
GeS ₂	8	0.1628	1	1
Cl ₂ Rb ₂	9	0.1396	1	1
Na	9	0.0095	1	4
As ₂ Fe ₂	9	0.163	1	1
In	9	0.0444	1	4
K ₂ PdS ₂	10	0.5035	1	1
K ₂ PtTe ₂	10	0.6146	1	1
H ₂ Na ₂ Pd	10	0.1627	1	1
FKO ₂ Se	10	0.1155	1	1
ClKO ₃	10	0.009	1	1
K ₂ PtSe ₂	10	0.5323	1	1
K ₂ PdSe ₂	10	0.5145	1	1
K ₂ PtS ₂	10	0.5003	1	1
BrKO ₃	10	0.0045	1	1
I ₂ Lu ₂ Se ₂	11	0.1205	1	1
Hf ₂ Se ₂ Si ₂	11	0.1631	1	1
Cl ₄ Cu ₂	11	0.1253	1	1
Gd ₂ I ₂ S ₂	11	0.1171	1	1
Cl ₄ Mg ₂	11	0.0337	1	1
I ₂ S ₂ Tb ₂	11	0.1176	1	1
Cl ₂ Ga ₂ Te ₂	11	0.1201	1	1
Cl ₂ Cu	11	0.1088	1	2
Sn	11	0.1271	1	6
Br ₂ Ga ₂ Te ₂	11	0.1196	1	1
Ca ₄ Cu ₂	11	0.1181	1	1
CuO ₂	11	0.142	1	2
Dy ₂ I ₂ S ₂	11	0.1179	1	1
Cl ₄ KTl	11	0.1475	1	1
Sb ₂	12	0.1637	2	1
I ₂ Zn	13	0.1635	2	1
Bi ₂ Se ₂	13	0.1157	1	2
Mg ₂	13	0.0384	1	4
Br ₂ Er ₂	14	0.1632	2	1
Cl ₂ La ₂	14	0.1633	2	1
Br ₂ Gd ₂	14	0.1632	2	1
In ₂ Se ₂	14	0.1634	2	1
As ₂ Sn ₂	14	0.1632	2	1
Br ₂ La ₂	14	0.1637	2	1
Li ₂ P ₂ Pr	15	0.1638	2	1
FKO ₂ Se	15	0.1094	1	2
Ho ₂ I ₂ S ₂	16	0.1549	2	1
AlH ₄ Na	16	0.155	2	1
Ga ₂ Ge ₂ Te ₂	16	0.1638	2	1
I ₂ S ₂ Yb ₂	16	0.1551	2	1
F ₂ Lu ₂ Se ₂	16	0.1636	2	1
C ₄ Ca ₂	16	0.1738	2	1
I ₂ Sb ₂ Te ₂	16	0.1513	2	1
Er ₂ I ₂ S ₂	16	0.155	2	1
I ₂ S ₂ Tm ₂	16	0.1551	2	1
I ₂ Lu ₂ Se ₂	17	0.0677	1	2

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

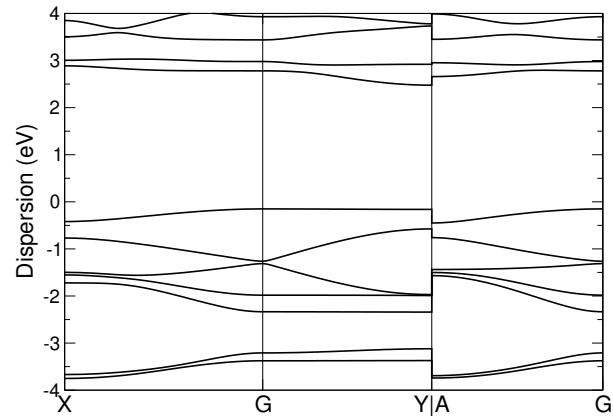
Formula	N° atoms	strain	cell size 1	cell size 2
I ₂ La ₂ P	445	0.0001	25	64
Br ₂ Mg	368	0.0001	25	81
CrI ₂	368	0.0002	25	81
Te ₂ Zr	227	0.0002	16	49
Br ₂ Hf ₂	21	0.0002	1	4
Ba ₂ F ₂ I ₂	675	0.0002	39	80
I ₂ Pr ₂ S ₂	74	0.0002	4	9
FeI ₂	368	0.0002	25	81
PbTe ₂	120	0.0003	9	25
O ₂ Sn ₂	499	0.0003	27	91
MnNaTe ₂	145	0.0003	9	25
NbSe ₂	17	0.0004	1	4
Br ₂ OV	55	0.0005	3	10
CoH ₂ O ₂	485	0.0005	16	81
S ₂ Sn ₂	511	0.0005	35	84
Cu ₃ Se ₃	374	0.0006	16	49
BrNZr	17	0.0006	1	4
I ₂ Pb	47	0.0006	4	9
In ₂ Se ₃	325	0.0006	16	49
C ₂ F ₂	301	0.0007	9	64
HfTe ₂	227	0.0007	16	49
SSb ₂ Te ₂	170	0.0007	9	25
O ₄ PTl	675	0.0007	39	80
AsSe ₂	17	0.0007	1	4
BrCdI	120	0.0007	9	25
Sm	109	0.0008	9	64
GdI ₂	317	0.0009	25	64
Ba ₂ N	227	0.0009	16	49
As ₂ O ₃	490	0.0009	37	61
Er ₂ F ₂ Se ₂	374	0.0009	16	49
Ag ₂	38	0.0009	4	9
Cu ₂ Sr ₂	381	0.001	25	64
NSr ₂	368	0.001	25	81
Te ₄ TiZr	736	0.0011	50	81
Br ₂ Er ₂ S ₂	821	0.0012	49	96
AlH ₄ Na	684	0.0012	42	79
Ba ₂ Pt	47	0.0012	4	9
Se ₂ Sn	368	0.0013	25	81
GeTe ₂	368	0.0013	25	81
Pt ₂ Te ₂	276	0.0014	16	49
Br ₂ Gd ₂ Ge	170	0.0015	9	25
Cu ₂ I ₂	145	0.0015	9	25
Cl ₂ Y ₂	530	0.0015	25	81
I ₂ Ni	368	0.0015	25	81
ReS ₂	323	0.0015	16	81
HNiO ₂	241	0.0015	9	49
NaPSn	227	0.0016	16	49
AgClO ₂	633	0.0016	37	112
Se ₂ Ta	17	0.0016	1	4
NbSe ₂	17	0.0017	1	4

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Hg₃S₂ (C2/m (12))

Structural and electronic properties

	Formula	Hg ₃ S ₂
	Spacegroup	C2/m (12)
	Prototype	Br ₂ Hg ₃
	Parent 3D	Hg ₃ Bi ₂ S ₂ Cl ₈
	Source DB	ICSD
	DB ID	237618
DF2-C09	Binding energy [meV/ Å²]	222.02
RVV10	Binding energy [meV/ Å²]	94.77
	Band gap (PBE) [eV]	0.0

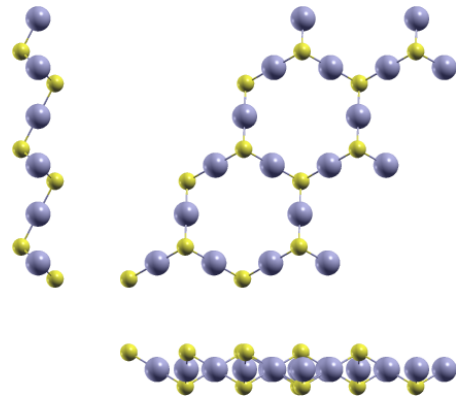


Band structure: Electronic band structure of Hg₃S₂ (C2/m (12)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Hg₃S₂ (C2/m (12)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		7.59816466	−0.00005812	0.00000000
a₂		3.90254259	6.51937631	0.00000000
a₃		0.00000000	0.00000000	22.25193804
		x [Å]	y [Å]	z [Å]
●	S	3.84316543	2.17854583	12.26118866
●	Hg	1.95544382	1.10846751	11.12596910
●	Hg	5.75452628	1.10843853	11.12596905
●	Hg	3.90671527	4.36815582	11.12596911
●	S	0.06771766	0.03838661	9.99074917



Orthographic projections: views of Hg₃S₂ (C2/m (12)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
CKN	8	0.2442	1	1
Fe ₂ Te ₂	9	0.1616	1	1
Ca ₂ Cl ₂	9	0.1617	1	1
Cl ₂ Rb ₂	9	0.1127	1	1
Cu ₂ S ₂	9	0.1628	1	1
O ₂ Sn ₂	9	0.163	1	1
Br ₃ Cs	9	0.2611	1	1
P ₂ Rh ₂	9	0.1627	1	1
F ₂ Tl ₂	9	0.1627	1	1
As ₂ Ru ₂	9	0.1617	1	1
IO ₃ Tl	10	0.2559	1	1
ClKO ₃	10	0.2659	1	1
KNO ₃	10	0.2419	1	1
Br ₂ Ca ₂ H ₂	11	0.1623	1	1
Br ₂ O ₂ Tm ₂	11	0.1618	1	1
Br ₂ O ₂ Y ₂	11	0.1628	1	1
Hg ₄ O ₂	11	0.1402	1	1
Br ₂ Er ₂ O ₂	11	0.1621	1	1
Br ₂ Dy ₂ O ₂	11	0.1628	1	1
Cl ₄ Mg ₂	11	0.032	1	1
Br ₂ Ho ₂ O ₂	11	0.1624	1	1
Br ₂ O ₂ Yb ₂	11	0.1615	1	1
AuI ₄ Li	11	0.5739	1	1
Ca ₂ Mn ₂ Si ₂	11	0.1624	1	1
CS ₃ Tl ₂	11	0.63	1	1
Cl ₄ KTl	11	0.1167	1	1
Br ₂ Ca ₃ Si	11	0.1189	1	1
HgO	13	0.0452	1	4
AsSb	13	0.009	1	4
Pb ₂ Se ₂	13	0.4259	1	2
Au ₂ Se ₂	13	0.0128	1	2
BiTe	13	0.1632	2	1
SbSe ₂ Tl	13	0.0326	1	2
AlLiTe ₂	14	0.1631	2	1
CKN	14	0.2337	1	3
F ₂ Ni	14	0.1143	1	3
Bi ₂ Te ₃	15	0.1632	2	1
K	16	0.0489	2	6
Hg ₄ O ₂	16	0.1003	2	1
Ge ₂ I ₂ La ₂	16	0.1635	2	1
CdCl ₂	17	0.0138	1	4
Bi ₂ In ₂	17	0.2166	1	3
PSn ₂	17	0.0134	1	4
Br ₂ Zn	17	0.0049	1	4
Cu ₄ Te ₂	17	0.1418	1	2
InSe ₂	17	0.0142	1	4
AsSn ₂	17	0.0101	1	4
GeTe ₂	17	0.0128	1	4
SiTe ₂	17	0.0047	1	4
I ₂ Mn	17	0.014	1	4

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

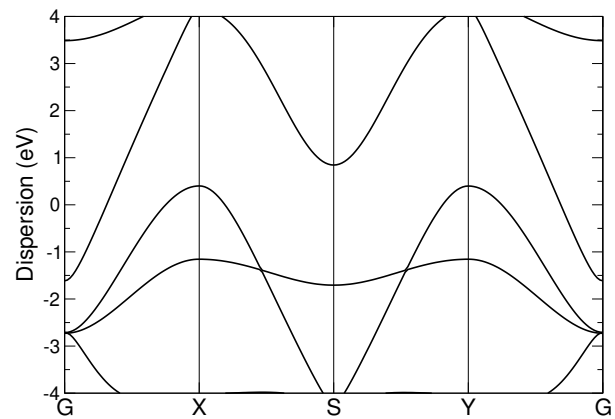
Formula	N° atoms	strain	cell size 1	cell size 2
Br ₂ O ₂ Yb ₂	768	0.0002	30	103
SbSe ₂ Tl	668	0.0004	48	107
Fe ₂ Te ₂	562	0.0005	30	103
Ca ₂ Cl ₂	617	0.0007	33	113
Cu ₂ K ₂ Te ₂	405	0.0007	21	50
H ₂ Li ₂ Pt	515	0.0007	17	86
Gd ₂ I ₂ Se ₂	930	0.0007	54	110
As ₂ Ru ₂	617	0.0008	33	113
SbSe ₂ Tl	655	0.0009	47	105
Ca ₂ Cl ₂	562	0.0009	30	103
Br ₂ O ₂ Tm ₂	843	0.0009	33	113
SbSe ₂ Tl	543	0.001	39	87
Hg ₄ O ₂	653	0.001	67	53
Ca ₂ Cl ₂	486	0.0011	26	89
Fe ₂ Te ₂	486	0.0011	26	89
As ₂ Ru ₂	562	0.0011	30	103
As ₂ Ru ₂	486	0.0011	26	89
O ₄ PSn	405	0.0012	21	50
Hg ₄ O ₂	566	0.0012	58	46
ClKO ₃	1000	0.0012	90	110
CNRb	447	0.0012	39	84
Br ₂ O ₂ Yb ₂	664	0.0012	26	89
Br ₂ O ₂ Tm ₂	664	0.0013	26	89
I ₂ Se ₂ Tb ₂	930	0.0013	54	110
P ₄	720	0.0014	40	130
I ₂ Se ₂ Yb ₂	528	0.0014	30	63
Br ₂ O ₂ Yb ₂	589	0.0014	23	79
Ca ₄ Cu ₂	935	0.0014	55	110
Cl ₄ Mg ₂	625	0.0014	35	75
AlH ₄ Na	751	0.0014	41	91
Ho ₂ I ₂ Se ₂	942	0.0015	54	112
Fe ₂ Te ₂	431	0.0015	23	79
I ₂ Se ₂ Tm ₂	528	0.0015	30	63
H ₂ Li ₂ Pt	395	0.0016	13	66
SbSe ₂ Tl	530	0.0016	38	85
Hg ₄ O ₂	234	0.0017	24	19
Br ₂ Er ₂ Se ₂	642	0.0017	36	77
Ca ₂ Cl ₂	431	0.0017	23	79
KNO ₃	980	0.0017	84	112
Sn ₂ Te ₂	305	0.0017	21	50
Br ₃ Cs	720	0.0017	72	90
C ₄ Ca ₂	316	0.0018	14	41
Bi ₂ Se ₂	499	0.0018	31	86
Br ₂ O ₂ Ti ₂	532	0.0018	20	72
HgO	215	0.0018	15	70
As ₂ Ru ₂	431	0.0018	23	79
ClKO ₃	895	0.002	80	99
Br ₂ O ₂ Tm ₂	589	0.002	23	79
Pd ₂ S ₄	573	0.0021	39	63
O ₂ Sn ₂	416	0.0021	20	79

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

HgO (Pmmm (47))

Structural and electronic properties

	Formula	HgO
	Spacegroup	Pmmm (47)
	Prototype	FeSe
	Parent 3D	HgO
	Source DB	COD
	DB ID	2310656
DF2-C09	Binding energy [meV/ Å²]	N/A
RVV10	Binding energy [meV/ Å²]	74.3
	Band gap (PBE) [eV]	0.0

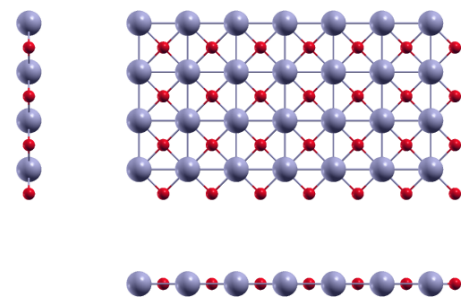


Band structure: Electronic band structure of HgO (Pmmm (47)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of HgO (Pmmm (47)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.24429924	0.00000000	0.00000000
a₂	0.00000000	3.24690129	0.00000000
a₃	0.00000000	0.00000000	20.00000000
	x [Å]	y [Å]	z [Å]
● Hg	1.34638474	1.62345064	10.00000000
● O	2.96853326	3.24690129	10.00000000



Orthographic projections: views of HgO (Pmmm (47)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Na	3	0.1482	1	1
AsSb	4	0.1906	1	1
Tl	4	0.9788	1	2
As ₂	4	0.156	1	1
CaCl	4	0.3804	1	1
Cl ₂ Zn	5	0.1549	1	1
CdCl ₂	5	0.1972	1	1
MoTe ₂	5	0.1503	1	1
AgTe ₂	5	0.0089	1	1
Nd	5	0.6527	1	3
PSn ₂	5	0.1654	1	1
ReSe ₂	5	0.1373	1	1
Br ₂ Zn	5	0.1778	1	1
HfS ₂	5	0.1588	1	1
InSe ₂	5	0.7518	1	1
AsSn ₂	5	0.1697	1	1
GeTe ₂	5	0.1959	1	1
SiTe ₂	5	0.1828	1	1
Te ₂ V	5	0.1522	1	1
I ₂ Mn	5	0.1974	1	1
CuTe ₂	5	0.1584	1	1
S ₂ Zr	5	0.1646	1	1
NSr ₂	5	0.1927	1	1
PbS ₂	5	0.1872	1	1
Br ₂ Co	5	0.1555	1	1
Ca ₂ N	5	0.1565	1	1
LiO ₂	5	0.1154	1	1
Cl ₂ Zn	5	1.1108	1	1
FeI ₂	5	0.1944	1	1
I ₂ Ni	5	0.1961	1	1
S ₂ Ti	5	0.1326	1	1
Te ₂ Ti	5	0.1781	1	1
CrI ₂	5	0.1938	1	1
Te ₂ Zn	5	0.1502	1	1
RhTe ₂	5	0.1729	1	1
Bi ₂ Pd	5	0.0097	1	1
Br ₂ Mn	5	0.1537	1	1
Cl ₂ Ni	5	0.1381	1	1
Cl ₂ Co	5	0.1324	1	1
CrTe ₂	5	0.1433	1	1
PtS ₂	5	0.1492	1	1
CoTe ₂	5	0.1591	1	1
Br ₂ V	5	0.1367	1	1
ClNZr	5	0.135	1	1
Cl ₂ Fe	5	0.1318	1	1
CdClO	5	0.1517	1	1
Se ₂ Ti	5	0.1467	1	1
Br ₂ Ti	5	0.1428	1	1
Te ₂ W	5	0.1505	1	1
AsSe ₂	5	0.1393	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

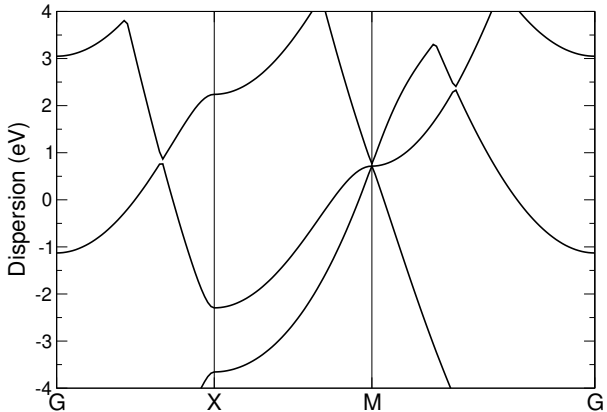
Formula	N° atoms	strain	cell size 1	cell size 2
Ca ₂ Mn ₂ Si ₂	536	0.0002	85	61
Fe ₂ Se ₂	742	0.0002	145	113
F ₂ I ₂ Yb ₂	806	0.0002	136	89
Ca ₂ Cl ₂ H ₂	422	0.0002	64	49
Br ₂ Ho ₂ O ₂	536	0.0002	85	61
Co ₂ S ₂	524	0.0002	100	81
Bi ₂ In ₂	396	0.0003	100	49
Ge ₂ Hf ₂ Te ₂	736	0.0003	113	85
Br ₂ Ca ₂ H ₂	536	0.0003	85	61
CaCl	366	0.0003	101	82
Hf ₂ Si ₂ Te ₂	546	0.0003	81	64
I ₂ Sb ₂ Te ₂	144	0.0003	36	12
As ₂ Cd ₂ K ₂	248	0.0003	49	25
Co ₂ Se ₂	418	0.0004	81	64
F ₄ Sn	407	0.0004	81	49
Eu ₂ H ₂ I ₂	806	0.0004	136	89
Ba ₂ Ge ₂ Mn ₂	806	0.0004	136	89
Cl ₂ Zn	275	0.0004	64	49
MnSe ₂	448	0.0004	101	82
Ni ₂ Se ₂	172	0.0004	36	25
Hf ₃ Te ₂	380	0.0004	65	50
Si ₂ Te ₂ Zr ₂	968	0.0005	145	113
F ₂ Ni	629	0.0006	145	113
Cu ₂ Rb ₂ Te ₂	494	0.0006	100	49
I ₂ O ₂ Pr ₂	146	0.0006	25	16
F ₂ I ₂ Sm ₂	146	0.0006	25	16
CeI ₂	147	0.0006	36	25
O ₄ PSn	248	0.0007	49	25
Ga ₂ I ₂ Y ₂	722	0.0007	118	81
I ₂ O ₂ Sm ₂	806	0.0007	136	89
BaF ₂	479	0.0007	118	81
Br ₂ Eu ₂ O ₂	222	0.0007	36	25
Hf ₃ Te ₂	373	0.0007	64	49
Br ₂ Ca ₃ Si	276	0.0007	63	25
O ₂ Pb ₂	114	0.0008	25	16
I ₃ Sn	424	0.0008	130	41
As ₂ Co ₂ Li ₂	736	0.0008	113	85
CaCl	362	0.0008	100	81
ClH ₃ O	612	0.0008	131	70
I ₂ S ₂ Tl ₂	968	0.0009	145	113
Bi ₂ Cl ₂ O ₂	222	0.0009	36	25
Ca ₂ Cl ₂	942	0.0009	181	145
CaI ₂	411	0.0009	108	65
SbSe ₂ Tl	246	0.0009	63	30
MnSe ₂	443	0.0009	100	81
Fe ₂ O ₄	892	0.0009	110	112
Cr ₂ O ₄	642	0.001	81	80
As ₂ Co ₂	424	0.001	82	65
Ba ₂ H ₂ I ₂	742	0.001	149	74
Br ₂ CsF	594	0.001	149	74

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

In (P4/mmm (123))

Structural and electronic properties


	Formula	In
	Spacegroup	P4/mmm (123)
	Prototype	Sn
	Parent 3D	In
	Source DB	COD
	DB ID	1512513
DF2-C09	Binding energy [meV/ Å²]	71.92
RVV10	Binding energy [meV/ Å²]	64.5
	Band gap (PBE) [eV]	0.0

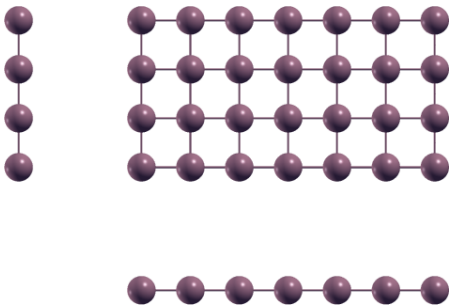


Band structure: Electronic band structure of In (P4/mmm (123)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of In (P4/mmm (123)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	2.98137769	0.00000000	0.00000000
a₂	0.00000000	2.98137769	0.00000000
a₃	0.00000000	0.00000000	20.00000000
	x [Å]	y [Å]	z [Å]
 In	1.49068884	1.49068884	10.00000000



Orthographic projections: views of In (P4/mmm (123)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	2	0.1569	1	1
Sn	2	0.0044	1	1
Na	2	0.1937	1	1
In	2	0.1356	1	1
As ₂	3	0.7711	1	1
LiO	3	0.1445	1	1
Na	3	0.1529	2	1
P ₂	3	0.1516	1	1
C ₂	3	0.1097	1	1
Gd	3	0.3014	2	1
Cl ₂ Zn	4	0.767	1	1
S ₂ V	4	0.1382	1	1
MoS ₂	4	0.1388	1	1
Cl ₂ Mn	4	0.1629	1	1
MoTe ₂	4	0.1967	1	1
MoSe ₂	4	0.1561	1	1
ReSe ₂	4	0.1779	1	1
S ₂ Ta	4	0.1652	1	1
HfS ₂	4	0.7817	1	1
CuTe ₂	4	0.7802	1	1
NiO ₂	4	0.1085	1	1
Br ₂ Co	4	0.7694	1	1
Ca ₂ N	4	0.7731	1	1
Cl ₂ Ti	4	0.1518	1	1
S ₂ Ti	4	0.1708	1	1
NbS ₂	4	0.1647	1	1
Te ₂ Zn	4	0.1965	1	1
S ₂ W	4	0.1388	1	1
Bi ₂ Pd	4	0.382	1	1
Cl ₂ Ni	4	0.179	1	1
Cl ₂ Co	4	0.1704	1	1
CrTe ₂	4	0.1867	1	1
PtS ₂	4	0.195	1	1
NbS ₂	4	0.16	1	1
CoTe ₂	4	0.7829	1	1
Br ₂ V	4	0.177	1	1
ClN ₂ Zr	4	0.1745	1	1
Cl ₂ Fe	4	0.1696	1	1
CdClO	4	0.7548	1	1
S ₂ Ta	4	0.1591	1	1
CKN	4	2.5697	1	1
Se ₂ V	4	0.1577	1	1
Se ₂ Ti	4	0.1915	1	1
Br ₂ Ti	4	0.1859	1	1
Te ₂ W	4	0.1969	1	1
AsSe ₂	4	0.1808	1	1
Cl ₂ V	4	0.1423	1	1
CdO ₂	4	0.1702	1	1
BrN ₂ Zr	4	0.1825	1	1
NbSe ₂	4	0.1796	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

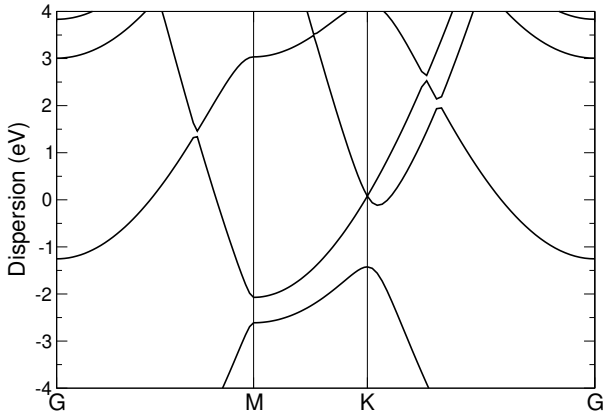
Formula	N° atoms	strain	cell size 1	cell size 2
As ₂ Ru ₂	366	0.0	106	65
Hf ₂ Se ₂ Si ₂	451	0.0001	85	61
Ag ₂ K ₂ Te ₂	214	0.0001	64	25
Cu ₂ Se ₂	492	0.0001	136	89
Br ₂ Ho ₂ O ₂	375	0.0001	81	49
Bi ₂ Pd	343	0.0001	100	81
Cu ₂ F ₄	376	0.0002	130	41
Br ₂ HLa	368	0.0002	108	65
Ca ₂ Cl ₂	366	0.0002	106	65
Br ₂ O ₂ Tm ₂	496	0.0002	106	65
F ₄ Sn	174	0.0002	49	25
Ca ₂ Mn ₂ Si ₂	375	0.0003	81	49
I ₂ S ₂ Tl ₂	670	0.0003	136	89
As ₂ Ir ₂	52	0.0003	16	9
AsCuLi ₂	368	0.0004	108	65
O ₂ Sn ₂	329	0.0004	97	58
Br ₂ O ₂ Tb ₂	445	0.0004	97	58
Bi ₂ Se ₂	6	0.0004	2	1
Ni ₂ Se ₂	485	0.0005	145	85
CeLi ₂ P ₂	433	0.0005	108	65
Br ₂ Ca ₂ H ₂	375	0.0005	81	49
Ge ₂ Mn ₂ Sr ₂	70	0.0005	16	9
Ca ₂ Cl ₂ F ₂	859	0.0005	181	113
Au ₂ Br ₂	296	0.0005	100	49
As ₂ Fe ₂	329	0.0005	85	61
HgI ₂	21	0.0006	9	4
I ₂ Pr ₂ Si ₂	498	0.0006	108	65
F ₂ Ni	403	0.0006	136	89
Si ₂ Te ₂ Zr ₂	670	0.0006	136	89
Br ₂ Mg	361	0.0006	118	81
FeI ₂	361	0.0006	118	81
Fe ₂ Te ₂	366	0.0006	106	65
Cl ₂ S ₂ Tl ₂	79	0.0007	25	9
N ₄	315	0.0007	63	63
Ga ₂ Te ₂	368	0.0007	108	65
Ba ₂ Ni ₃	433	0.0007	108	65
CeI ₂	400	0.0007	145	85
Cu ₂ Te ₂	89	0.0007	25	16
CrI ₂	361	0.0007	118	81
Bi ₂ Cl ₂ O ₂	655	0.0008	145	85
Br ₂ Eu ₂ O ₂	655	0.0008	145	85
CrO ₂	243	0.0008	48	65
Br ₂ Cu ₂	329	0.0008	97	58
AlLiTe ₂	411	0.0009	131	70
Fe ₂ S ₂	136	0.0009	36	25
GeI ₂	303	0.0009	108	65
I ₂ S ₂ Tb ₂	469	0.0009	139	55
C ₂ Cl ₂ Y ₂	663	0.0009	129	89
I ₂ La ₂ Sb	275	0.0009	80	39
Se ₂ Ta ₄	823	0.001	145	113

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

In (P6/mmm (191))

Structural and electronic properties

	Formula	In
	Spacegroup	P6/mmm (191)
	Prototype	In
	Parent 3D	NbInSe ₂
	Source DB	ICSD
	DB ID	53102
DF2-C09	Binding energy [meV/ Å²]	61.68
RVV10	Binding energy [meV/ Å²]	59.87
	Band gap (PBE) [eV]	0.0

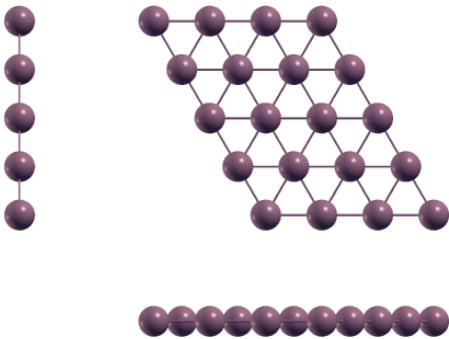


Band structure: Electronic band structure of In (P6/mmm (191)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of In (P6/mmm (191)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.16034140	0.00000000	0.00000000
a₂	−1.58017070	2.73693594	0.00000000
a₃	0.00000000	0.00000000	20.00000000
	x [Å]	y [Å]	z [Å]
● In	0.00000000	0.00000000	10.00000000



Orthographic projections: views of In (P6/mmm (191)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Sn	2	0.1426	1	1
Na	2	0.4736	1	1
In	2	0.1466	1	1
As ₂	3	0.4943	1	1
Cl ₂ Zn	4	2.8507	1	1
S ₂ V	4	0.0032	1	1
MoS ₂	4	0.004	1	1
MoTe ₂	4	0.4794	1	1
PSn ₂	4	2.9803	1	1
HfS ₂	4	0.5016	1	1
FeO ₂	4	0.261	1	1
AsSn ₂	4	3.0309	1	1
Te ₂ V	4	0.4844	1	1
CuTe ₂	4	0.5006	1	1
S ₂ Zr	4	2.9701	1	1
NiO ₂	4	0.2628	1	1
Br ₂ Co	4	0.4932	1	1
ReS ₂	4	0.0086	1	1
Ca ₂ N	4	0.4957	1	1
MnO ₂	4	0.2484	1	1
I ₂ Zn	4	13.6876	1	1
Te ₂ Zn	4	0.479	1	1
S ₂ W	4	0.004	1	1
Br ₂ Mn	4	2.8355	1	1
CrTe ₂	4	0.46	1	1
PtS ₂	4	0.4762	1	1
CoTe ₂	4	2.9035	1	1
CdClO	4	0.4831	1	1
Se ₂ Ti	4	0.4695	1	1
Br ₂ Ti	4	0.4586	1	1
Te ₂ W	4	0.4798	1	1
AsSe ₂	4	0.4486	1	1
S ₂ Sn	4	2.9736	1	1
Cl ₂ V	4	0.0081	1	1
Se ₂ Zr	4	3.189	1	1
PtSe ₂	4	3.0396	1	1
OTl ₂	4	0.4836	1	1
BrNZr	4	0.4518	1	1
Br ₂ Fe	4	0.4934	1	1
Br ₂ Cr	4	0.4593	1	1
Br ₂ Ni	4	2.925	1	1
FeSe ₂	4	0.1371	1	1
NbTe ₂	4	2.9674	1	1
NbSe ₂	4	0.4492	1	1
MoS ₂	4	0.0042	1	1
Cl ₂ Mg	4	2.9257	1	1
CrSe ₂	4	0.0069	1	1
Se ₂ Ta	4	0.4567	1	1
CrSe ₂	4	0.0094	1	1
O ₂ Pt	4	0.0015	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

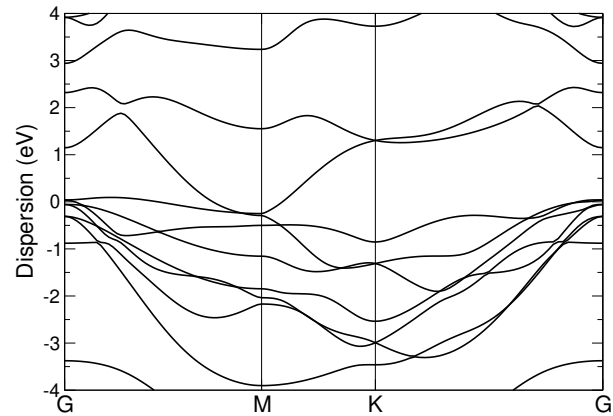
Formula	N° atoms	strain	cell size 1	cell size 2
DyI ₂	247	0.0	100	49
CdClO	244	0.0	73	57
PtS ₂	273	0.0001	81	64
Ca ₂ N	211	0.0001	64	49
OTl ₂	244	0.0002	73	57
Cl ₂ Hf ₂ N ₂	415	0.0002	73	57
Br ₂ F ₂ Pb ₂	159	0.0002	39	20
SiTe ₂	111	0.0002	36	25
Cl ₂ La ₂	209	0.0003	61	37
In ₂ Se ₂	277	0.0003	81	49
Br ₂ F ₂ Sr ₂	159	0.0003	39	20
Nd	85	0.0003	36	49
IKO ₃	161	0.0003	81	16
BaF ₂	43	0.0003	16	9
NiTe ₂	111	0.0003	36	25
Ga ₂ S ₂	229	0.0004	57	43
As ₂	162	0.0004	64	49
C ₂ Br ₂ La ₂	249	0.0004	57	32
I ₂ S ₂ Tb ₂	394	0.0004	100	49
Cu ₂ K ₂ Te ₂	454	0.0004	130	54
CrTe ₂	343	0.0005	100	81
Te ₂ V	244	0.0005	73	57
Cl ₂ Er ₂ O ₂	186	0.0005	36	25
Li ₂ Tl ₂	164	0.0005	64	25
NS ₂ Zr	337	0.0005	81	64
Cl ₂ Sc ₂	424	0.0005	100	81
CCL ₂ Lu ₂	309	0.0005	64	49
I ₄ Sr ₂	21	0.0006	9	2
Ga ₂ I ₂ Y ₂	70	0.0006	16	9
Ga ₂ S ₃	401	0.0006	81	64
CrO ₂	214	0.0006	43	57
STl ₂	43	0.0006	16	9
Cd ₂ I ₃	174	0.0006	49	25
Se ₂ Si ₂ Zr ₂	604	0.0006	118	81
MnO ₂	241	0.0006	49	64
Br ₂ Zr ₂	383	0.0006	91	73
AsI ₂ La ₂	174	0.0006	49	25
Se ₂ Zr	111	0.0007	36	25
PTe ₂ Ti ₂	272	0.0007	57	43
Dy ₂ I ₂ S ₂	394	0.0007	100	49
Ga ₂ S ₂	229	0.0007	57	43
O ₄ PSn	403	0.0007	115	48
Br ₂ Hf ₂ N ₂	358	0.0007	64	49
Br ₂ Cr	343	0.0007	100	81
Br ₂ Fe	211	0.0008	64	49
Br ₂ Ni	186	0.0008	57	43
Br ₂ Co	211	0.0008	64	49
CoTe ₂	186	0.0008	57	43
Br ₂ H ₂ Zr ₂	586	0.0008	100	81
Cl ₂ Mg	186	0.0009	57	43

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

In₂Te₃ (P-3m1 (164))

Structural and electronic properties

Formula	In ₂ Te ₃
Spacegroup	P-3m1 (164)
Prototype	As
Parent 3D	In ₂ Te ₃
Source DB	ICSD
DB ID	657607
DF2-C09 Binding energy [meV/ Å²]	31.86
RVV10 Binding energy [meV/ Å²]	36.65
Band gap (PBE) [eV]	0.0

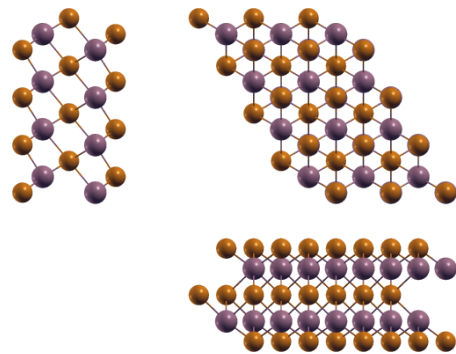


Band structure: Electronic band structure of In₂Te₃ (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of In₂Te₃ (P-3m1 (164)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.22907424	−0.00000000	0.00000000
a₂	−2.11453712	3.66248572	0.00000000
a₃	0.00000000	0.00000000	26.98600478
	x [Å]	y [Å]	z [Å]
● In	2.11453712	3.66248572	11.46579704
● Te	2.11453712	3.66248572	17.07975783
● Te	0.00000000	2.44165715	13.49300239
● In	2.11453712	1.22082857	15.52020774
● Te	2.11453712	1.22082857	9.90624695



Orthographic projections: views of In₂Te₃ (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
InSe	7	0.0018	1	1
AsSb	7	0.2744	1	1
Bi ₂	7	0.0077	1	1
AgTl	7	0.1542	1	1
As ₂	7	1.5317	1	1
P ₂	7	4.8599	1	1
PbTe	7	0.0036	1	1
CaCl	7	0.1141	1	1
Cl ₂ Zn	8	1.5243	1	1
I ₂ Mg	8	0.0083	1	1
CdI ₂	8	0.0053	1	1
PSn ₂	8	1.5964	1	1
Br ₂ Zn	8	0.2597	1	1
Br ₂ Ca	8	0.0066	1	1
HfS ₂	8	1.5513	1	1
AsSn ₂	8	0.2504	1	1
SiTe ₂	8	0.2655	1	1
I ₂ Pr	8	0.1379	1	1
S ₂ Zr	8	1.5908	1	1
Br ₂ La	8	0.008	1	1
Br ₂ Cu	8	0.7246	1	1
Ca ₂ Si	8	0.4543	1	1
PbS ₂	8	0.2706	1	1
Br ₂ Co	8	1.5287	1	1
BiClTe	8	0.0057	1	1
Ca ₂ N	8	1.5355	1	1
Cl ₂ Ti	8	4.8632	1	1
BrCdI	8	0.0053	1	1
Cl ₂ Zn	8	0.1212	1	1
Te ₂ Ti	8	0.2601	1	1
BaF ₂	8	0.002	1	1
RhTe ₂	8	0.2541	1	1
CoTe ₂	8	1.5537	1	1
AsKSn	8	0.0035	1	1
PbTe ₂	8	0.0063	1	1
I ₂ Nd	8	0.1387	1	1
NiTe ₂	8	0.2646	1	1
Cl ₂ Cu	8	0.067	1	1
S ₂ Sn	8	1.5927	1	1
I ₂ V	8	0.2674	1	1
GeI ₂	8	0.0038	1	1
Se ₂ Zr	8	0.2661	1	1
I ₂ Pb	8	0.4477	1	1
STl ₂	8	0.0011	1	1
PtSe ₂	8	1.6294	1	1
CoI ₂	8	0.275	1	1
Br ₂ Fe	8	1.5292	1	1
TaTe ₂	8	0.2496	1	1
MnSe ₂	8	0.1141	1	1
Br ₂ Ni	8	1.5657	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

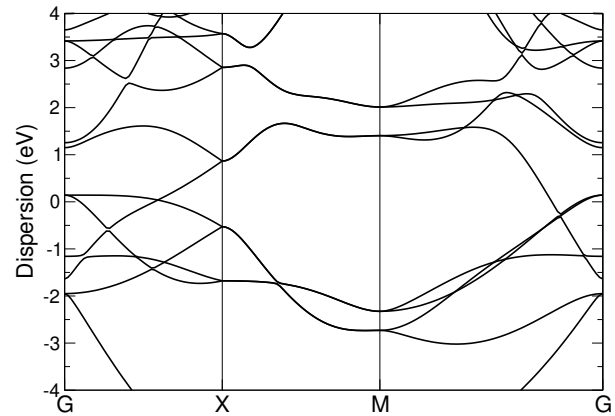
Formula	N° atoms	strain	cell size 1	cell size 2
S ₂ Sn	386	0.0	43	57
Sb ₂ SeTe ₂	10	0.0001	1	1
As ₂ O ₃	490	0.0001	61	37
I ₂ N ₂ Zr ₂	723	0.0001	57	73
I ₂ V	705	0.0001	81	100
HNiO ₂	511	0.0001	39	79
CCL ₂ Gd ₂	725	0.0002	64	81
HN ₃ OZn	551	0.0002	37	61
CaH ₂ O ₂	425	0.0002	36	49
N ₂ W	272	0.0002	25	49
S ₂ Zr	386	0.0002	43	57
NiTe ₂	638	0.0002	73	91
Cu ₂ O ₂	355	0.0002	39	40
TaTe ₂	437	0.0002	49	64
CuTe ₂	327	0.0002	36	49
Cl ₂ Hf ₂	180	0.0003	16	25
CoO ₂	47	0.0003	4	9
Br ₂ Zn	563	0.0003	64	81
Hf ₂ I ₂ N ₂	629	0.0003	49	64
CdClHO	501	0.0003	49	64
CaClHO	729	0.0004	73	91
CBr ₂ Y ₂	725	0.0004	64	81
Bi ₂ Se ₂ Te	10	0.0004	1	1
NbTe ₂	386	0.0004	43	57
Cl ₂ N ₂ Zr ₂	474	0.0004	36	49
Mg ₂	541	0.0004	65	108
FeO ₂	47	0.0005	4	9
CS ₂ Ta ₂	650	0.0005	49	81
Cl ₂ O ₂ Tm ₂	911	0.0005	73	91
Al ₂ Cl ₂ O ₂	39	0.0005	3	4
PSn ₂	386	0.0005	43	57
Cl ₂ Ti	488	0.0006	49	81
Ho ₂ S ₂	355	0.0006	39	40
Te ₂ Ti	563	0.0006	64	81
HfSe ₂	563	0.0006	64	81
H ₂ MgO ₂	125	0.0006	9	16
HfS ₂	327	0.0006	36	49
Br ₃ Cs	420	0.0006	64	25
La ₂ S ₂	50	0.0007	6	5
P ₂	407	0.0007	49	81
Sn ₂ Te ₂	599	0.0008	75	56
NiO ₂	47	0.0008	4	9
SiTe ₂	638	0.0008	73	91
AsSn ₂	437	0.0008	49	64
ClH ₃ O	725	0.0009	81	64
LiNbS ₂	180	0.0009	16	25
GeI ₂ Y ₂	10	0.0009	1	1
S ₂ Ta	155	0.0009	16	25
CoTe ₂	327	0.0009	36	49
As ₄	539	0.001	63	56

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

InBi (P4/nmm (129))

Structural and electronic properties

	Formula	InBi
	Spacegroup	P4/nmm (129)
	Prototype	FeSe
	Parent 3D	In ₂ Bi ₂
	Source DB	COD
	DB ID	1527695
DF2-C09	Binding energy [meV/ Å²]	50.23
RVV10	Binding energy [meV/ Å²]	49.86
	Band gap (PBE) [eV]	0.0

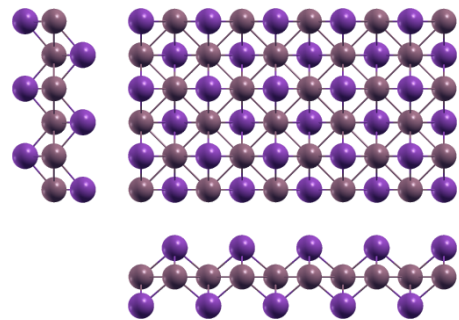


Band structure: Electronic band structure of InBi (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of InBi (P4/nmm (129)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.63453411	0.00000000	0.00000000
a₂	0.00000000	4.63453411	0.00000000
a₃	0.00000000	0.00000000	23.90735389
	x [Å]	y [Å]	z [Å]
● Bi	0.00000000	2.31726705	13.94018123
● In	0.00000000	0.00000000	11.95367695
● In	2.31726705	2.31726705	11.95367695
● Bi	2.31726705	0.00000000	9.96717267



Orthographic projections: views of InBi (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
AsSb	6	0.1095	1	1
AgTl	6	0.621	1	1
Sm	6	0.1435	1	2
SiTe ₂	7	0.1108	1	1
Br ₂ Cu	7	0.1013	1	1
NSr ₂	7	0.1091	1	1
FeI ₂	7	0.1089	1	1
CrI ₂	7	0.1089	1	1
Ba ₂ Hg	7	0.221	1	1
CNRb	7	0.0404	1	1
CKN	7	0.0491	1	1
NiTe ₂	7	0.111	1	1
I ₂ V	7	0.1105	1	1
Se ₂ Zr	7	0.1107	1	1
BiITe	7	0.1085	1	1
CoI ₂	7	0.1094	1	1
Br ₂ Mg	7	0.1089	1	1
I ₂ La	7	0.5596	1	1
Se ₂ Sn	7	0.1092	1	1
Li ₂ Tl ₂	8	0.1468	1	1
Cu ₂ I ₂	8	0.2093	1	1
Ag ₂ Br ₂	8	0.5611	1	1
S ₂ Sn ₂	8	0.212	1	1
K	8	2.3052	1	4
N ₃ Na	8	0.026	1	1
As ₂ Ir ₂	8	0.568	1	1
O ₂ Pb ₂	8	0.5978	1	1
Ga ₂ Se ₂	8	0.1102	1	1
P ₄	8	0.1674	1	1
CaClHO	8	0.1111	1	1
Bi ₂ O ₂	8	0.2071	1	1
PbS ₂ Sn	8	0.2215	1	1
As ₂ Rh ₂	8	0.5604	1	1
Br ₂ CsF	8	0.002	1	1
Sn ₂ Te ₂	8	0.0077	1	1
As ₂ O ₃	9	0.184	1	1
F ₄ Sn	9	0.22	1	1
Bi ₂ Te ₃	9	0.1085	1	1
PTe ₂ Zr ₂	9	0.1096	1	1
FKO ₂ Se	9	1.3928	1	1
F ₄ Nb	9	0.2134	1	1
NaO ₄	9	0.1561	1	1
AgNO ₃	9	0.1569	1	1
Cl ₄ Mn	9	0.0057	1	1
Ba ₂ H ₂ I ₂	10	0.0039	1	1
Br ₂ Ho ₂ S ₂	10	0.0632	1	1
Br ₂ F ₂ Sr ₂	10	0.2115	1	1
Au ₂ K ₂ S ₂	10	2.5142	1	1
Cu ₄ Te ₂	10	0.3443	1	1
Eu ₂ F ₂ I ₂	10	0.2066	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

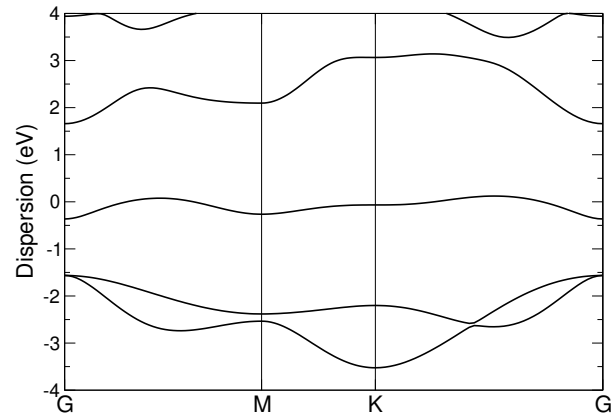
Formula	N° atoms	strain	cell size 1	cell size 2
F ₄ Sn	833	0.0	82	101
Br ₂ Cu ₂	244	0.0	25	36
Co ₂ S ₂	520	0.0	49	81
Ca ₂ Cl ₂ H ₂	214	0.0001	16	25
Fe ₂ S ₂	620	0.0001	58	97
Br ₂ O ₂ Yb ₂	530	0.0001	41	61
O ₂ Pb ₂	460	0.0002	50	65
BiClTe	387	0.0002	48	65
F ₄ Nb	670	0.0002	65	82
Te ₂ W	197	0.0002	20	39
Bi ₂ Pd	247	0.0002	25	49
Ge ₂ Mn ₂ Sr ₂	438	0.0002	36	49
I ₂ Pr	387	0.0002	48	65
MoTe ₂	197	0.0002	20	39
Gd ₂ GeI ₂	517	0.0003	48	65
HgO	396	0.0003	49	100
Br ₂ Eu ₂ F ₂	754	0.0003	61	85
Cu ₂ Rb ₂ Te ₂	10	0.0003	1	1
I ₂ O ₂ Pr ₂	580	0.0003	49	64
F ₂ I ₂ Sm ₂	590	0.0003	50	65
Te ₂ Zn	197	0.0003	20	39
Er ₂ I ₂ O ₂	754	0.0003	61	85
Br ₂ O ₂ Tb ₂	316	0.0004	25	36
CdI ₂	387	0.0004	48	65
I ₂ O ₂ Tm ₂	754	0.0004	61	85
FHOZn	736	0.0004	54	130
Ge ₂ Se ₂ Zr ₂	896	0.0005	65	106
Ca ₂ Cl ₂	684	0.0005	65	106
Hf ₃ Te ₂	189	0.0005	16	25
CdH ₂ O ₂	275	0.0005	20	39
TaTe ₂	339	0.0005	36	65
CrSe ₂	606	0.0005	54	130
K ₂ PdS ₂	244	0.0005	36	20
Er ₂ I ₂ S ₂	708	0.0005	72	70
F ₄ Sn	824	0.0005	81	100
Cl ₂ Zn	139	0.0006	16	25
F ₄ Nb	661	0.0006	64	81
Br ₂ F ₂ Yb ₂	316	0.0006	25	36
HfLiS ₂	236	0.0006	20	39
CaCl	358	0.0006	49	81
K ₂ PdSe ₂	300	0.0006	45	24
Eu ₂ F ₂ I ₂	590	0.0006	50	65
Br ₂ La ₂ O ₂	590	0.0006	50	65
CeLi ₂ P ₂	914	0.0006	81	118
As ₂ Ir ₂	340	0.0007	36	49
Br ₂ La ₂ P	517	0.0007	48	65
MnSe ₂	439	0.0007	49	81
Br ₂ HLa	796	0.0007	81	118
Bi ₂ Se ₂	716	0.0007	81	98
Cl ₂ V	606	0.0007	54	130

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

InSe (P3m1 (156))

Structural and electronic properties

	Formula	InSe
	Spacegroup	P3m1 (156)
	Prototype	GeTe
	Parent 3D	In ₂ Se ₃
	Source DB	COD
	DB ID	1528775
DF2-C09	Binding energy [meV/ Å²]	48.86
RVV10	Binding energy [meV/ Å²]	48.97
	Band gap (PBE) [eV]	0.0

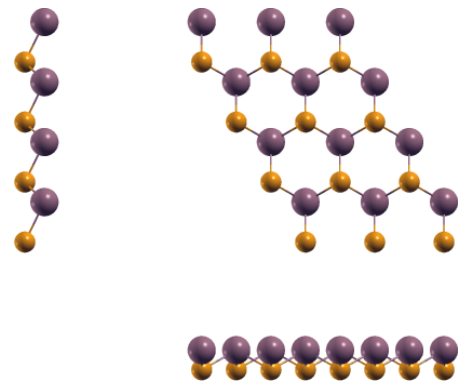


Band structure: Electronic band structure of InSe (P3m1 (156)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of InSe (P3m1 (156)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.24507727	−0.00000000	0.00000000
a₂	−2.12253863	3.67634475	0.00000000
a₃	0.00000000	0.00000000	21.31663417
	x [Å]	y [Å]	z [Å]
● Se	2.12253863	1.22544825	11.25843689
● In	2.12253863	3.67634475	10.05819727



Orthographic projections: views of InSe (P3m1 (156)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
AsSb	4	0.2717	1	1
Bi ₂	4	0.0059	1	1
AgTl	4	0.1525	1	1
PbTe	4	0.0018	1	1
CaCl	4	0.1134	1	1
CdI ₂	5	0.0035	1	1
PSn ₂	5	1.5833	1	1
Br ₂ Zn	5	0.2572	1	1
Br ₂ Ca	5	0.0048	1	1
HfS ₂	5	1.5385	1	1
AsSn ₂	5	0.248	1	1
SiTe ₂	5	0.263	1	1
I ₂ Pr	5	0.1365	1	1
Br ₂ Cu	5	0.7182	1	1
NSr ₂	5	0.2741	1	1
Ca ₂ Si	5	0.4499	1	1
PbS ₂	5	0.268	1	1
BiClTe	5	0.0039	1	1
Ca ₂ N	5	1.5228	1	1
BrCdI	5	0.007	1	1
Cl ₂ Zn	5	0.1202	1	1
HgI ₂	5	0.2086	1	1
Te ₂ Ti	5	0.2576	1	1
CrI ₂	5	0.2754	1	1
BaF ₂	5	0.0038	1	1
BiBrTe	5	0.0096	1	1
RhTe ₂	5	1.6323	1	1
CoTe ₂	5	1.5409	1	1
AsKSn	5	0.0052	1	1
PbTe ₂	5	0.008	1	1
I ₂ Nd	5	0.1372	1	1
NiTe ₂	5	0.2621	1	1
Cl ₂ Cu	5	0.0675	1	1
I ₂ V	5	0.2649	1	1
GeI ₂	5	0.002	1	1
Se ₂ Zr	5	0.2635	1	1
STl ₂	5	0.0029	1	1
PtSe ₂	5	0.2489	1	1
CoI ₂	5	0.2724	1	1
GeS ₂	5	0.4329	1	1
TaTe ₂	5	0.2472	1	1
MnSe ₂	5	0.1134	1	1
Br ₂ Ni	5	1.5528	1	1
CeI ₂	5	0.1359	1	1
Br ₂ Mg	5	0.2758	1	1
I ₂ Ti	5	0.2729	1	1
Cl ₂ Mg	5	1.5531	1	1
F ₂ Ni	5	0.1181	1	1
I ₂ La	5	0.1412	1	1
F ₂ Na	5	0.26	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

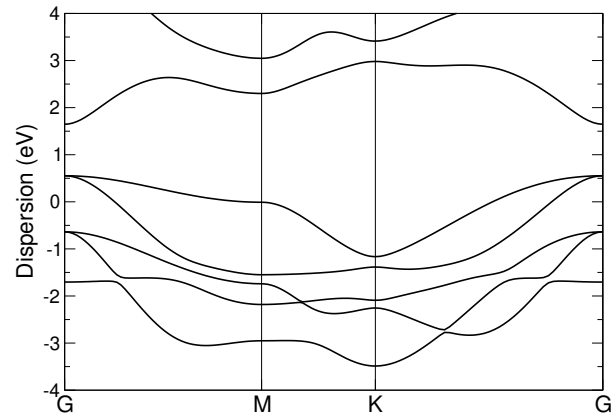
Formula	N° atoms	strain	cell size 1	cell size 2
F ₂ Se ₂ Y ₂	422	0.0	64	49
As ₂ Li ₂ Pr	7	0.0	1	1
Br ₂ Y ₂	562	0.0	81	100
Cl ₂ Y ₂	406	0.0001	57	73
I ₂ La ₂ Si ₂	8	0.0001	1	1
HNiO ₂	498	0.0001	49	100
Se ₂ Ti	158	0.0002	25	36
Ba ₂ H ₂ I ₂	418	0.0002	65	48
PbS ₂	462	0.0003	81	100
S ₂ V	66	0.0003	9	16
AsLi ₃	6	0.0003	1	1
PtSe ₂	290	0.0003	49	64
Br ₂ Pr ₂	452	0.0003	64	81
Ga ₂ Se ₂	562	0.0003	81	100
Ga ₂ S ₂	268	0.0003	36	49
I ₂ V	419	0.0004	73	91
Cl ₂ O ₂ Yb ₂	614	0.0004	64	81
MoS ₂	66	0.0004	9	16
F ₂ Na	371	0.0005	64	81
S ₂ W	66	0.0005	9	16
Bi ₂ Te ₂	374	0.0005	73	57
Br ₂ O ₂ Ti ₂	350	0.0005	40	45
Se ₂ Zr	419	0.0005	73	91
Br ₂ Zr ₂	194	0.0006	25	36
H ₂ Li ₂ Pd	670	0.0006	65	108
CBr ₂ Y ₂	479	0.0006	57	73
C ₂ Br ₂ Gd ₂	716	0.0006	82	92
MoS ₂	66	0.0006	9	16
Ga ₂ Se ₂	406	0.0007	57	73
As ₂ Li ₂ Nd	7	0.0007	1	1
Ge ₂ Se ₂	518	0.0007	91	84
PTe ₂ Ti ₂	317	0.0007	36	49
Ag ₂ K ₂ Te ₂	722	0.0007	118	81
Ga ₂ S ₂	268	0.0007	36	49
Cl ₂ Er ₂ O ₂	692	0.0007	73	91
Cl ₂ Ho ₂ O ₂	692	0.0007	73	91
FeH ₂ O ₂	295	0.0008	25	49
Br ₂ Ni	219	0.0008	36	49
CoTe ₂	219	0.0008	36	49
Cl ₂ O ₂ Y ₂	762	0.0008	81	100
Cl ₂ Mg	219	0.0009	36	49
Te ₄ W ₂	530	0.0009	85	60
GeI ₂ Y ₂	7	0.0009	1	1
ClH ₃ O	482	0.0009	81	64
Bi ₂ STe ₂	7	0.0009	1	1
AsSn ₂	290	0.0009	49	64
SiTe ₂	419	0.001	73	91
NiO ₂	35	0.001	4	9
C ₂ Br ₂ Tb ₂	716	0.001	82	92
I ₂ Lu ₂ S ₂	522	0.001	81	60

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

InSe₂ (P3m1 (156))

Structural and electronic properties

	Formula	InSe ₂
	Spacegroup	P3m1 (156)
	Prototype	InSe2
	Parent 3D	In ₂ Se ₃
	Source DB	COD
	DB ID	1528775
DF2-C09	Binding energy [meV/ Å²]	48.86
RVV10	Binding energy [meV/ Å²]	48.97
	Band gap (PBE) [eV]	0.0

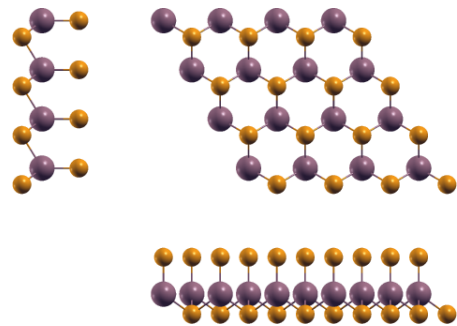


Band structure: Electronic band structure of InSe₂ (P3m1 (156)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of InSe₂ (P3m1 (156)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.88761569	−0.00000000	0.00000000
a₂	−1.94380785	3.36677395	0.00000000
a₃	0.00000000	0.00000000	23.93546534
	x [Å]	y [Å]	z [Å]
● In	−0.00000000	2.24451597	12.53314529
● Se	−0.00000000	2.24451597	10.00310878
● Se	1.94380785	1.12225798	13.90816589



Orthographic projections: views of InSe₂ (P3m1 (156)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	4	1.5355	1	1
HgO	5	0.4435	1	1
AsSb	5	0.0053	1	1
Bi ₂	5	0.4552	1	1
GeTe	5	0.0007	1	1
S ₂	5	0.0023	1	1
CaCl	5	0.1389	1	1
IrTe ₂	6	0.0016	1	1
CdCl ₂	6	0.0004	1	1
CdI ₂	6	0.4495	1	1
AgTe ₂	6	0.4229	1	1
MoSe ₂	6	1.5302	1	1
ReSe ₂	6	0.2594	1	1
S ₂ Ta	6	1.5923	1	1
Br ₂ Ca	6	0.4525	1	1
CaI ₂	6	2.9306	1	1
GeTe ₂	6	0.0014	1	1
I ₂ Mn	6	0.0003	1	1
NSr ₂	6	0.0037	1	1
I ₂ Yb	6	0.5013	1	1
PbS ₂	6	0.0078	1	1
BiClTe	6	0.4504	1	1
LiO ₂	6	0.0671	1	1
Cl ₂ Zn	6	0.152	1	1
FeI ₂	6	0.0024	1	1
I ₂ Ni	6	0.0012	1	1
S ₂ Ti	6	1.6294	1	1
NbS ₂	6	1.589	1	1
CrI ₂	6	0.0028	1	1
BiBrTe	6	0.4641	1	1
Bi ₂ Pd	6	0.1143	1	1
N ₂ W	6	4.8612	1	1
Cl ₂ Ni	6	0.2607	1	1
Cl ₂ Co	6	1.6267	1	1
CrTe ₂	6	0.2694	1	1
Br ₂ V	6	0.2583	1	1
ClNZr	6	0.2554	1	1
Cl ₂ Fe	6	0.2498	1	1
S ₂ Ta	6	1.5513	1	1
Se ₂ V	6	1.5416	1	1
Se ₂ Ti	6	0.2749	1	1
Br ₂ Ti	6	0.2686	1	1
AsSe ₂	6	0.2627	1	1
I ₂ Tm	6	2.9153	1	1
BiTe	6	0.4808	1	1
CdO ₂	6	0.2506	1	1
BrNZr	6	0.2646	1	1
NbSe ₂	6	0.2613	1	1
CoI ₂	6	0.0049	1	1
GeS ₂	6	0.1296	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

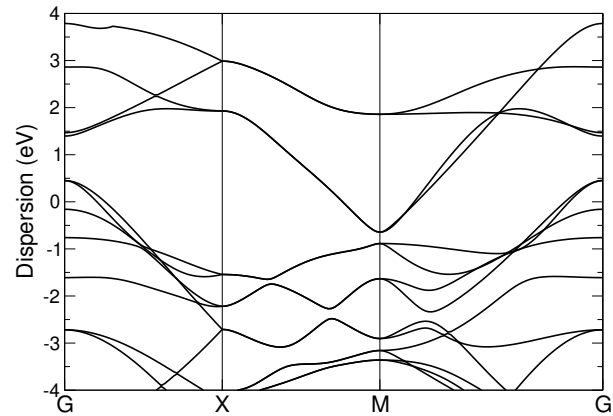
Formula	N° atoms	strain	cell size 1	cell size 2
S ₂ Ta	300	0.0	43	57
ClNZr	390	0.0	57	73
LiNbS ₂	357	0.0001	43	57
I ₂ Tm	300	0.0001	57	43
FeH ₂ O ₂	416	0.0001	37	61
ReSe ₂	435	0.0001	64	81
Cu ₂ Sr ₂	565	0.0001	91	73
Se ₂ Ta	543	0.0001	81	100
Cl ₂ H ₂ Sc ₂	843	0.0001	81	100
Cu ₄ Te ₂	786	0.0001	100	81
Cl ₂ Er ₂ H ₂	9	0.0001	1	1
GeI ₂ La ₂	386	0.0002	57	43
BrNZr	492	0.0002	73	91
Gd ₂ I ₂ S ₂	363	0.0002	49	36
Br ₂ Hf ₂	583	0.0002	73	91
I ₂ Mn	6	0.0003	1	1
CNNa	411	0.0003	77	60
H ₂ Si ₂	7	0.0003	1	1
Br ₂ Cr ₂ O ₂	675	0.0003	73	76
F ₂ I ₂ Pb ₂	483	0.0003	65	48
CdCl ₂	6	0.0004	1	1
Cl ₂ Fe	339	0.0004	49	64
N ₃ W ₂	107	0.0004	9	16
Ba ₂ Cd	339	0.0005	65	48
NbS ₂	300	0.0005	43	57
Br ₂ Ca ₃ Si	363	0.0005	49	36
Br ₂ H ₂ Zr ₂	609	0.0005	57	73
Ni ₂ Te ₂	7	0.0006	1	1
S ₂ Ta	255	0.0006	36	49
Ca ₂ Si	183	0.0006	36	25
Ce ₂ I ₂ S ₂	258	0.0006	36	25
N ₂ W	390	0.0007	49	81
Sb ₂ Te ₂	208	0.0007	36	25
Br ₂ Ti	543	0.0007	81	100
GeTe	5	0.0007	1	1
Sb ₂ Te ₃	705	0.0007	100	81
AlLiTe ₂	499	0.0007	81	64
Br ₂ V	435	0.0007	64	81
Se ₂ V	255	0.0007	36	49
F ₂ Se ₂ Y ₂	171	0.0008	25	16
Cl ₂ Zr	339	0.0008	49	64
I ₂ La ₂ P	638	0.0008	91	73
Cl ₂ Cu	375	0.0008	61	64
NbSe ₂	492	0.0008	73	91
Br ₂ H ₂ Zr ₂	843	0.0009	81	100
In ₂ S ₃	8	0.0009	1	1
CCl ₂ Sc ₂	536	0.0009	57	73
Ge ₂ I ₂ La ₂	486	0.0009	64	49
BiTe	390	0.0009	73	57
Br ₂ Cr	543	0.001	81	100

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Ir₂As₂ (P4/nmm)

Structural and electronic properties

	Formula	Ir ₂ As ₂
	Spacegroup	P4/nmm
	Prototype	FeSe
	Parent 3D	As ₂ Ir ₂ K
	Source DB	MPDS
	DB ID	S2110353
DF2-C09	Binding energy [meV/ Å²]	72.11
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

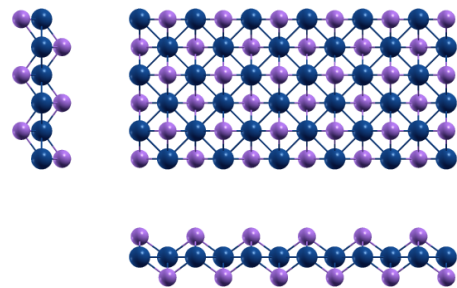


Band structure: Electronic band structure of Ir₂As₂ (P4/nmm) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ir₂As₂ (P4/nmm) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.97796811	0.00000000	0.00000000
a₂		0.00000000	3.97796811	0.00000000
a₃		0.00000000	0.00000000	17.65191260
		x [Å]	y [Å]	z [Å]
●	As	-0.99449203	-0.99449203	1.45458307
●	As	0.99449203	-2.98347608	-1.45458307
●	Ir	0.99449203	-0.99449203	0.00000000
●	Ir	-0.99449203	-2.98347608	0.00000000



Orthographic projections: views of Ir₂As₂ (P4/nmm) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.1736	1	1
Tl	5	0.1088	1	1
InSe	6	0.1381	1	1
Bi ₂	6	0.1431	1	1
AgTl	6	0.0156	1	1
Ag ₂	6	0.1801	1	1
P ₂	6	0.1099	1	1
PbTe	6	0.1396	1	1
I ₂ Mg	7	0.1302	1	1
CdI ₂	7	0.1411	1	1
Nd	7	0.1877	1	3
MoSe ₂	7	0.109	1	1
Ba ₂ Pt	7	0.1798	1	1
Br ₂ Ca	7	0.1421	1	1
CaI ₂	7	0.1632	1	1
I ₂ Pr	7	0.0084	1	1
Br ₂ La	7	0.1305	1	1
Br ₂ Cu	7	0.1021	1	1
Ca ₂ Si	7	0.1854	1	1
I ₂ Yb	7	0.1605	1	1
BiClTe	7	0.1414	1	1
Cl ₂ Ti	7	0.1099	1	1
BrCdI	7	0.1325	1	1
HgI ₂	7	0.3956	1	1
BaF ₂	7	0.1351	1	1
BiBrTe	7	0.1463	1	1
AsKSn	7	0.1339	1	1
PbTe ₂	7	0.1318	1	1
I ₂ Nd	7	0.0075	1	1
Cl ₂ Cu	7	0.0971	1	1
I ₂ Tm	7	0.1619	1	1
GeI ₂	7	0.1398	1	1
I ₂ Pb	7	0.1821	1	1
STl ₂	7	0.1358	1	1
BiITe	7	0.1525	1	1
GeS ₂	7	0.2088	1	1
DyI ₂	7	0.1663	1	1
CeI ₂	7	0.0092	1	1
GdI ₂	7	0.149	1	1
I ₂ La	7	0.0029	1	1
CdI ₂	7	0.1407	1	1
I ₂ Pr	7	0.1414	1	1
Se ₂ W	7	0.109	1	1
Bi ₂ In ₂	8	1.1589	1	1
Cu ₂ Sr ₂	8	0.1472	1	1
LiMnTe ₂	8	0.1401	1	1
Ir ₂ P ₂	8	0.0077	1	1
Ag ₂ Br ₂	8	0.0024	1	1
AsLi ₃	8	0.1384	1	1
O ₂ Sn ₂	8	0.0257	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

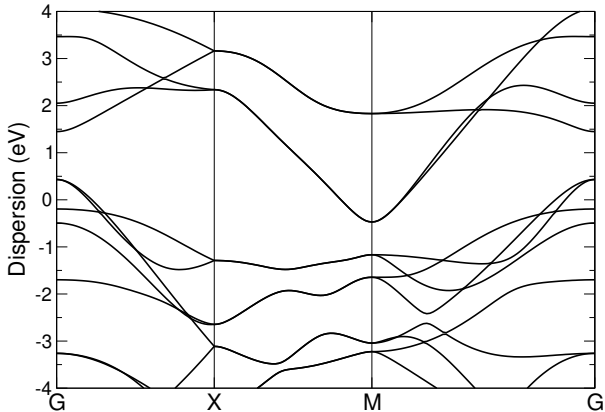
Formula	N° atoms	strain	cell size 1	cell size 2
Fe ₂ S ₂	732	0.0	82	101
AgTe ₂	139	0.0002	16	25
S ₂ Sn	387	0.0002	48	65
HgI ₂	516	0.0002	81	64
Cu ₂ F ₄	118	0.0003	16	9
Pb ₂ Se ₂	472	0.0003	65	53
Ag ₂ K ₂ Te ₂	294	0.0003	36	25
Bi ₂ Se ₂	68	0.0003	9	8
S ₂ Zr	387	0.0003	48	65
In	52	0.0003	9	16
Cl ₂ S ₂ Tl ₂	196	0.0003	25	16
Ho ₂ S ₂	696	0.0004	85	89
GeS ₂	887	0.0004	113	145
CrS ₂	197	0.0004	20	39
Bi ₂ Pd	208	0.0005	25	36
NbTe ₂	387	0.0005	48	65
O ₄ PSn	550	0.0005	64	49
As ₂ Cd ₂ K ₂	550	0.0005	64	49
Ag ₂ K ₂ Se ₂	718	0.0005	82	65
Fe ₂ S ₂	724	0.0006	81	100
PSn ₂	387	0.0006	48	65
Cl ₄ Mn	645	0.0006	85	61
H ₄ Ti	717	0.0006	58	97
Bi ₂ In ₂	340	0.0007	49	36
AgNO ₃	877	0.0007	118	81
NaO ₄	877	0.0008	118	81
Cl ₂ O ₂ Sc ₂	76	0.0008	7	8
Ca ₂ O ₂	244	0.0008	25	36
I ₂ N ₂ Ti ₂	86	0.0008	8	9
F ₄ Pb	814	0.0008	101	82
Ge ₂ Mn ₂ Sr ₂	10	0.0008	1	1
Se ₂ Ti	678	0.0009	81	118
Cu ₂ Rb ₂ Te ₂	412	0.001	49	36
Ba ₂ H ₂ I ₂	962	0.001	113	85
Ca ₂ H ₂ I ₂	10	0.001	1	1
Se ₂ Si ₂ Zr ₂	752	0.001	65	82
Br ₂ O ₂ Sc ₂	96	0.001	9	10
Na	442	0.0011	81	118
H ₂ Li ₂ Pd	717	0.0012	58	97
Cl ₂ Er ₂ S ₂	34	0.0012	4	3
Br ₂ Zr ₂	796	0.0013	81	118
CNNa	752	0.0013	110	104
Ag ₂ I ₂	580	0.0013	81	64
Ag ₂ K ₂ Se ₂	708	0.0013	81	64
H ₂ Na ₂ O ₂	438	0.0013	36	49
Mg ₃	578	0.0013	65	106
CNRb	388	0.0014	64	44
Cl ₂ Rb ₂	492	0.0014	89	34
Br ₂ OV	640	0.0014	71	89
F ₄ Pb	805	0.0014	100	81

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Ir₂P₂ (P4/nmm)

Structural and electronic properties

	Formula	Ir ₂ P ₂
	Spacegroup	P4/nmm
	Prototype	FeSe
	Parent 3D	Ir ₂ KP ₂
	Source DB	MPDS
	DB ID	S2110351
DF2-C09	Binding energy [meV/ Å²]	85.81
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

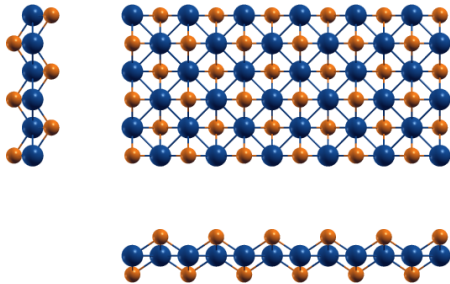


Band structure: Electronic band structure of Ir₂P₂ (P4/nmm) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ir₂P₂ (P4/nmm) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.91230452	0.00000000	0.00000000
a₂		0.00000000	3.91230452	0.00000000
a₃		0.00000000	0.00000000	17.17905620
		x [Å]	y [Å]	z [Å]
●	P	-0.97807613	-0.97807613	-1.30799921
●	P	0.97807613	-2.93422839	1.30799921
●	Ir	-0.97807613	-2.93422839	0.00000000
●	Ir	0.97807613	-0.97807613	0.00000000



Orthographic projections: views of Ir₂P₂ (P4/nmm) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.1831	1	1
InSe	6	0.1449	1	1
Bi ₂	6	0.1503	1	1
AgTl	6	0.0217	1	1
Ag ₂	6	0.1901	1	1
LiO	6	0.1099	1	1
PbTe	6	0.1465	1	1
Sb ₂	6	0.1318	1	1
I ₂ Mg	7	0.1362	1	1
MoS ₂	7	0.1114	1	1
CdI ₂	7	0.1481	1	1
Nd	7	0.7531	1	3
Ba ₂ Pt	7	0.1897	1	1
Br ₂ Ca	7	0.1493	1	1
CaI ₂	7	0.172	1	1
AsSn ₂	7	0.1085	1	1
I ₂ Pr	7	0.0008	1	1
Br ₂ La	7	0.1364	1	1
Br ₂ Cu	7	0.1052	1	1
Ca ₂ Si	7	0.1957	1	1
I ₂ Yb	7	0.1691	1	1
BiClTe	7	0.1485	1	1
BrCdI	7	0.1387	1	1
HgI ₂	7	1.1131	1	1
I ₂ Zn	7	0.1295	1	1
BaF ₂	7	0.1415	1	1
BiBrTe	7	0.1538	1	1
S ₂ W	7	0.1114	1	1
GeI ₂	7	0.1347	1	1
AsKSn	7	0.1403	1	1
PbTe ₂	7	0.1379	1	1
I ₂ Nd	7	0.0002	1	1
Cl ₂ Cu	7	0.0984	1	1
I ₂ Tm	7	0.1707	1	1
SnTe ₂	7	0.133	1	1
Cl ₂ V	7	0.1104	1	1
GeI ₂	7	0.1467	1	1
I ₂ Pb	7	0.1921	1	1
STl ₂	7	0.1424	1	1
PtSe ₂	7	0.1087	1	1
BiTe	7	0.1605	1	1
GeS ₂	7	0.2175	1	1
DyI ₂	7	0.1753	1	1
CeI ₂	7	0.0015	1	1
Se ₂ Yb	7	0.1349	1	1
MoS ₂	7	0.1113	1	1
BiTe ₂	7	0.1351	1	1
GdI ₂	7	0.1567	1	1
CrSe ₂	7	0.1107	1	1
I ₂ La	7	0.005	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

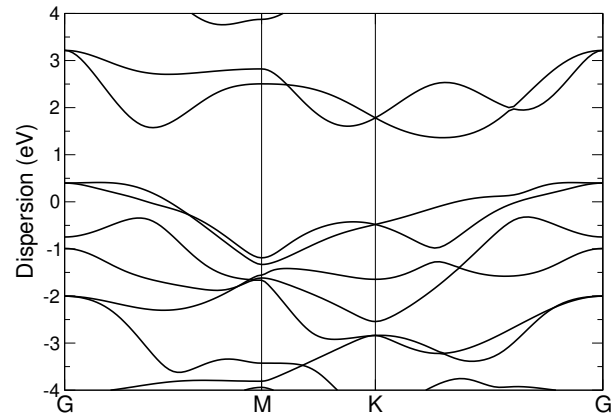
Formula	N° atoms	strain	cell size 1	cell size 2
Ag ₂ K ₂ Te ₂	490	0.0001	61	41
Br ₂ O ₂ Sm ₂	10	0.0002	1	1
Ca ₂ N	387	0.0002	48	65
I ₂ Nd	7	0.0002	1	1
Ag ₂ K ₂ Se ₂	560	0.0002	65	50
Tl	492	0.0002	89	136
Hf ₂ Se ₂ Si ₂	924	0.0003	81	100
Cu ₂ K ₂ Te ₂	412	0.0003	49	36
Cu ₂ Na ₂ Te ₂	886	0.0003	100	81
Br ₂ CsF	584	0.0003	85	61
Bi ₂ Pd	499	0.0004	61	85
I ₂ O ₂ Yb ₂	10	0.0004	1	1
C ₂ Cl ₂ Y ₂	880	0.0005	79	94
Cl ₄ Mn	269	0.0005	36	25
Mo ₂ Te ₄	824	0.0005	101	70
As ₂	322	0.0006	48	65
Mg ₄	900	0.0006	89	136
Cl ₂ Cu	676	0.0006	88	108
F ₄ Pb	644	0.0006	81	64
C ₂ Li ₂	672	0.0006	84	84
BrNZr	678	0.0006	81	118
Br ₂ Hf ₂ N ₂	582	0.0006	48	65
HgI ₂	403	0.0006	64	49
CCL ₂ Lu ₂	517	0.0007	48	65
H ₂ Li ₂ Pd	790	0.0007	65	106
I ₂ Pr	7	0.0008	1	1
AgBrO ₂	724	0.0008	88	93
As ₂ Fe ₂	724	0.0008	81	100
NS ₂ Ta	236	0.0008	20	39
Ag ₂ K ₂ Se ₂	550	0.0009	64	49
Mg ₃	139	0.0009	16	25
As ₂ O ₃	757	0.0009	108	65
Br ₂ Fe	387	0.0009	48	65
Ca ₂ O ₂	584	0.0009	61	85
O ₂ Sn ₂	900	0.001	101	124
Br ₂ Co	387	0.001	48	65
C ₂ Cl ₂ Y ₂	804	0.0011	72	86
Se ₂ V	694	0.0011	79	126
O ₄ PTl	962	0.0011	113	85
Ba ₂ F ₂ I ₂	962	0.0012	113	85
Cl ₂ N ₂ Zr ₂	582	0.0012	48	65
NbSe ₂	678	0.0012	81	118
Mg ₂	472	0.0012	65	106
AuI ₄ Li	558	0.0012	81	39
H ₄ Ti	790	0.0013	65	106
I ₂ O ₂ Tm ₂	10	0.0013	1	1
Cu ₂ Rb ₂ Te ₂	706	0.0013	85	61
Cl ₂ Cu	362	0.0014	47	58
N ₂ W	197	0.0014	20	39
CaH ₂ O ₂	517	0.0014	48	65

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

IrTe₂ (P-3m1 (164))

Structural and electronic properties

	Formula	IrTe ₂
	Spacegroup	P-3m1 (164)
	Prototype	CdI2
	Parent 3D	IrTe ₂
	Source DB	COD
	DB ID	9009106
DF2-C09	Binding energy [meV/ Å²]	55.02
RVV10	Binding energy [meV/ Å²]	55.09
	Band gap (PBE) [eV]	0.0

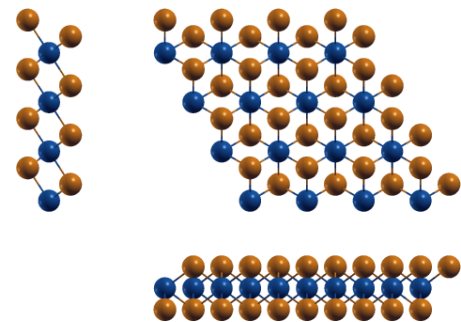


Band structure: Electronic band structure of IrTe₂ (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of IrTe₂ (P-3m1 (164)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.90084044	0.00000000	0.00000000
a₂	-1.95042022	3.37822692	0.00000000
a₃	0.00000000	0.00000000	22.83213713
	x [Å]	y [Å]	z [Å]
● Te	1.95042022	1.12607564	9.94672255
● Te	0.00000000	2.25215128	12.88541458
● Ir	0.00000000	0.00000000	11.41606857



Orthographic projections: views of IrTe₂ (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	4	3.0315	1	1
Tl	4	1.5241	1	1
Na	4	0.275	1	1
AsSb	5	0.0069	1	1
Bi ₂	5	0.4512	1	1
GeTe	5	0.0009	1	1
S ₂	5	0.0007	1	1
CaCl	5	0.1376	1	1
CdCl ₂	6	0.002	1	1
Cl ₂ Mn	6	1.5654	1	1
ReSe ₂	6	0.2572	1	1
S ₂ Ta	6	1.5805	1	1
Br ₂ Ca	6	0.4486	1	1
CaI ₂	6	2.9097	1	1
InSe ₂	6	0.0016	1	1
GeTe ₂	6	0.003	1	1
HfTe ₂	6	0.0085	1	1
I ₂ Mn	6	0.0018	1	1
NSr ₂	6	0.0053	1	1
I ₂ Yb	6	0.497	1	1
LiO ₂	6	0.0678	1	1
Cl ₂ Zn	6	0.1504	1	1
FeI ₂	6	0.004	1	1
I ₂ Ni	6	0.0028	1	1
S ₂ Ti	6	0.2491	1	1
CrI ₂	6	0.0044	1	1
BiBrTe	6	0.4601	1	1
Bi ₂ Pd	6	0.1136	1	1
Cl ₂ Ni	6	0.2585	1	1
Cl ₂ Co	6	0.2486	1	1
CrTe ₂	6	0.2671	1	1
Br ₂ V	6	0.2561	1	1
ClN ₂ Zr	6	1.641	1	1
Cl ₂ Fe	6	0.2477	1	1
S ₂ Ta	6	1.5398	1	1
Se ₂ V	6	1.5302	1	1
Se ₂ Ti	6	0.2726	1	1
Br ₂ Ti	6	0.2662	1	1
Te ₂ Zr	6	0.009	1	1
AsSe ₂	6	0.2605	1	1
I ₂ Tm	6	0.5006	1	1
BiTe	6	0.4766	1	1
CdO ₂	6	0.2484	1	1
BrN ₂ Zr	6	0.2623	1	1
NbSe ₂	6	0.2591	1	1
CoI ₂	6	0.0064	1	1
GeS ₂	6	0.1285	1	1
MnSe ₂	6	0.1375	1	1
Br ₂ Cr	6	0.2667	1	1
Cl ₂ Zr	6	0.2482	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

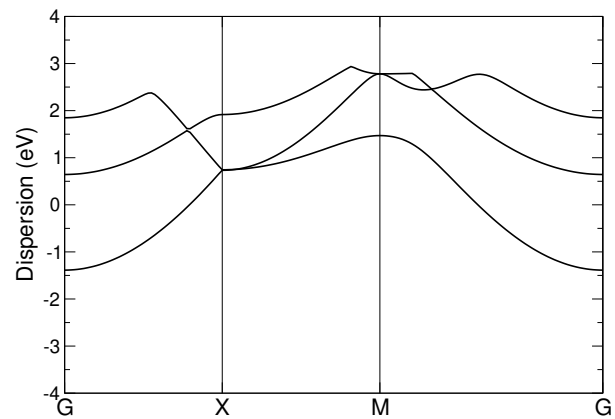
Formula	N° atoms	strain	cell size 1	cell size 2
Se ₂ Ta	435	0.0001	64	81
S ₂ Ti	339	0.0001	49	64
Cl ₂ H ₂ Zr ₂	402	0.0001	36	49
GdI ₂	492	0.0001	91	73
NbS ₂	255	0.0001	36	49
BrKO ₃	368	0.0002	81	25
ClKO ₃	227	0.0002	49	16
Bi ₂ Te ₃	563	0.0002	81	64
NbSe ₂	435	0.0002	64	81
Ga ₂ Se ₂	7	0.0002	1	1
I ₂ La ₂ Te	327	0.0002	49	36
BiTe	435	0.0002	81	64
Cl ₂ Zr ₂	463	0.0003	57	73
Br ₂ Ca ₃ Si	363	0.0004	49	36
CrTe ₂	543	0.0004	81	100
H ₂ MnO ₂	107	0.0004	9	16
CaI ₂	300	0.0004	57	43
Cl ₂ Hf ₂	357	0.0004	43	57
AsI ₂ La ₂	504	0.0004	73	57
Ba ₂ Cu ₂	388	0.0004	64	49
BiBrTe	543	0.0004	100	81
Cl ₂ Sc ₂	643	0.0004	81	100
Cd ₂ I ₃	504	0.0004	73	57
Br ₂ V	390	0.0005	57	73
Cl ₂ Co	339	0.0005	49	64
O ₂ Zn	294	0.0006	37	61
Se ₂ Ta	492	0.0006	73	91
Cu ₂ Sr ₂	624	0.0006	100	81
Cl ₂ Ni	435	0.0006	64	81
I ₂ Yb	339	0.0006	64	49
CdO ₂	339	0.0006	49	64
Br ₂ Cr	543	0.0006	81	100
S ₂	5	0.0007	1	1
CCl ₂ Sc ₂	536	0.0007	57	73
In ₂ S ₃	8	0.0007	1	1
Gd ₂ I ₂ Se ₂	624	0.0007	100	54
Br ₂ H ₂ Zr ₂	843	0.0008	81	100
I ₂ N ₂ Ti ₂	828	0.0008	96	90
I ₂ La ₂ P	638	0.0008	91	73
Cl ₂ H ₂ Sc ₂	765	0.0008	73	91
Cl ₂ Zr	339	0.0008	49	64
Ni ₂ SbTe ₂	8	0.0008	1	1
AsSe ₂	435	0.0009	64	81
AlLiTe ₂	499	0.0009	81	64
C ₂ F ₂	48	0.0009	4	9
GeTe	5	0.0009	1	1
Cl ₂ Fe ₂ O ₂	711	0.0009	73	82
Br ₂ Ti	543	0.0009	81	100
Ce ₂ I ₂ S ₂	258	0.001	36	25
Ca ₂ Si	183	0.001	36	25

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

K (P4/mmm (123))

Structural and electronic properties


	Formula	K
	Spacegroup	P4/mmm (123)
	Prototype	Sn
	Parent 3D	KNi ₂ Se ₂
	Source DB	COD
	DB ID	4117903
DF2-C09	Binding energy [meV/ Å²]	88.58
RVV10	Binding energy [meV/ Å²]	86.3
	Band gap (PBE) [eV]	0.0

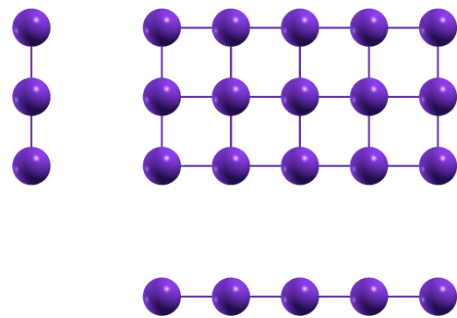


Band structure: Electronic band structure of K (P4/mmm (123)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of K (P4/mmm (123)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.31767713	0.00000000	0.00000000
a₂	0.00000000	4.31767713	0.00000000
a₃	0.00000000	0.00000000	20.00000000
	x [Å]	y [Å]	z [Å]
 K	2.15883856	2.15883856	10.00000000



Orthographic projections: views of K (P4/mmm (123)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	2	0.1355	1	1
Na	2	0.1104	1	1
Ag ₂	3	0.14	1	1
As ₂	3	0.1087	1	1
Sb ₂	3	0.1089	1	1
Cl ₂ Zn	4	0.1089	1	1
MoTe ₂	4	0.1099	1	1
Nd	4	0.1452	1	3
Ba ₂ Pt	4	0.1398	1	1
Te ₂ V	4	0.1095	1	1
Ca ₂ Si	4	0.1437	1	1
Br ₂ Co	4	0.1088	1	1
Br ₂ Mn	4	0.1092	1	1
PtS ₂	4	0.1102	1	1
CdClO	4	0.1096	1	1
CKN	4	0.4069	1	1
Se ₂ Ti	4	0.1108	1	1
Te ₂ W	4	0.1099	1	1
I ₂ Pb	4	0.1413	1	1
OTl ₂	4	0.1096	1	1
Br ₂ Fe	4	0.1088	1	1
DyI ₂	4	0.1307	1	1
CeI ₂	4	0.2213	1	1
F ₂ Zn	4	0.2176	1	1
Bi ₂ Te ₂	5	0.1558	1	1
Fe ₂ Te ₂	5	0.2079	1	1
Li ₂ Tl ₂	5	0.1832	1	1
Ca ₂ Cl ₂	5	0.2084	1	1
Cl ₂ OOS	5	0.5669	1	1
NS ₂ Zr	5	0.1103	1	1
S ₂ Sn ₂	5	0.0197	1	1
Cu ₂ S ₂	5	0.214	1	1
Au ₂ Br ₂	5	0.0086	1	1
Br ₂ Cu ₂	5	0.2161	1	1
N ₃ Na	5	0.0287	1	1
Tl	5	0.0767	2	3
AgBrO ₂	5	0.1272	1	1
Ge ₂ S ₂	5	0.0459	1	1
Br ₂ Zr ₂	5	0.1109	1	1
O ₂ Sn ₂	5	0.2147	1	1
KS ₂ Ti	5	0.1091	1	1
P ₂ Rh ₂	5	0.2133	1	1
F ₂ Tl ₂	5	0.2134	1	1
BN	5	0.1481	1	2
Sb ₂ Te ₂	5	0.1425	1	1
Ge ₂ Se ₂	5	0.0281	1	1
Cu ₂ Se ₂	5	0.5602	1	1
Ag ₂ Te ₂	5	0.2153	1	1
As ₂ Ru ₂	5	0.2086	1	1
AgClO ₂	5	0.121	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

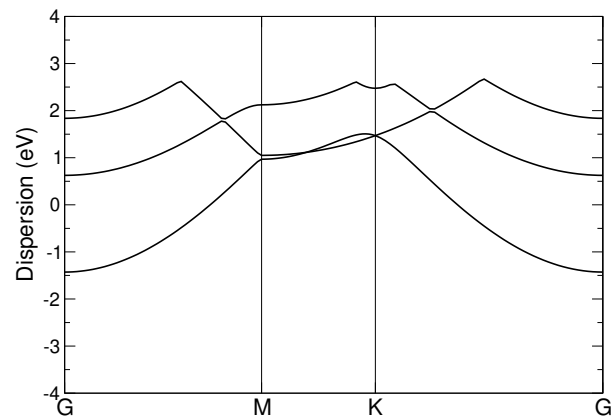
Formula	N° atoms	strain	cell size 1	cell size 2
Ca ₂ Cl ₂ F ₂	433	0.0001	49	64
F ₂ Tl ₂	393	0.0001	65	82
MnSe ₂	133	0.0002	25	36
Bi ₂ Cl ₂ O ₂	681	0.0002	81	100
Cl ₂ S ₂ Tl ₂	623	0.0002	113	85
Cl ₄ Cu ₂	427	0.0002	109	53
P ₂ Rh ₂	393	0.0003	65	82
Br ₂ Cu ₂	869	0.0003	145	181
CaCl	97	0.0003	25	36
Tl	59	0.0003	20	39
Bi ₂ Se ₂	441	0.0003	85	89
Br ₂ Dy ₂ O ₂	557	0.0003	65	82
As ₂ Mg ₂ Na ₂	7	0.0003	1	1
Br ₂ O ₂ Y ₂	557	0.0003	65	82
Br ₂ O ₂ Tm ₂	983	0.0003	113	145
Hf ₃ Te ₂	281	0.0004	36	49
Ca ₂ Ge ₂ Mn ₂	681	0.0004	81	100
Cu ₂ S ₂	393	0.0004	65	82
Se ₂ Ta ₄	701	0.0004	65	106
Ba ₂ N	243	0.0005	48	65
P ₂ Rh ₂	388	0.0005	64	81
AgClO ₄	472	0.0005	82	65
Br ₂ F ₂ Tm ₂	681	0.0005	81	100
Ge ₂ Hf ₂ Te ₂	763	0.0005	85	113
As ₂ Ru ₂	693	0.0006	113	145
Hf ₂ Si ₂ Te ₂	571	0.0006	61	85
I ₂ Lu ₂ O ₂	681	0.0006	81	100
Br ₂ O ₂ V ₂	267	0.0006	27	40
AsSb	317	0.0006	81	118
F ₂ Tl ₂	388	0.0006	64	81
Se ₂ V	137	0.0007	20	39
Br ₂ Ho ₂ O ₂	550	0.0007	64	81
Cu ₃ Se ₃	438	0.0007	48	65
Ca ₂ Cl ₂	693	0.0007	113	145
CoI ₂	435	0.0007	81	118
Fe ₂ Li ₂ P ₂	571	0.0008	61	85
Se ₂ W	137	0.0008	20	39
Bi ₂ Pd	520	0.0008	85	145
Ca ₂ Mn ₂ Si ₂	550	0.0008	64	81
Cl ₂ O ₂ V ₂	465	0.0009	45	70
Ni ₂ Se ₂	486	0.0009	82	101
Co ₂ S ₂	169	0.0009	25	36
Ca ₂ Cl ₂ H ₂	330	0.0009	36	49
H ₂ Na ₂ O ₂	901	0.0009	85	136
O ₂ Sn ₂	393	0.001	65	82
MoSe ₂	137	0.001	20	39
PTe ₂ Zr ₂	671	0.001	81	118
Ho ₂ S ₂	313	0.001	53	65
I ₄ Zr ₂	296	0.001	56	40
S ₂ Sn	457	0.001	79	126

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

K (P6/mmm (191))

Structural and electronic properties


	Formula	K
	Spacegroup	P6/mmm (191)
	Prototype	In
	Parent 3D	KSnS ₂
	Source DB	ICSD
	DB ID	23448
DF2-C09	Binding energy [meV/ Å²]	109.86
RVV10	Binding energy [meV/ Å²]	114.65
	Band gap (PBE) [eV]	0.0

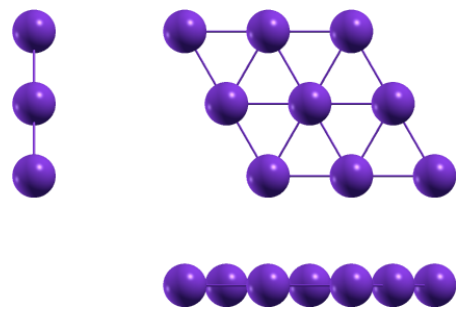


Band structure: Electronic band structure of K (P6/mmm (191)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of K (P6/mmm (191)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.57595034	0.00000000	0.00000000
a₂	-2.28797517	3.96288924	0.00000000
a₃	0.00000000	0.00000000	20.00000000
	x [Å]	y [Å]	z [Å]
 K	0.00000000	0.00000000	10.00000000



Orthographic projections: views of K (P6/mmm (191)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	2	0.1467	1	1
Na	2	4.845	1	1
GeTe	3	1.522	1	1
AgTl	3	0.1242	1	1
Ag ₂	3	0.0055	1	1
Sb ₂	3	0.2652	1	1
IrTe ₂	4	1.5285	1	1
I ₂ Mg	4	0.2735	1	1
Ba ₂ Pt	4	0.0053	1	1
CaI ₂	4	0.009	1	1
HfTe ₂	4	1.5887	1	1
I ₂ Pr	4	0.1147	1	1
Br ₂ La	4	0.274	1	1
AuTe ₂	4	0.2543	1	1
PdTe ₂	4	1.6283	1	1
I ₂ Zn	4	0.2606	1	1
GeI ₂	4	0.2707	1	1
Ba ₂ Hg	4	0.134	1	1
PtS ₂	4	4.8669	1	1
Ba ₂ N	4	1.6	1	1
Te ₂ Zr	4	1.5923	1	1
I ₂ Nd	4	0.1151	1	1
Cl ₂ Cu	4	0.1904	1	1
SnTe ₂	4	0.2674	1	1
I ₂ V	4	1.4472	1	1
I ₂ Pb	4	0.0071	1	1
DyI ₂	4	0.0063	1	1
CeI ₂	4	0.1144	1	1
Se ₂ Yb	4	0.2711	1	1
BiTe ₂	4	0.2715	1	1
PtTe ₂	4	0.2538	1	1
Br ₂ Cd	4	0.2498	1	1
I ₂ La	4	0.1173	1	1
F ₂ Zn	4	0.1131	1	1
Ba ₂ Cd	4	0.1361	1	1
NaPSn	4	1.5821	1	1
Li ₂ Tl ₂	5	0.4535	1	1
Cu ₂ I ₂	5	0.1266	1	1
In ₂ Se ₂	5	0.1673	1	1
Cu ₂ Te ₂	5	0.1121	1	1
Ir ₂ P ₂	5	0.115	1	1
Ag ₂ Br ₂	5	0.1176	1	1
Br ₂ Er ₂	5	0.255	1	1
O ₂ Sn ₂	5	0.1139	1	1
Cu ₂ S ₂	5	0.1119	1	1
Au ₂ Br ₂	5	0.1333	1	1
HgI ₂	5	0.2304	2	1
Mg ₃	5	0.1548	2	1
Ge ₂ Te ₂	5	0.148	1	1
Br ₂ Tb ₂	5	1.6328	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

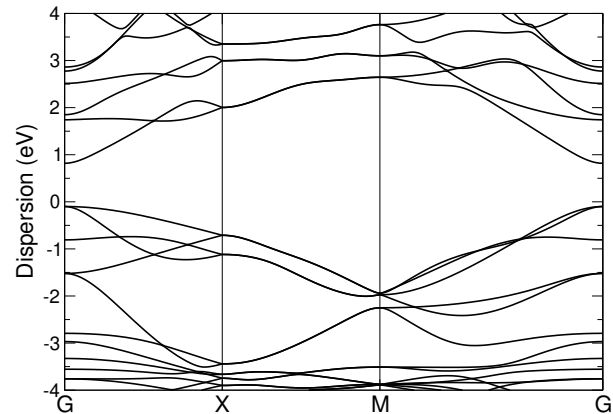
Formula	N° atoms	strain	cell size 1	cell size 2
Te ₂ Zr	214	0.0	43	57
Te ₂ Zn	220	0.0	37	61
CBr ₂ Lu ₂	141	0.0001	16	25
Cl ₂ O ₂ Y ₂	241	0.0001	25	36
Cl ₂ V	276	0.0001	39	79
N ₂ Re	217	0.0001	25	64
SnTe ₂	381	0.0001	81	100
Br ₂ N ₂ Zr ₂	166	0.0001	16	25
I ₂ Lu ₂ S ₂	172	0.0001	28	24
Sm	65	0.0002	16	49
BH ₄ Li	681	0.0002	81	100
In ₂ Se ₂	388	0.0002	64	81
MoTe ₂	220	0.0002	37	61
Br ₂ PY ₂	369	0.0002	49	64
C ₄ Ca ₂	624	0.0002	84	90
Br ₂ Gd ₂	349	0.0002	57	73
HfLiS ₂	281	0.0002	37	61
Ca ₄ Cu ₂	177	0.0003	33	24
Cl ₂ Gd ₂	232	0.0003	36	49
Br ₂ Er ₂	349	0.0003	57	73
As ₂ Sn ₂	349	0.0003	57	73
I ₂ S ₂ Sm ₂	7	0.0003	1	1
I ₂ La ₂ Sb	6	0.0004	1	1
Te ₂ W	220	0.0004	37	61
PtS ₂	292	0.0004	49	81
Br ₂ La ₂	437	0.0004	73	91
Br ₂ Cd	241	0.0004	49	64
ClNZr	57	0.0004	9	16
In ₂ Se ₃	328	0.0005	43	57
CrSe ₂	349	0.0005	49	100
CrO ₂	84	0.0005	9	25
Br ₂ Er ₂ S ₂	194	0.0005	32	27
HfTe ₂	214	0.0005	43	57
Ga ₂ Se ₂	169	0.0006	25	36
NaO ₄	401	0.0006	81	64
FHOZn	449	0.0006	49	100
S ₂ Zn ₂	232	0.0006	36	49
Sb ₂	255	0.0006	73	91
Cl ₂ Ho ₂ O ₂	241	0.0006	25	36
P ₄	523	0.0007	91	108
Er ₂ F ₂ Se ₂	385	0.0007	43	57
Cu ₃ Se ₃	385	0.0008	43	57
CdH ₂ O ₂	342	0.0008	37	61
F ₂ Se ₂ Yb ₂	330	0.0008	36	49
F ₂ Ho ₂ Se ₂	433	0.0008	49	64
CeLi ₂ P ₂	581	0.0008	81	100
C	73	0.0008	9	64
AuTe ₂	276	0.0009	57	73
Br ₂ Y ₂	169	0.0009	25	36
Cl ₂ N ₂ Ti ₂	94	0.0009	10	14

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

K₂Ag₂Te₂ (Pm)

Structural and electronic properties

Formula	K ₂ Ag ₂ Te ₂
Spacegroup	Pm
Prototype	PbClF
Parent 3D	Ag ₂ Ce ₂ K ₂ Te ₈
Source DB	MPDS
DB ID	S1623484
DF2-C09 Binding energy [meV/ Å²]	37.64
RVV10 Binding energy [meV/ Å²]	N/A
Band gap (PBE) [eV]	0.92

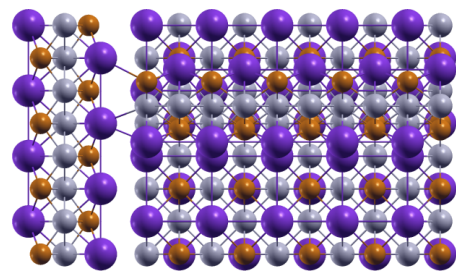


Band structure: Electronic band structure of K₂Ag₂Te₂ (Pm) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of K₂Ag₂Te₂ (Pm) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		0.00000000	-4.77080685	0.00000000
a₂		-4.77079690	0.00000000	0.00000000
a₃		0.00000000	0.00000000	24.55655227
		x [Å]	y [Å]	z [Å]
●	K	-2.51744441	-2.38540343	-2.64103158
●	K	-0.13179811	0.00000000	2.64045681
●	Ag	-2.51636881	0.00000000	0.00021045
●	Ag	-0.13035290	-2.38540343	0.00014459
●	Te	-2.51759430	-2.38540343	1.75550091
●	Te	-0.13261811	0.00000000	-1.75528119



Orthographic projections: views of K₂Ag₂Te₂ (Pm) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
GeTe	8	0.1112	1	1
IrTe ₂	9	0.111	1	1
CdCl ₂	9	0.1114	1	1
InSe ₂	9	0.1113	1	1
HfTe ₂	9	0.1091	1	1
I ₂ Mn	9	0.1114	1	1
Ba ₂ Hg	9	0.5979	1	1
CNRb	9	0.0341	1	1
CKN	9	0.2398	1	1
Ba ₂ N	9	0.1088	1	1
Te ₂ Zr	9	0.109	1	1
Ba ₂ Cd	9	0.2086	1	1
NaPSn	9	0.1093	1	1
H ₂ Si ₂	10	0.1113	1	1
Li ₂ Tl ₂	10	0.1352	1	1
Cu ₂ I ₂	10	0.567	1	1
Au ₂ Br ₂	10	0.2234	1	1
Ge ₂ Te ₂	10	0.2154	1	1
N ₃ Na	10	0.2288	1	1
S ₂ Zn ₂	10	0.1105	1	1
As ₄	10	0.1836	1	1
P ₂ Sn ₂	10	0.1106	1	1
LiMnSe ₂	10	0.1099	1	1
Ga ₂ Se ₂	10	0.1109	1	1
Au ₂ I ₂	10	0.6305	1	1
Ni ₂ Te ₂	10	0.1115	1	1
Bi ₂ O ₂	10	0.5612	1	1
AgClO ₂	10	0.3385	1	1
La ₂ S ₂	10	0.216	1	1
PbS ₂ Sn	10	0.2147	1	1
Pt ₂ Te ₂	10	0.1093	1	1
Se ₂ Sn ₂	10	0.221	1	1
Cl ₂ Tb ₂	10	0.1101	1	1
Sm	10	0.1492	1	4
As ₂ O ₃	11	0.1677	1	1
F ₄ Sn	11	0.5955	1	1
In ₂ Se ₃	11	0.1091	1	1
FKO ₂ Se	11	1.306	1	1
NaO ₄	11	0.1431	1	1
AgNO ₃	11	0.1438	1	1
Cl ₄ Mn	11	0.0079	1	1
In ₂ S ₃	11	0.1111	1	1
Ni ₂ SbTe ₂	11	0.1108	1	1
Ho ₂ I ₂ S ₂	12	0.0548	1	1
Eu ₂ F ₂ I ₂	12	0.5596	1	1
AlH ₄ Na	12	0.0054	1	1
NiO ₂	12	0.1517	1	2
Br ₂ Ca ₃ Si	12	0.5986	1	1
Br ₂ S ₂ Y ₂	12	0.3405	1	1
Gd ₂ I ₂ S ₂	12	0.0539	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

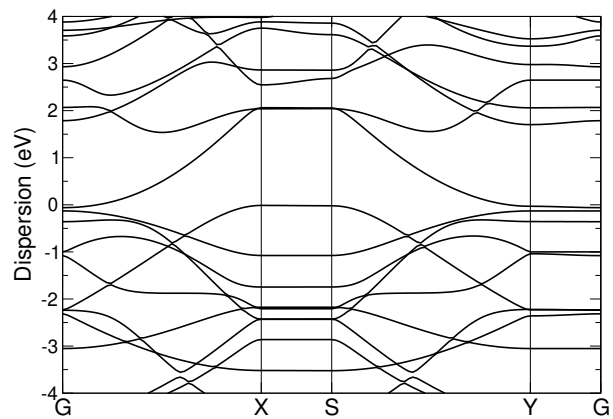
Formula	N° atoms	strain	cell size 1	cell size 2
In	214	0.0001	25	64
Br ₂ Ca ₃ Si	690	0.0001	50	65
Ir ₂ P ₂	490	0.0001	41	61
Ba ₂ Hg	495	0.0001	50	65
F ₄ Sn	614	0.0002	49	64
Cl ₂ Zn	537	0.0002	49	81
S ₂ Zr	237	0.0002	20	39
NbTe ₂	237	0.0002	20	39
As ₂ Ir ₂	294	0.0003	25	36
Cu ₂ I ₂	412	0.0003	36	49
Ca ₂ Cl ₂ H ₂	780	0.0003	49	81
S ₂ Sn	237	0.0003	20	39
Bi ₂ Se ₂	278	0.0004	25	32
AgTe ₂	51	0.0004	4	9
Cu ₂ Te ₂	814	0.0004	65	106
Er ₂ I ₂ S ₂	852	0.0005	70	72
Cu ₂ Se ₂	736	0.0005	58	97
Cu ₂ Se ₂ Tl ₂	510	0.0006	36	49
Ge ₂ Mn ₂ Sr ₂	366	0.0006	25	36
AsLi ₃	958	0.0006	81	118
Pd ₂ S ₄	588	0.0006	56	42
InSe	722	0.0007	81	118
Br ₂ Y ₂	476	0.0007	36	65
Br ₂ Er ₂ O ₂	246	0.0007	16	25
Br ₂ H ₂ Sr ₂	510	0.0007	36	49
Ag ₂ Te ₂	588	0.0008	48	75
I ₂ S ₂ Tl ₂	930	0.0008	58	97
Sn	293	0.0008	34	89
I ₂ Nd ₂ O ₂	876	0.0008	61	85
PSn ₂	237	0.0008	20	39
Ca ₂ O ₂	754	0.0008	53	109
Fe ₂ S ₂	118	0.0008	9	16
Hf ₃ Te ₂	699	0.0009	49	81
Er ₂ I ₂ S ₂	840	0.0009	69	71
Cl ₂ Ho ₂ O ₂	606	0.0009	36	65
Br ₂ Ho ₂ S ₂	738	0.0009	60	63
PbS ₂	411	0.0009	36	65
Br ₂ O ₂ Tm ₂	246	0.0009	16	25
Ba ₂ Hg	486	0.001	49	64
Br ₂ O ₂ Sc ₂	234	0.001	15	24
F ₂ Ni	639	0.0011	58	97
Si ₂ Te ₂ Zr ₂	930	0.0011	58	97
MoSe ₂	633	0.0011	48	115
Cl ₂ La ₂	978	0.0011	79	126
BrKO ₃	684	0.0011	79	42
Cl ₂ Er ₂ S ₂	624	0.0012	50	54
As ₂ Ru ₂	196	0.0012	16	25
Se ₂ W	633	0.0012	48	115
Br ₂ Ca ₃ Si	678	0.0012	49	64
I ₂ S ₂ Tb ₂	954	0.0012	79	80

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

K₂PdS₂ (Pmmm (47))

Structural and electronic properties

	Formula	K ₂ PdS ₂
	Spacegroup	Pmmm (47)
	Prototype	K ₂ PtSe ₂
	Parent 3D	K ₂ PdS ₂
	Source DB	ICSD
	DB ID	641296
DF2-C09	Binding energy [meV/ Å²]	107.63
RVV10	Binding energy [meV/ Å²]	112.31
	Band gap (PBE) [eV]	0.0

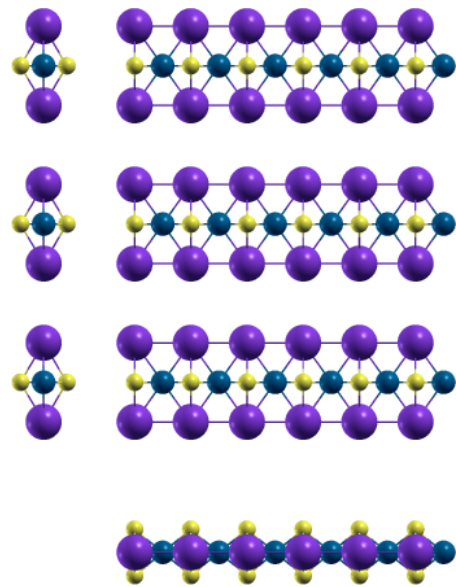


Band structure: Electronic band structure of K₂PdS₂ (Pmmm (47)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of K₂PdS₂ (Pmmm (47)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.70372430	0.00000000	0.00000000
a₂		0.00000000	10.44002100	0.00000000
a₃		0.00000000	0.00000000	23.07788193
		x [Å]	y [Å]	z [Å]
●	K	0.00000000	2.61149000	11.53894096
●	S	0.00000000	5.22001050	13.06697701
●	K	0.00000000	7.82853100	11.53894096
●	Pd	1.85186215	5.22001050	11.53894096
●	S	0.00000000	5.22001050	10.01090492



Orthographic projections: views of K₂PdS₂ (Pmmm (47)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Br ₃ Cs	9	0.5754	1	1
SbSe ₂ Tl	9	0.4864	1	1
Hg ₃ N ₂	10	0.6138	1	1
ClKO ₃	10	0.5855	1	1
K ₂ PdSe ₂	10	0.0139	1	1
K ₂ PtS ₂	10	0.0036	1	1
GeTe	11	0.0496	1	3
CKN	11	0.045	1	2
S ₂	11	0.0502	1	3
I ₄ Sr ₂	11	0.6675	1	1
Sb ₂	11	0.0653	1	3
CS ₃ Tl ₂	11	4.0696	1	1
IrTe ₂	14	0.05	1	3
I ₂ Mg	14	0.0702	1	3
CdCl ₂	14	0.0492	1	3
InSe ₂	14	0.0493	1	3
HfTe ₂	14	0.0541	1	3
I ₂ Mn	14	0.0492	1	3
Br ₂ La	14	0.0705	1	3
NSr ₂	14	0.0481	1	3
AuTe ₂	14	0.0592	1	3
LiO ₂	14	0.1028	1	3
Cl ₂ Zn	14	0.023	1	3
PdTe ₂	14	0.0575	1	3
FeI ₂	14	0.0485	1	3
I ₂ Ni	14	0.0489	1	3
CrI ₂	14	0.0484	1	3
I ₂ Zn	14	0.0626	1	3
Bi ₂ Pd	14	0.0747	1	3
GeI ₂	14	0.0686	1	3
Ba ₂ N	14	0.055	1	3
Te ₂ Zr	14	0.0544	1	3
Cl ₂ Cu	14	0.1082	1	3
SnTe ₂	14	0.0666	1	3
GeS ₂	14	0.0173	1	3
Br ₂ Mg	14	0.0484	1	3
CuO ₂	14	0.0806	1	3
Se ₂ Yb	14	0.0688	1	3
BiTe ₂	14	0.069	1	3
F ₂ Ni	14	0.0199	1	3
PtTe ₂	14	0.0589	1	3
Br ₂ Cd	14	0.0569	1	3
NaPSn	14	0.0536	1	3
O ₄ PSn	16	0.1589	2	1
Cu ₂ K ₂ Te ₂	16	0.1591	2	1
CS ₃ Tl ₂	16	1.1485	2	1
H ₂ Si ₂	17	0.0495	1	3
CrS ₂	17	0.0802	1	4
Br ₂ Ho ₂ S ₂	17	0.0358	1	2
Cl ₂ Gd ₂	17	0.0513	1	3

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

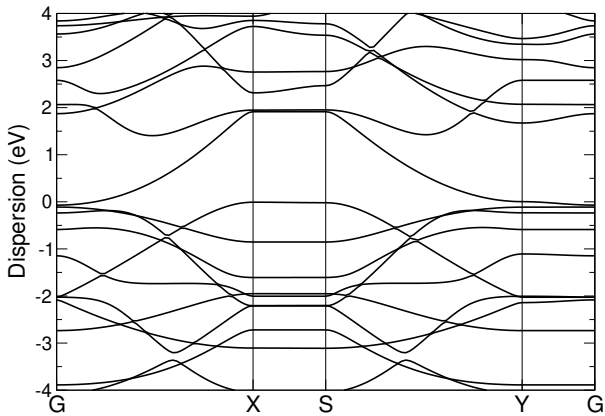
Formula	N° atoms	strain	cell size 1	cell size 2
I ₂ Sb ₂ Te ₂	605	0.0002	49	60
Bi ₂ In ₂	244	0.0005	20	36
Cu ₂ Rb ₂ Te ₂	316	0.0006	20	36
F ₄ Sn	290	0.0007	18	40
PdTe ₂	519	0.0012	39	108
I ₂ La ₂ O ₂	330	0.0013	18	40
Ho ₂ S ₂	668	0.0013	44	112
N ₂ W	177	0.0013	9	44
Br ₂ Tb ₂	627	0.0013	39	108
PtTe ₂	159	0.0014	12	33
IO ₃ Tl	995	0.0014	100	99
Br ₂ Ho ₂	192	0.0014	12	33
Ba ₂ Hg	210	0.0014	18	40
GeI ₂ Y ₂	980	0.0014	56	140
Bi ₂ S ₃	735	0.0015	39	108
AuTe ₂	159	0.0015	12	33
Bi ₂ S ₃	225	0.0015	12	33
Br ₂ Cd	519	0.0015	39	108
CCl ₂ Sc ₂	620	0.0015	26	98
Br ₂ H ₂ Zr ₂	718	0.0016	26	98
Cl ₂ Zr ₂	522	0.0016	26	98
Ag ₂ K ₂ Se ₂	300	0.0016	18	35
Br ₂ PY ₂	735	0.0016	39	108
Br ₂ Ca ₃ Si	330	0.0016	18	40
Br ₂ Tb ₂	192	0.0017	12	33
Br ₂ PY ₂	265	0.0018	14	39
ClN ₂ Zr	424	0.0018	26	98
Br ₂ Cd	187	0.0018	14	39
ClN ₂ Zr	393	0.0018	24	91
NaO ₄	725	0.0019	54	91
Br ₂ Er ₂	192	0.0019	12	33
F ₂ Ho ₂ Se ₂	304	0.0019	14	39
Br ₂ V	424	0.002	26	98
C	121	0.002	6	91
Ca ₄ Cu ₂	970	0.002	68	105
PdTe ₂	332	0.002	25	69
Cu ₂ K ₂ Te ₂	932	0.002	58	107
Br ₂ H ₂ Zr ₂	666	0.0021	24	91
In	75	0.0021	8	35
PdTe ₂	159	0.0021	12	33
Br ₂ CsF	244	0.0021	20	36
Ag ₂	229	0.0022	25	52
I ₂ Pr ₂ S ₂	437	0.0022	25	52
Ba ₂ Pt	281	0.0022	25	52
Hg ₄ O ₂	565	0.0022	65	40
CCl ₂ Sc ₂	575	0.0023	24	91
P ₄	484	0.0023	32	81
AgNO ₃	725	0.0023	54	91
Ga ₂ Gd ₂ I ₂	679	0.0023	35	84
Br ₂ Gd ₂	192	0.0023	12	33

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

K₂PdSe₂ (Pmmm (47))

Structural and electronic properties

	Formula	K ₂ PdSe ₂
	Spacegroup	Pmmm (47)
	Prototype	K ₂ PtSe ₂
	Parent 3D	K ₂ PdSe ₂
	Source DB	ICSD
	DB ID	641298
DF2-C09	Binding energy [meV/ Å²]	90.38
RVV10	Binding energy [meV/ Å²]	94.69
	Band gap (PBE) [eV]	0.0

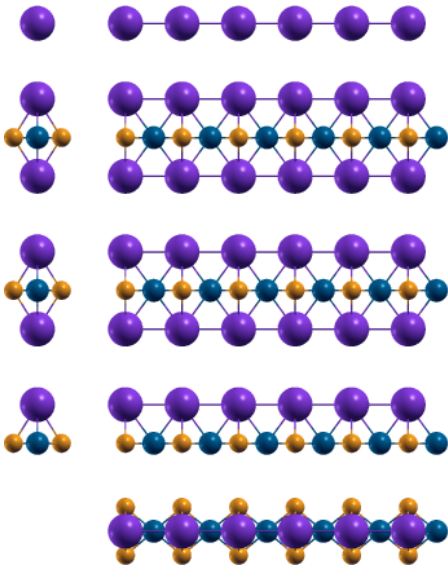


Band structure: Electronic band structure of K₂PdSe₂ (Pmmm (47)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of K₂PdSe₂ (Pmmm (47)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.85542547	0.00000000	0.00000000
a₂		0.00000000	10.42196176	0.00000000
a₃		0.00000000	0.00000000	23.34459305
		x [Å]	y [Å]	z [Å]
●	Se	0.00000000	0.00000000	13.30949288
●	K	0.00000000	7.78642611	11.67229652
●	K	0.00000000	2.63553566	11.67229652
●	Pd	1.92771274	0.00000000	11.67229652
●	Se	0.00000000	0.00000000	10.03510017



Orthographic projections: views of K₂PdSe₂ (Pmmm (47)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Br ₃ Cs	9	0.5351	1	1
SbSe ₂ Tl	9	0.4435	1	1
K ₂ PdS ₂	10	0.0129	1	1
Hg ₃ N ₂	10	0.5711	1	1
K ₂ PtSe ₂	10	0.0086	1	1
K ₂ PtS ₂	10	0.0162	1	1
CKN	11	0.0288	1	2
I ₄ Sr ₂	11	3.2161	1	1
Sb ₂	11	0.056	1	3
I ₂ Mg	14	0.0602	1	3
Br ₂ La	14	0.0605	1	3
AuTe ₂	14	0.0511	1	3
BrCdI	14	0.0627	1	3
PdTe ₂	14	0.0498	1	3
I ₂ Zn	14	0.0538	1	3
GeI ₂	14	0.0588	1	3
AsKSn	14	0.0643	1	3
PbTe ₂	14	0.0619	1	3
SnTe ₂	14	0.0571	1	3
GeS ₂	14	0.0288	1	3
Se ₂ Yb	14	0.0589	1	3
BiTe ₂	14	0.0591	1	3
PtTe ₂	14	0.0508	1	3
Br ₂ Cd	14	0.0493	1	3
K	15	0.0718	2	5
CS ₃ Tl ₂	16	1.0493	2	1
Br ₂ Ho ₂ S ₂	17	0.0206	1	2
S ₂ V	17	0.1537	1	4
MoS ₂	17	0.1543	1	4
Ho ₂ I ₂ S ₂	17	0.0312	1	2
Cu ₄ Te ₂	17	0.1282	1	2
Br ₂ Er ₂	17	0.0514	1	3
ReS ₂	17	0.1451	1	4
Br ₂ Tb ₂	17	0.0501	1	3
S ₂ W	17	0.1544	1	4
Gd ₂ I ₂ S ₂	17	0.1179	1	2
N ₂ W	17	0.0851	1	4
Tl	17	0.0649	2	7
Cl ₂ La ₂	17	0.0524	1	3
Br ₂ Gd ₂	17	0.0517	1	3
MnNaTe ₂	17	0.0624	1	3
I ₂ S ₂ Yb ₂	17	0.0255	1	2
Br ₂ Dy ₂ S ₂	17	0.023	1	2
Br ₂ OV	17	0.0838	1	3
AsCuLi ₂	17	0.0584	1	3
Cu ₂ I ₂	17	0.061	1	3
Sn	17	0.0864	2	7
Br ₂ Lu ₂ S ₂	17	0.0102	1	2
I ₂ La ₂	17	0.0639	1	3
Br ₂ S ₂ Yb ₂	17	0.0164	1	2

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

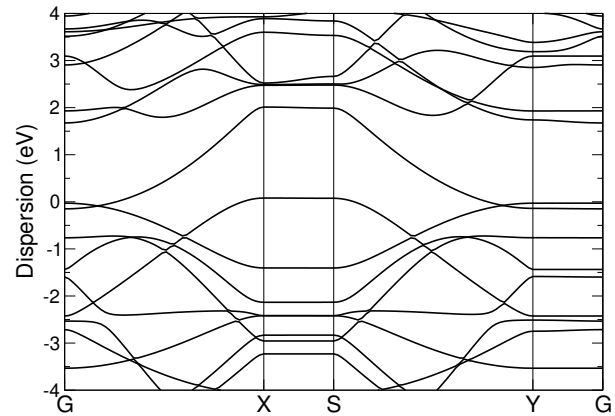
Formula	N° atoms	strain	cell size 1	cell size 2
Ba ₂ Pt	345	0.0001	30	65
Ag ₂	280	0.0002	30	65
Cu ₂ Rb ₂ Te ₂	390	0.0003	24	45
Bi ₂ In ₂	300	0.0006	24	45
Au ₂ I ₂	562	0.0007	42	88
NS ₂ Ta	179	0.0008	7	36
Dy ₂ I ₂ S ₂	393	0.0008	21	48
ClNZr	269	0.0008	16	63
I ₂ Pr ₂ S ₂	540	0.0009	30	65
NaO ₄	165	0.0009	12	21
PbS ₂ Sn	280	0.001	20	45
C	83	0.0011	4	63
Br ₂ H ₂ Zr ₂	458	0.0012	16	63
C ₂ I ₂ La ₂	40	0.0012	2	5
DyI ₂	249	0.0013	21	48
P ₄	372	0.0013	24	63
I ₂ Sb ₂ Te ₂	795	0.0013	63	80
I ₃ Sn	147	0.0014	15	18
CCl ₂ Sc ₂	395	0.0015	16	63
Br ₂ CsF	300	0.0015	24	45
AgNO ₃	165	0.0015	12	21
Bi ₂ Se ₂	392	0.0016	28	63
I ₂ S ₂ Tb ₂	393	0.0016	21	48
Gd ₂ GeI ₂	880	0.0016	50	126
HgI ₂	231	0.0017	21	42
Bi ₂ Te ₂	260	0.0017	20	40
Ag ₂ I ₂	273	0.0017	21	42
Cl ₂ Zr ₂	332	0.0018	16	63
Sb ₂ Te ₂	825	0.0019	61	130
In	133	0.002	14	63
I ₂ Nd ₂ S ₂	540	0.002	30	65
CaI ₂	249	0.002	21	48
Hg ₃ N ₂	960	0.0021	98	94
As ₂ O ₃	815	0.0021	63	100
Sb ₂ Te ₂	665	0.0022	49	105
Br ₂ Tb ₂	379	0.0023	23	66
Bi ₂ S ₃	445	0.0023	23	66
PdTe ₂	313	0.0024	23	66
C ₂ I ₂ Y ₂	608	0.0024	28	78
C ₂ I ₂ Y ₂	585	0.0025	27	75
Ag ₂ K ₂ Se ₂	771	0.0025	45	91
Cl ₂ O ₂ V ₂	300	0.0025	12	40
Br ₂ V	269	0.0026	16	63
Ag ₂ K ₂ Se ₂	357	0.0026	21	42
N ₂ W	143	0.0026	7	36
Ho ₂ S ₂	654	0.0026	42	111
PtTe ₂	313	0.0027	23	66
PtTe ₂	271	0.0027	20	57
AuTe ₂	271	0.0027	20	57
Br ₂ Cd	313	0.0028	23	66

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

K₂PtS₂ (Pmmm (47))

Structural and electronic properties






	Formula	K ₂ PtS ₂
	Spacegroup	Pmmm (47)
	Prototype	K ₂ PtSe ₂
	Parent 3D	K ₂ PtS ₂
	Source DB	ICSD
	DB ID	26258
DF2-C09	Binding energy [meV/ Å²]	97.83
RVV10	Binding energy [meV/ Å²]	102.38
	Band gap (PBE) [eV]	0.0

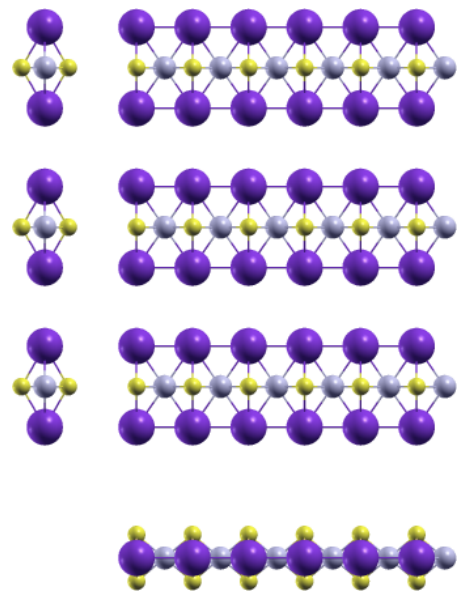


Band structure: Electronic band structure of K₂PtS₂ (Pmmm (47)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of K₂PtS₂ (Pmmm (47)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.66376130	0.00000000	0.00000000
a₂		0.00000000	10.43948047	0.00000000
a₃		0.00000000	0.00000000	23.06033738
		x [Å]	y [Å]	z [Å]
	K	0.00000000	2.56925221	11.53016869
	S	0.00000000	5.21974023	13.05768816
	K	0.00000000	7.87022826	11.53016869
	Pt	1.83188065	5.21974023	11.53016869
	S	0.00000000	5.21974023	10.00264922



Orthographic projections: views of K₂PtS₂ (Pmmm (47)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Br ₃ Cs	9	0.5871	1	1
K ₂ PdS ₂	10	0.0037	1	1
Hg ₃ N ₂	10	0.6262	1	1
ClKO ₃	10	0.5974	1	1
K ₂ PdSe ₂	10	0.0179	1	1
AsSb	11	0.0493	1	3
GeTe	11	0.0516	1	3
CKN	11	0.0496	1	2
S ₂	11	0.0524	1	3
Sb ₂	11	0.0684	1	3
CaCl	11	0.013	1	3
CS ₃ Tl ₂	11	4.1419	1	1
SbSe ₂ Tl	13	0.609	1	2
IrTe ₂	14	0.052	1	3
CdCl ₂	14	0.0511	1	3
InSe ₂	14	0.0513	1	3
GeTe ₂	14	0.0507	1	3
HfTe ₂	14	0.0566	1	3
I ₂ Mn	14	0.0512	1	3
NSr ₂	14	0.0498	1	3
AuTe ₂	14	0.062	1	3
PdTe ₂	14	0.0602	1	3
FeI ₂	14	0.0503	1	3
I ₂ Ni	14	0.0508	1	3
CrI ₂	14	0.0501	1	3
I ₂ Zn	14	0.0656	1	3
GeI ₂	14	0.0718	1	3
Ba ₂ N	14	0.0576	1	3
Te ₂ Zr	14	0.0569	1	3
Cl ₂ Cu	14	0.1109	1	3
SnTe ₂	14	0.0698	1	3
CoI ₂	14	0.0494	1	3
GeS ₂	14	0.0141	1	3
MnSe ₂	14	0.013	1	3
Br ₂ Mg	14	0.0502	1	3
CuO ₂	14	0.0788	1	3
I ₂ Ti	14	0.0495	1	3
Se ₂ Yb	14	0.072	1	3
BiTe ₂	14	0.0723	1	3
F ₂ Ni	14	0.0198	1	3
PtTe ₂	14	0.0617	1	3
Br ₂ Cd	14	0.0596	1	3
Se ₂ Sn	14	0.0497	1	3
NaPSn	14	0.0561	1	3
H ₂ Si ₂	17	0.0515	1	3
Br ₂ Ho ₂ S ₂	17	0.0402	1	2
Cl ₂ Gd ₂	17	0.0535	1	3
Ho ₂ I ₂ S ₂	17	0.052	1	2
Br ₂ Er ₂	17	0.0624	1	3
Cl ₂ OV	17	0.0793	1	3

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

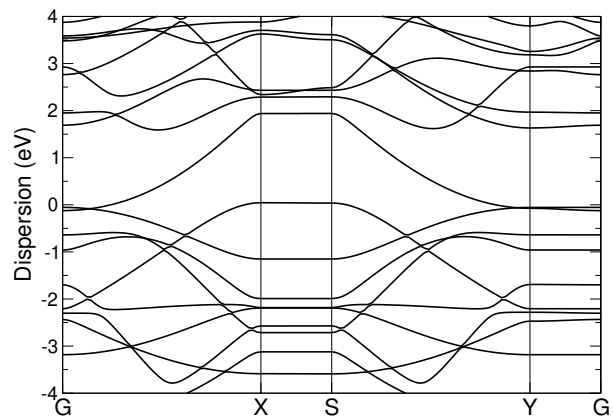
Formula	N° atoms	strain	cell size 1	cell size 2
Ba ₂ Hg	185	0.0007	16	35
Br ₂ Ca ₃ Si	290	0.0008	16	35
F ₄ Sn	255	0.0009	16	35
Br ₂ Cd	159	0.0013	12	33
NS ₂ Ta	221	0.0013	9	44
Br ₂ PY ₂	225	0.0013	12	33
Cl ₂ Ga ₂ Te ₂	578	0.0013	40	63
Au ₂ I ₂	403	0.0013	31	62
Bi ₂ Se ₂	488	0.0014	36	77
Ca ₄ Cu ₂	454	0.0014	32	49
Br ₂ Ho ₂	525	0.0015	33	90
Bi ₂ S ₃	615	0.0016	33	90
PdTe ₂	159	0.0016	12	33
Br ₂ Tb ₂	525	0.0016	33	90
Ga ₂ I ₂ Tb ₂	679	0.0017	35	84
Ga ₂ Gd ₂ I ₂	679	0.0017	35	84
F ₂ Ho ₂ Se ₂	258	0.0018	12	33
PbS ₂ Sn	190	0.0018	14	30
Gd ₂ GeI ₂	990	0.0018	58	140
PtTe ₂	435	0.0019	33	90
IO ₃ Tl	545	0.0019	55	54
Mg ₃	300	0.0019	18	70
Br ₂ Tb ₂	192	0.002	12	33
P ₄	540	0.002	36	90
I ₂ La ₂	840	0.0021	56	140
AuTe ₂	435	0.0021	33	90
Gd ₂ GeI ₂	595	0.0021	35	84
Bi ₂ S ₃	430	0.0022	23	63
Bi ₂ S ₃	225	0.0022	12	33
I ₂ La ₂ O ₂	910	0.0022	50	110
Sn ₂ Te ₂	718	0.0023	58	107
Br ₂ Ho ₂	367	0.0023	23	63
Ho ₂ S ₂	668	0.0024	44	112
Br ₂ Ho ₂	192	0.0024	12	33
I ₂ La ₂ O ₂	290	0.0024	16	35
Br ₂ Er ₂	525	0.0025	33	90
N ₂ W	177	0.0025	9	44
Ge ₂ Te ₂	316	0.0026	24	49
Br ₂ Er ₂	491	0.0027	31	84
Bi ₂ Se ₂	354	0.0028	26	56
Bi ₂ In ₂	676	0.0028	56	99
Au ₂ K ₂ S ₂	912	0.0028	96	72
Au ₂ K ₂ S ₂	711	0.0028	75	56
PtTe ₂	276	0.0028	21	57
Cl ₄ KTl	465	0.0028	45	40
AuTe ₂	276	0.0029	21	57
Br ₂ Gd ₂	491	0.0029	31	84
Ba ₂ Cd	185	0.0029	16	35
Br ₂ Er ₂	333	0.003	21	57
Cu ₂ Rb ₂ Te ₂	874	0.003	56	99

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

K₂PtSe₂ (Pmmm (47))

Structural and electronic properties






Formula	K ₂ PtSe ₂
Spacegroup	Pmmm (47)
Prototype	K ₂ PtSe ₂
Parent 3D	K ₂ PtSe ₂
Source DB	ICSD
DB ID	40430
DF2-C09 Binding energy [meV/ Å²]	81.92
RVV10 Binding energy [meV/ Å²]	86.41
Band gap (PBE) [eV]	0.0

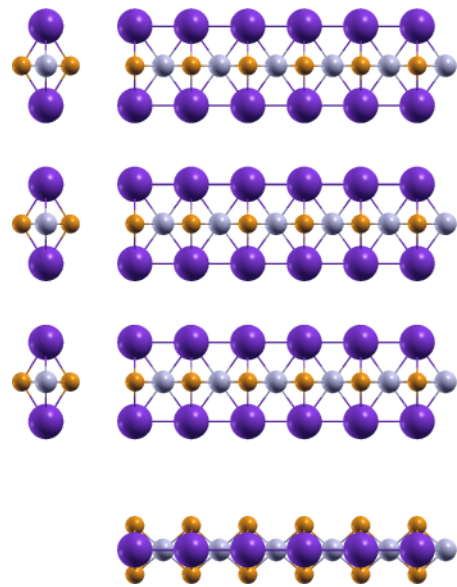


Band structure: Electronic band structure of K₂PtSe₂ (Pmmm (47)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of K₂PtSe₂ (Pmmm (47)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.80918286	0.00000000	0.00000000
a₂		0.00000000	10.65933858	0.00000000
a₃		0.00000000	0.00000000	23.33500346
		x [Å]	y [Å]	z [Å]
	K	0.00000000	2.65813425	11.66750173
	Se	0.00000000	5.32966929	13.31229441
	K	0.00000000	8.00120433	11.66750173
	Pt	1.90459143	5.32966929	11.66750173
	Se	0.00000000	5.32966929	10.02270905



Orthographic projections: views of K₂PtSe₂ (Pmmm (47)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
In	9	0.0814	1	4
Hg ₃ N ₂	10	0.5758	1	1
K ₂ PdSe ₂	10	0.0084	1	1
InSe	11	0.0686	1	3
Sb ₂	11	0.0561	1	3
CaCl	11	0.0183	1	3
I ₂ Mg	14	0.0601	1	3
HfTe ₂	14	0.0482	1	3
Br ₂ La	14	0.0603	1	3
AuTe ₂	14	0.0515	1	3
BrCdI	14	0.0625	1	3
PdTe ₂	14	0.0503	1	3
I ₂ Zn	14	0.0541	1	3
BaF ₂	14	0.0652	1	3
GeI ₂	14	0.0587	1	3
Ba ₂ N	14	0.0488	1	3
AsKSn	14	0.064	1	3
Te ₂ Zr	14	0.0484	1	3
PbTe ₂	14	0.0617	1	3
SnTe ₂	14	0.0571	1	3
STl ₂	14	0.066	1	3
GeS ₂	14	0.0256	1	3
MnSe ₂	14	0.0184	1	3
Se ₂ Yb	14	0.0589	1	3
BiTe ₂	14	0.0591	1	3
PtTe ₂	14	0.0513	1	3
Br ₂ Cd	14	0.0499	1	3
NaPSn	14	0.0479	1	3
K	15	0.0477	2	5
CrS ₂	17	0.0811	1	4
Fe ₂ Te ₂	17	0.0242	1	3
Br ₂ Ho ₂ S ₂	17	0.0245	1	2
Ca ₂ Cl ₂	17	0.0245	1	3
Ho ₂ I ₂ S ₂	17	0.0354	1	2
C ₂ I ₂ La ₂	17	0.1313	1	2
Br ₂ Er ₂	17	0.0518	1	3
ReS ₂	17	0.081	1	4
Gd ₂ I ₂ Se ₂	17	0.128	1	2
Cl ₂ OV	17	0.0786	1	3
Br ₂ S ₂ Y ₂	17	0.0213	1	2
Br ₂ Tb ₂	17	0.0506	1	3
Gd ₂ I ₂ S ₂	17	0.0414	1	2
N ₂ W	17	0.0818	1	4
Cl ₂ La ₂	17	0.0527	1	3
I ₂ S ₂ Tb ₂	17	0.0389	1	2
Br ₂ Gd ₂	17	0.0521	1	3
MnNaTe ₂	17	0.0622	1	3
I ₂ S ₂ Yb ₂	17	0.0296	1	2
Br ₂ Dy ₂ S ₂	17	0.0268	1	2
Br ₂ OV	17	0.0286	1	3

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

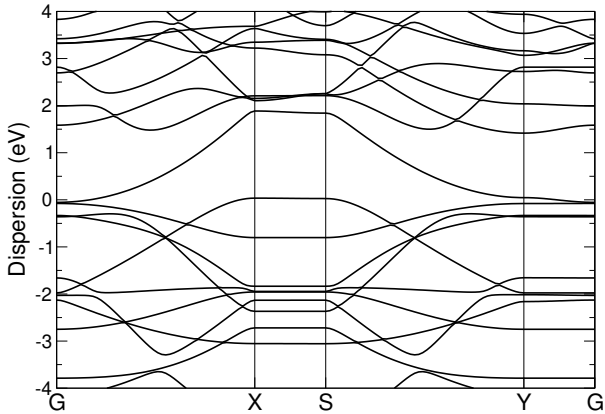
Formula	N° atoms	strain	cell size 1	cell size 2
Br ₂ La ₂	226	0.0001	14	39
Cl ₂ Hg ₂ N ₂	240	0.0001	18	25
Sb ₂	148	0.0002	14	39
Cu ₂ K ₂ Te ₂	300	0.0003	18	35
I ₂ S ₂ Tb ₂	158	0.0005	10	18
Li ₂ P ₂ Pr	265	0.0007	14	39
Ga ₂ Ge ₂ Te ₂	304	0.0008	14	39
CrTe ₂	393	0.0011	24	91
Au ₂ Br ₂	530	0.0012	38	85
Cl ₂ Sc ₂	484	0.0012	24	91
Br ₂ Cr	393	0.0014	24	91
Mg ₂	110	0.0015	8	35
Br ₂ H ₂ Zr ₂	666	0.0015	24	91
Mo ₂ Te ₄	960	0.0016	60	110
Cu ₂ Te ₂	314	0.0016	18	56
F ₂ Lu ₂ Se ₂	304	0.0016	14	39
Gd ₂ I ₂ S ₂	897	0.0017	57	102
Br ₂ Ti	393	0.0017	24	91
Dy ₂ I ₂ S ₂	158	0.0017	10	18
Cl ₄ Mg ₂	405	0.0017	39	35
SnTe ₂	187	0.0017	14	39
AgTe ₂	255	0.0018	15	60
Gd ₂ I ₂ S ₂	158	0.0019	10	18
BH ₄ Li	843	0.0019	39	108
BH ₄ Li	304	0.002	14	39
Ca ₄ Cu ₂	815	0.002	55	90
Au ₂ Br ₂	250	0.002	18	40
O ₄ PSn	300	0.0021	18	35
CdO ₂	765	0.0021	45	180
Cu ₂ F ₄	95	0.0022	7	10
Ho ₂ I ₂ S ₂	875	0.0022	55	100
Ho ₂ I ₂ S ₂	858	0.0022	54	98
CeLi ₂ P ₂	735	0.0022	39	108
Br ₂ Zr ₂	522	0.0022	26	98
Cl ₂ H ₂ Sc ₂	666	0.0022	24	91
Mo ₂ Te ₄	915	0.0023	57	105
Br ₂ Zr ₂	484	0.0023	24	91
Sn ₂ Te ₂	230	0.0023	18	35
H ₂ I ₂ Sr ₂	330	0.0023	18	40
CrS ₂	80	0.0023	4	20
Gd ₂ I ₂ S ₂	141	0.0023	9	16
Gd	35	0.0024	3	20
PbS ₂	73	0.0024	5	16
ClKO ₃	450	0.0024	45	45
Ho ₂ I ₂ S ₂	841	0.0024	53	96
Se ₂ Ti	424	0.0024	26	98
Cl ₂ O ₂ Ti ₂	426	0.0024	18	56
C ₂	370	0.0024	18	140
I ₂ Zn	215	0.0024	16	45
Br ₂ Ti	362	0.0024	22	84

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

K₂PtTe₂ (Pmmm (47))

Structural and electronic properties

	Formula	K ₂ PtTe ₂
	Spacegroup	Pmmm (47)
	Prototype	K ₂ PtSe ₂
	Parent 3D	K ₂ PtTe ₂
	Source DB	ICSD
	DB ID	40432
DF2-C09	Binding energy [meV/ Å²]	67.05
RVV10	Binding energy [meV/ Å²]	71.32
	Band gap (PBE) [eV]	0.0

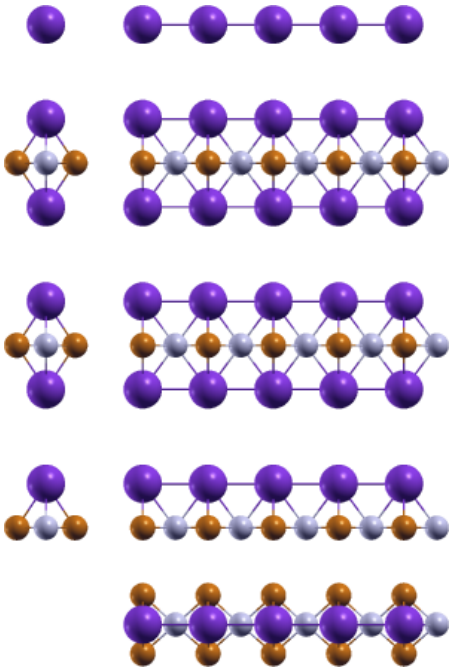


Band structure: Electronic band structure of K₂PtTe₂ (Pmmm (47)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of K₂PtTe₂ (Pmmm (47)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		4.04534442	0.00000000	0.00000000
a₂		0.00000000	11.30161692	0.00000000
a₃		0.00000000	0.00000000	23.60988343
		x [Å]	y [Å]	z [Å]
●	Te	0.00000000	0.00000000	13.60730100
●	Pt	2.02267221	0.00000000	11.80494171
●	K	0.00000000	8.57501979	11.80494171
●	K	0.00000000	2.72659713	11.80494171
●	Te	0.00000000	0.00000000	10.00258243



Orthographic projections: views of K₂PtTe₂ (Pmmm (47)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	9	0.0813	1	4
As ₂ O ₃	10	2.0526	1	1
Hg ₃ N ₂	10	0.4972	1	1
InSe	11	0.0495	1	3
Bi ₂	11	0.0522	1	3
PbTe	11	0.0502	1	3
CaCl	11	0.0753	1	3
In ₂ Se ₂	13	0.0049	1	2
P ₂	13	0.0812	1	4
I ₃ Sn	13	0.2485	1	2
CdI ₂	14	0.0511	1	3
Br ₂ Ca	14	0.0517	1	3
I ₂ Yb	14	0.0647	1	3
BiClTe	14	0.0512	1	3
Cl ₂ Zn	14	0.0268	1	3
BaF ₂	14	0.048	1	3
BiBrTe	14	0.0543	1	3
I ₂ Tm	14	0.0659	1	3
GeI ₂	14	0.0503	1	3
STl ₂	14	0.0483	1	3
BiTe	14	0.0586	1	3
MnSe ₂	14	0.0753	1	3
GdI ₂	14	0.0561	1	3
CdI ₂	14	0.0508	1	3
I ₂ Pr	14	0.0513	1	3
KNO ₃	15	0.3574	1	2
Fe ₂ Te ₂	17	0.0197	1	3
Br ₂ Ho ₂ S ₂	17	0.0206	1	2
S ₂ V	17	0.0824	1	4
MoS ₂	17	0.0823	1	4
Cl ₂ Mn	17	0.145	1	4
Ca ₂ Cl ₂	17	0.0195	1	3
MoSe ₂	17	0.0812	1	4
Cu ₄ Te ₂	17	0.1223	1	2
Cu ₂ Sr ₂	17	0.0549	1	3
Cl ₂ OOS	17	0.0336	1	3
LiMnTe ₂	17	0.0505	1	3
AgNO ₂	17	0.5478	1	3
AsLi ₃	17	0.0496	1	3
Cl ₂ Ti	17	0.0812	1	4
I ₂ Se ₂ Tb ₂	17	0.022	1	2
Gd ₂ I ₂ Se ₂	17	0.024	1	2
Br ₂ S ₂ Y ₂	17	0.0174	1	2
AlLiTe ₂	17	0.0578	1	3
S ₂ W	17	0.0823	1	4
Cl ₂ ORu	17	0.0759	1	3
As ₂ Co ₂	17	0.0756	1	3
Br ₂ Er ₂ Se ₂	17	0.0076	1	2
NbS ₂	17	0.0815	1	4
Cu ₂ Te ₂	17	0.025	1	3

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

Formula	N° atoms	strain	cell size 1	cell size 2
RhTe ₂	393	0.0005	24	91
GdI ₂	187	0.0005	14	39
I ₂ La ₂ P	265	0.0007	14	39
AgClO ₄	300	0.0007	18	35
I ₂ N ₂ Zr ₂	666	0.0009	24	91
Cl ₂ Rb ₂	300	0.0009	32	35
CdClHO	484	0.0011	24	91
CuTe ₂	765	0.0013	45	180
Se ₂ Ta ₄	435	0.0014	15	60
Cu ₂ Sr ₂	226	0.0015	14	39
O ₄ PTl	370	0.0016	20	45
As ₂ Cd ₂ K ₂	330	0.0017	18	40
Sm	230	0.0018	18	140
Ga ₂ Se ₂	484	0.0019	24	91
BiBrTe	215	0.0019	16	45
I ₂ Pr ₂ S ₂	788	0.002	40	98
Ba ₂ F ₂ I ₂	370	0.002	20	45
HgO	110	0.002	8	35
Ba ₂ F ₂ I ₂	330	0.0021	18	40
N ₃ W ₂	940	0.0021	26	162
Ga ₂ S ₃	545	0.0022	21	88
As ₂ O ₃	280	0.0022	20	36
CdClHO	446	0.0023	22	84
Ag ₂	396	0.0023	40	98
PtSe ₂	362	0.0023	22	84
O ₄ PSn	330	0.0024	18	40
Cu ₄ Te ₂	350	0.0024	16	45
Ba ₂ Pt	494	0.0024	40	98
BiBrTe	187	0.0025	14	39
AgCuTe ₂	220	0.0025	12	40
Ag ₂ I ₂	280	0.0025	20	45
Sm	140	0.0026	11	85
Sb ₂ Te ₂	592	0.0026	40	98
Cl ₂ Y ₂	484	0.0026	24	91
RhTe ₂	362	0.0026	22	84
AsSn ₂	362	0.0026	22	84
AlLiTe ₂	627	0.0026	39	108
Au ₂ K ₂ Se ₂	580	0.0026	56	50
O ₄ PTl	330	0.0026	18	40
Br ₂ Gd ₂	89	0.0026	5	16
Br ₂ Cr ₂ S ₂	650	0.0027	28	85
AuCrTe ₄	778	0.0028	50	88
Au ₂ K ₂ S ₂	935	0.0028	91	80
Sb ₂ Te ₃	305	0.0028	16	45
Pb ₂ Se ₂	546	0.0028	38	89
F ₂ Se ₂ Y ₂	330	0.0029	18	40
CBr ₂ Y ₂	620	0.0029	26	98
CuTe ₂	686	0.0029	40	162
AlLiTe ₂	226	0.0029	14	39
Te ₂ Zn	369	0.003	21	88

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.







KAuS (Pmma (51))

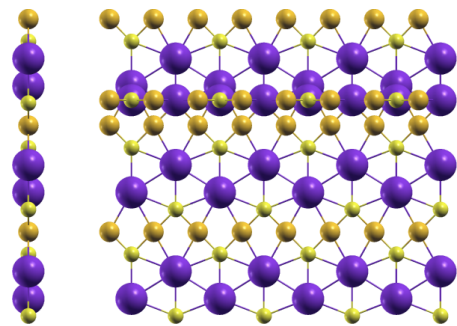
Structural and electronic properties

Formula	KAuS
Spacegroup	Pmma (51)
Prototype	AuKS
Parent 3D	K ₂ Au ₂ S ₂
Source DB	COD
DB ID	1510204
DF2-C09 Binding energy [meV/ Å ²]	37.81
RVV10 Binding energy [meV/ Å ²]	42.52
Band gap (PBE) [eV]	1.67

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of KAuS (Pmma (51)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		6.53716754	0.00000000	0.00000000
a₂		0.00000000	-7.87590247	0.00000000
a₃		0.00000000	0.00000000	-20.00000000
		x [Å]	y [Å]	z [Å]
	K	1.63429189	-4.95338405	-10.00000000
	K	4.90287566	-2.92251842	-10.00000000
	S	1.63429189	-1.65789854	-10.00000000
	S	4.90287566	-6.21800392	-10.00000000
	Au	0.00000000	-7.87590247	-10.00000000
	Au	3.26858377	-7.87590247	-10.00000000



Orthographic projections: views of KAuS (Pmma (51)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	8	0.1408	1	2
Bi ₂ In ₂	10	0.3378	1	1
Br ₂ CsF	10	0.3344	1	1
CaI ₂	12	0.1369	1	2
Ca ₂ Si	12	0.1457	1	2
Cl ₄ Cu ₂	12	0.6822	1	1
PdTe ₂	12	0.4594	1	2
Au ₂ K ₂ Se ₂	12	0.0061	1	1
Ba ₂ N	12	0.4505	1	2
Te ₂ Zr	12	0.448	1	2
Cu ₂ Rb ₂ Te ₂	12	0.3373	1	1
I ₂ Pb	12	0.1443	1	2
PtTe ₂	12	0.4643	1	2
Br ₂ Cd	12	0.4572	1	2
CS ₃ Tl ₂	12	0.0998	1	1
Br ₂ Tb ₂	14	0.4608	1	2
PbTe ₂	15	0.1279	1	3
Gd	15	0.0196	1	9
Cl ₂ Rb ₂	16	0.1511	2	1
Bi ₂ S ₃	16	0.4614	1	2
I ₂ La ₂ Te	16	0.1397	1	2
I ₃ Sn	16	0.3148	2	1
Na	17	0.1222	2	5
Bi ₂ Te ₂	18	0.1896	1	3
LiO ₂	18	0.2637	1	4
K	18	0.0172	2	6
Eu ₂ I ₂ O ₂	18	0.1362	1	2
Br ₂ Ca ₃ Si	18	0.1397	1	2
Cu ₃ Se ₃	18	0.4499	1	2
I ₂ La ₂	18	0.1293	1	3
AuI ₄ Li	18	0.2002	1	2
Br ₂ Ca ₃ Si	18	0.1391	1	2
Gd ₂ I ₂	18	0.127	1	3
I ₂ S ₂ Sm ₂	18	0.1406	1	2
I ₂ O ₂ Sm ₂	18	0.1365	1	2
AuCrTe ₄	18	0.333	1	2
Cl ₄ KTI	18	0.1528	2	1
SSb ₂ Te ₂	21	0.1285	1	3
Br ₂ Gd ₂ Ge	21	0.1272	1	3
GeI ₂ Y ₂	21	0.1325	1	3
Gd ₂ GeI ₂	21	0.1357	1	3
Cu ₂ Te ₂	22	0.0067	1	4
Tl	22	0.0107	2	10
O ₂ Sn ₂	22	0.1377	1	4
Na	22	0.0419	2	10
O ₂ Sn ₂	22	0.0831	1	4
O ₂ Sn ₂	22	0.0832	1	4
Cl ₂ Tb ₂	22	0.5281	1	4
CrS ₂	24	0.0485	1	6
I ₂ La ₂ Si ₂	24	0.1331	1	3

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

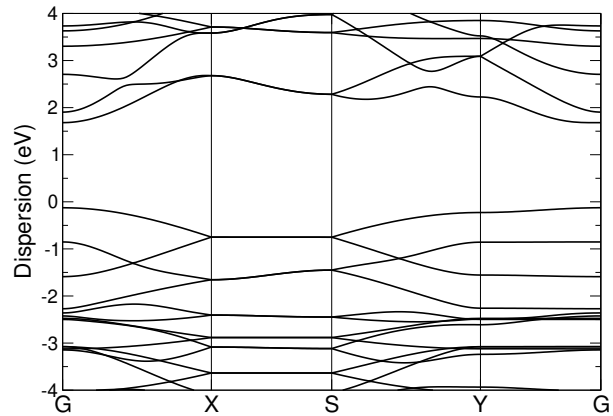
Formula	N° atoms	strain	cell size 1	cell size 2
Ga ₂ S ₂	480	0.0004	20	90
Au ₂ Se ₂	236	0.0005	16	35
CoTe ₂	390	0.0005	20	90
Br ₂ Hg ₃	614	0.0005	69	40
HfS ₂	390	0.0008	20	90
Ga ₂ S ₂	480	0.0009	20	90
Er ₂ I ₂ O ₂	78	0.0009	3	10
Br ₂ Eu ₂ F ₂	78	0.001	3	10
Bi ₂ Br ₂ O ₂	78	0.001	3	10
CuTe ₂	390	0.0011	20	90
Br ₂ Ca ₃ Si	210	0.0011	9	26
IKO ₃	819	0.0012	69	81
FeH ₂ O ₂	231	0.0012	6	39
PTe ₂ Ti ₂	570	0.0012	20	90
Ag ₂ F ₄	192	0.0013	12	20
I ₂ O ₂ Tm ₂	78	0.0013	3	10
N ₂ W	153	0.0013	6	39
CNRb	522	0.0014	41	92
Br ₂ Ni	390	0.0014	20	90
Cl ₂ N ₂ Ti ₂	30	0.0014	1	4
Cl ₂ Mg	390	0.0014	20	90
C ₂ F ₂	164	0.0015	4	35
Cl ₂ H ₂ Lu ₂	918	0.0015	28	125
I ₂ O ₂ Y ₂	78	0.0015	3	10
CaH ₂ O ₂	570	0.0015	20	90
S ₂	248	0.0016	18	70
F ₂ Se ₂ Yb ₂	528	0.0016	18	70
Br ₂ Nd ₂ O ₂	78	0.0017	3	10
Cl ₂ H ₂ Lu ₂	660	0.0017	20	90
I ₂ La ₂ Te	142	0.0017	7	20
Cl ₂ N ₂ Zr ₂	660	0.0018	20	90
Br ₂ Ca ₃ Si	162	0.0018	7	20
Ba ₂ H ₂ I ₂	888	0.0018	43	105
In ₂ Se ₂	946	0.0018	63	142
LiO ₂	381	0.0019	18	91
I ₂ S ₂ Sm ₂	162	0.0019	7	20
Sm	59	0.002	4	35
As ₂ O ₃	480	0.002	30	60
Br ₂ N ₂ Zr ₂	918	0.002	28	125
Cu ₂ Na ₂ Te ₂	222	0.002	10	27
K	62	0.0021	7	20
I ₂ Nd	48	0.0021	3	10
Hg ₃ S ₂	604	0.0022	54	56
Cl ₄ KTI	66	0.0022	5	6
Br ₂ O ₂ Sm ₂	78	0.0022	3	10
I ₃ Sn	722	0.0022	59	92
Li ₂ Tl ₂	552	0.0023	36	84
Br ₂ Hf ₂ N ₂	660	0.0023	20	90
Ir ₂ P ₂	58	0.0023	3	10
Br ₂ H ₂ Zr ₂	834	0.0023	24	115

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

KAuSe (P2/m (10))

Structural and electronic properties

	Formula	KAuSe
	Spacegroup	P2/m (10)
	Prototype	AuKS
	Parent 3D	K ₂ Au ₂ Se ₂
	Source DB	COD
	DB ID	1510205
DF2-C09	Binding energy [meV/ Å²]	34.57
RVV10	Binding energy [meV/ Å²]	39.08
	Band gap (PBE) [eV]	1.81

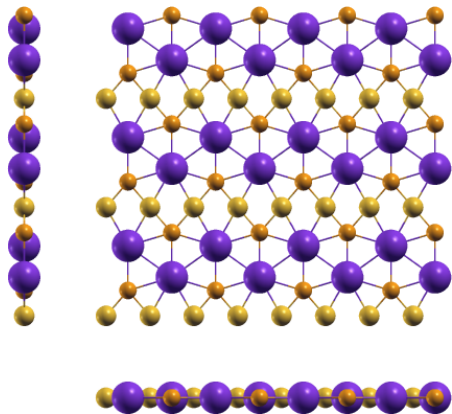


Band structure: Electronic band structure of KAuSe (P2/m (10)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of KAuSe (P2/m (10)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		6.43572052	−0.00003352	0.00000000
a₂		0.00001551	7.95457924	0.00000000
a₃		0.00000000	0.00000000	20.00000000
		x [Å]	y [Å]	z [Å]
●	K	1.60892781	5.12763866	10.00000000
●	K	4.82680822	2.82690706	10.00000000
●	Se	1.60893384	1.85872255	10.00000000
●	Se	4.82680219	6.09582317	10.00000000
●	Au	0.00000000	0.00000000	10.00000000
●	Au	3.21786026	−0.00001676	10.00000000



Orthographic projections: views of KAuSe (P2/m (10)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	8	0.1378	1	2
Br ₂ Cu	9	0.1556	1	1
Au ₂ K ₂ S ₂	12	0.0062	1	1
CaI ₂	12	0.1342	1	2
HfTe ₂	12	0.4567	1	2
Ca ₂ Si	12	0.1425	1	2
I ₂ Yb	12	0.1333	1	2
Ba ₂ N	12	0.4604	1	2
Te ₂ Zr	12	0.4579	1	2
I ₂ Tm	12	0.1338	1	2
I ₂ Pb	12	0.1411	1	2
AuI ₄ Li	12	0.1436	1	1
I ₂ La	12	0.1322	1	2
NaPSn	12	0.4546	1	2
Ag ₂ Br ₂	14	0.1323	1	2
Ba ₂ Cu ₂	14	0.1332	1	2
As ₂ Rh ₂	14	0.1323	1	2
Pt ₂ Te ₂	14	0.455	1	2
PbTe ₂	15	0.1311	1	3
SnTe ₂	15	0.1274	1	3
Gd	15	0.0251	1	9
Cl ₂ Rb ₂	16	0.1534	2	1
GeI ₂ La ₂	16	0.1337	1	2
In ₂ Se ₃	16	0.4568	1	2
I ₂ La ₂ Te	16	0.1368	1	2
K	18	0.0298	2	6
K	18	0.0769	2	6
GeNi ₃ Te ₂	18	0.4532	1	2
Br ₂ Ca ₃ Si	18	0.1368	1	2
Cl ₂ Cu	18	0.1569	2	2
Cu ₃ Se ₃	18	0.4598	1	2
I ₂ O ₂ Y ₂	18	0.1319	1	2
I ₂ La ₂	18	0.1326	1	3
H ₂ I ₂ Yb ₂	18	0.1321	1	2
Br ₂ Ca ₃ Si	18	0.1362	1	2
Bi ₂ Br ₂ O ₂	18	0.1317	1	2
Br ₂ Nd ₂ O ₂	18	0.1319	1	2
Gd ₂ I ₂	18	0.1302	1	3
I ₂ S ₂ Sm ₂	18	0.1377	1	2
SSb ₂ Te ₂	21	0.1317	1	3
Br ₂ Gd ₂ Ge	21	0.1304	1	3
GeI ₂ Y ₂	21	0.136	1	3
Gd ₂ GeI ₂	21	0.1393	1	3
Cu ₂ Te ₂	22	0.0054	1	4
AgCuTe ₂	22	0.0201	1	4
Tl	22	0.0059	2	10
CrS ₂	24	0.0464	1	6
InSe	24	0.0245	2	6
I ₂ La ₂ Si ₂	24	0.1366	1	3
I ₂ Pr ₂ Si ₂	24	0.1285	1	3

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

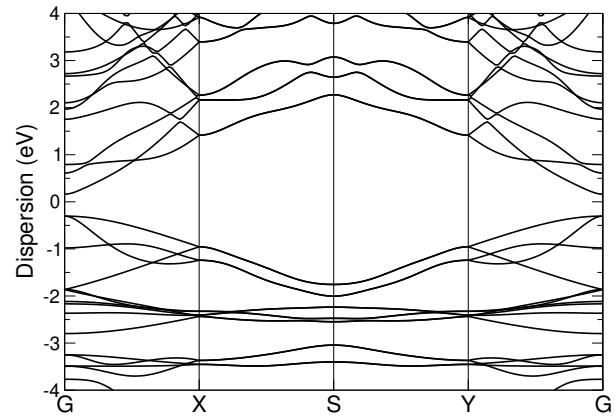
Formula	N° atoms	strain	cell size 1	cell size 2
CrS ₂	249	0.0002	10	63
PSn ₂	153	0.0003	8	35
Ga ₂ I ₂ Tb ₂	354	0.0004	14	45
S ₂ Sn	153	0.0004	8	35
Hg ₄ O ₂	786	0.0005	72	59
Se ₄ TiZr	306	0.0005	16	35
Br ₂ Ho ₂	722	0.0005	35	128
S ₂ Zr	153	0.0006	8	35
Ga ₂ Gd ₂ I ₂	354	0.0006	14	45
Br ₂ O ₂ Sc ₂	138	0.0007	5	18
NbTe ₂	153	0.0008	8	35
MnO ₂	264	0.0008	9	70
Gd ₂ GeI ₂	309	0.0012	14	45
Te ₂ Zn	696	0.0013	35	162
I ₂ Nd ₂ S ₂	114	0.0014	5	14
ReSe ₂	438	0.0014	21	104
CrO ₂	264	0.0015	9	70
Cl ₂ Rh ₂ Te ₂	372	0.0015	20	42
AgClO ₂	416	0.0015	20	74
Br ₂ V	438	0.0015	21	104
C ₂ I ₂ La ₂	750	0.0016	30	95
Pd ₂ S ₄	642	0.0016	40	67
Br ₂ S ₂ Yb ₂	204	0.0016	10	24
I ₂ La ₂ Sb	100	0.0016	5	14
F ₂ Se ₂ Tm ₂	690	0.0017	24	91
O ₄ PTl	588	0.0017	28	70
Br ₂ PY ₂	850	0.0017	35	128
LiMnSe ₂	508	0.0017	24	91
In ₂ Se ₂	734	0.0018	49	110
Cl ₂ Ni	438	0.0018	21	104
GeNi ₃ Te ₂	690	0.0018	24	91
Cl ₂ Tb ₂	702	0.0018	33	126
I ₃ Sn	814	0.0019	67	103
K	44	0.0019	5	14
Cl ₂ Cu	438	0.0019	24	98
Hg ₄ O ₂	654	0.002	60	49
Cl ₂ S ₂ Tl ₂	642	0.002	35	72
Cl ₂ Zr ₂	542	0.002	21	104
CBr ₂ Lu ₂	223	0.002	8	35
Br ₂ N ₂ Zr ₂	258	0.0021	8	35
I ₂ Lu ₂ S ₂	204	0.0021	10	24
NbSe ₂	438	0.0021	21	104
I ₂ Y ₂	508	0.0021	24	91
Ba ₂ F ₂ I ₂	588	0.0021	28	70
Hg ₄ O ₂	624	0.0021	57	47
Se ₂ Ta	438	0.0022	21	104
I ₂ Ti	270	0.0022	15	60
NaPSn	417	0.0022	24	91
Br ₂ Cu	486	0.0023	28	106
CCL ₂ Sc ₂	646	0.0023	21	104

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

KCuTe (Pmmn (59))

Structural and electronic properties

	Formula	KCuTe
	Spacegroup	Pmmn (59)
	Prototype	PbClF
	Parent 3D	K ₂ Ce ₂ Cu ₂ Te ₈
	Source DB	ICSD
	DB ID	86654
DF2-C09	Binding energy [meV/ Å²]	41.32
RVV10	Binding energy [meV/ Å²]	45.25
	Band gap (PBE) [eV]	0.47

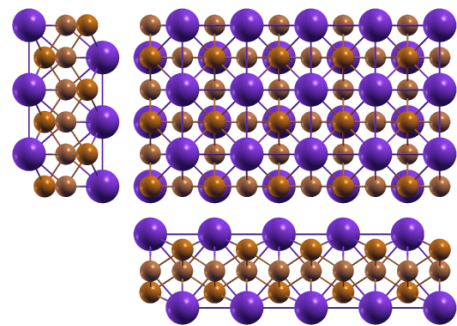


Band structure: Electronic band structure of KCuTe (Pmmn (59)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of KCuTe (Pmmn (59)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		4.56728918	0.00000000	0.00000000
a₂		0.00000000	4.56722374	0.00000000
a₃		0.00000000	0.00000000	25.91140994
		x [Å]	y [Å]	z [Å]
●	K	0.00000000	0.00000000	10.34794249
●	Cu	0.00000000	2.28361187	12.95569289
●	Te	2.28364459	2.28361187	11.44718860
●	K	2.28364459	2.28361187	15.56346745
●	Cu	2.28364459	0.00000000	12.95571705
●	Te	0.00000000	0.00000000	14.46422134



Orthographic projections: views of KCuTe (Pmmn (59)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
AgTl	8	0.2047	1	1
Sm	8	0.1456	1	2
Br ₂ Zn	9	0.1102	1	1
SiTe ₂	9	0.1093	1	1
I ₂ Pr	9	0.563	1	1
HgI ₂	9	0.0092	1	1
Te ₂ Ti	9	0.1101	1	1
BiBrTe	9	0.1086	1	1
RhTe ₂	9	0.1111	1	1
CNRb	9	0.0453	1	1
CKN	9	0.0516	1	1
I ₂ Nd	9	0.5658	1	1
NiTe ₂	9	0.1094	1	1
Cl ₂ Cu	9	0.1384	1	1
I ₂ V	9	0.109	1	1
Se ₂ Zr	9	0.1092	1	1
CeI ₂	9	0.5608	1	1
HfSe ₂	9	0.1101	1	1
Bi ₂ Te ₂	10	0.1324	1	1
Li ₂ Tl ₂	10	0.1534	1	1
Bi ₂ In ₂	10	0.007	1	1
Cu ₂ I ₂	10	0.2169	1	1
Cu ₂ Sr ₂	10	0.1088	1	1
Ir ₂ P ₂	10	0.5652	1	1
CdClHO	10	0.1113	1	1
S ₂ Sn ₂	10	0.22	1	1
Cl ₂ Y ₂	10	0.1105	1	1
As ₂ Ir ₂	10	0.5884	1	1
O ₂ Pb ₂	10	0.2132	1	1
Ga ₂ Se ₂	10	0.1087	1	1
Br ₂ OV	10	1.674	1	1
CaClHO	10	0.1096	1	1
Au ₂ I ₂	10	0.0237	1	1
O ₂ Sn ₂	10	0.5213	1	1
Ge ₂ Se ₂	10	0.2086	1	1
Bi ₂ O ₂	10	0.2146	1	1
Ni ₂ Se ₂	10	0.5602	1	1
Ag ₂ I ₂	10	0.0082	1	1
Br ₂ CsF	10	0.0049	1	1
Ga ₂ Se ₂	10	0.1106	1	1
Sn ₂ Te ₂	10	0.0021	1	1
O ₂ Sn ₂	10	0.5203	1	1
As ₂ O ₃	11	0.1929	1	1
I ₂ La ₂ P	11	0.1091	1	1
F ₄ Nb	11	0.2213	1	1
NaO ₄	11	0.1634	1	1
AgNO ₃	11	0.1643	1	1
ClH ₃ O	11	0.1301	1	1
Ba ₂ H ₂ I ₂	12	0.003	1	1
Br ₂ HO ₂ S ₂	12	0.3739	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

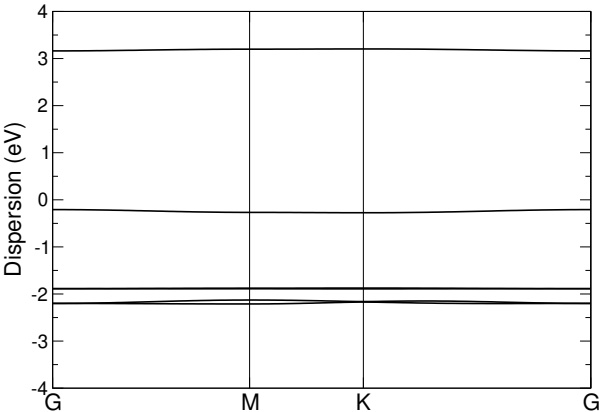
Formula	N° atoms	strain	cell size 1	cell size 2
Ca ₂ Cl ₂	294	0.0001	25	36
I ₂ O ₂ Sm ₂	690	0.0001	50	65
Hf ₂ Si ₂ Te ₂	246	0.0001	16	25
I ₂ Nd	363	0.0001	36	49
As ₂ Ru ₂	294	0.0001	25	36
Br ₂ O ₂ Sm ₂	510	0.0001	36	49
Br ₂ Ca ₂ F ₂	876	0.0002	61	85
AgTe ₂	645	0.0002	53	109
Eu ₂ I ₂ O ₂	678	0.0002	49	64
F ₂ I ₂ Sm ₂	870	0.0002	64	81
STl ₂	483	0.0003	48	65
Br ₂ F ₂ Yb ₂	876	0.0003	61	85
K ₂ Mn ₂ Sb ₂	678	0.0003	49	64
K ₂ PtSe ₂	300	0.0003	35	18
Br ₂ Ce ₂ O ₂	678	0.0003	49	64
Ir ₂ P ₂	412	0.0003	36	49
O ₂ Pb ₂	718	0.0003	65	82
Br ₂ O ₂ Tm ₂	366	0.0004	25	36
Se ₂ Si ₂ Zr ₂	780	0.0004	49	81
Ag ₂ Br ₂	962	0.0004	85	113
BrKO ₃	675	0.0004	80	39
Eu ₂ H ₂ I ₂	690	0.0004	50	65
O ₂ Pb ₂	708	0.0004	64	81
Eu ₂ F ₂ I ₂	882	0.0004	65	82
Br ₂ La ₂ O ₂	882	0.0004	65	82
In	454	0.0004	54	130
Fe ₂ Te ₂	294	0.0005	25	36
F ₂ Zn	621	0.0005	61	85
C ₄ Ca ₂	816	0.0006	61	75
In ₂ Se ₂	958	0.0006	81	118
As ₂ Rh ₂	962	0.0006	85	113
Co ₂ Se ₂	196	0.0007	16	25
I ₂ O ₂ Yb ₂	510	0.0007	36	49
Hg ₃ S ₂	405	0.0007	50	21
BaF ₂	483	0.0008	48	65
F ₂ I ₂ Yb ₂	690	0.0008	50	65
Mg ₆	894	0.0008	49	100
Br ₂ Gd ₂ O ₂	876	0.0008	61	85
Br ₂ Cu ₂	706	0.0008	61	85
I ₂ O ₂ Pr ₂	870	0.0009	64	81
CrTe ₂	237	0.0009	20	39
I ₂ La	849	0.0009	85	113
Br ₂ O ₂ Yb ₂	366	0.0009	25	36
O ₂ Sn ₂	916	0.0009	72	121
Bi ₂ O ₂	718	0.001	65	82
I ₂ O ₂ Tm ₂	510	0.001	36	49
Cl ₂ Sc ₂	276	0.001	20	39
Ga ₂ I ₂ Y ₂	678	0.001	48	65
CBr ₂ Lu ₂	541	0.001	36	65
I ₂ Mn	852	0.001	79	126

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

KNO₃ (P3m1)

Structural and electronic properties

	Formula	KNO ₃
	Spacegroup	P3m1
	Prototype	KNO3
	Parent 3D	K ₄ N ₄ O ₁₂
	Source DB	None
	DB ID	None
DF2-C09	Binding energy [meV/ Å²]	56.6
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	3.37

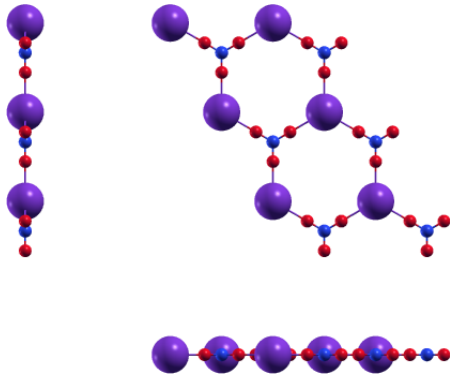


Band structure: Electronic band structure of KNO₃ (P3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of KNO₃ (P3m1) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		-3.28616859	-5.69181095	0.00000000
a₂		6.57233717	0.00000000	0.00000000
a₃		0.00000000	0.00000000	16.10446319
		x [Å]	y [Å]	z [Å]
•	N	0.00000000	-3.79454064	0.00023837
●	K	3.28616859	-1.89727032	-0.00094477
•	O	1.09144262	-3.16439594	0.00023546
•	O	-1.09144262	-3.16439594	0.00023546
•	O	0.00000000	-5.05483002	0.00023546



Orthographic projections: views of KNO₃ (P3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Br ₂ Cu	8	0.1443	1	1
Bi ₂ Pd	8	0.1627	1	1
Cl ₂ Cu	8	0.8465	1	1
AgNO ₂	9	0.1843	1	1
Ca ₂ O ₂	9	0.163	1	1
Tl	9	0.005	1	4
Ag ₂	9	0.2199	1	2
I ₃ Sn	9	0.1213	1	1
Hg ₃ S ₂	10	0.4981	1	1
Ba ₂ Pt	11	0.2195	1	2
Ca ₂ Si	11	0.2254	1	2
Cl ₄ Cu ₂	11	0.1462	1	1
I ₂ Se ₂ Tb ₂	11	0.1134	1	1
Gd ₂ I ₂ Se ₂	11	0.1133	1	1
Er ₂ I ₂ Se ₂	11	0.1138	1	1
I ₂ Se ₂ Tm ₂	11	0.114	1	1
I ₂ Pb	11	0.2219	1	2
Ag ₂ F ₄	11	0.1157	1	1
I ₂ Se ₂ Yb ₂	11	0.1141	1	1
Br ₂ Ca ₃ Si	11	0.1141	1	1
Ho ₂ I ₂ Se ₂	11	0.1137	1	1
AsSb	12	0.1634	2	1
CdCl ₂	13	0.1638	2	1
In ₂ Se ₂	13	0.1386	1	2
GeTe ₂	13	0.1637	2	1
I ₂ Mn	13	0.1638	2	1
NSr ₂	13	0.1635	2	1
PbS ₂	13	0.1632	2	1
Pb ₂ Se ₂	13	0.1485	1	2
FeI ₂	13	0.1636	2	1
I ₂ Ni	13	0.1637	2	1
HgI ₂	13	0.1549	2	1
CrI ₂	13	0.1636	2	1
Bi ₂ Se ₂	13	0.1316	1	2
Au ₂ Se ₂	13	0.4821	1	2
LiO	13	0.0077	1	4
CoI ₂	13	0.1634	2	1
Sb ₂ Te ₂	13	0.2237	1	2
P ₂	13	0.0003	1	4
Br ₂ Mg	13	0.1636	2	1
I ₂ Ti	13	0.1635	2	1
Se ₂ Sn	13	0.1635	2	1
N ₃ Na	14	0.1633	2	1
Ge ₂ S ₂	14	0.1676	2	1
Ga ₂ Se ₂	14	0.1632	2	1
Br ₂ Y ₂	14	0.1632	2	1
Ni ₂ Te ₂	14	0.1638	2	1
Ag ₂ I ₂	14	0.1548	2	1
K ₂ PtTe ₂	15	0.1171	2	1
Cl ₂ Y ₂	15	0.1635	2	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

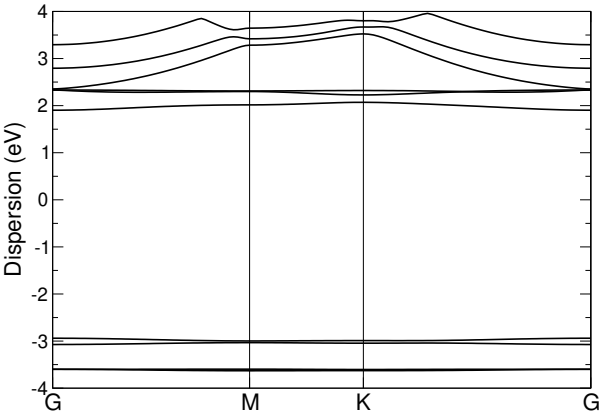
Formula	N° atoms	strain	cell size 1	cell size 2
CBr ₂ Y ₂	325	0.0	16	49
FeO ₂	192	0.0	9	49
CS ₂ Ta ₂	25	0.0	1	4
Cl ₂ Ti	17	0.0001	1	4
Li ₂ P ₂ Pr	445	0.0001	25	64
AlLiTe ₂	56	0.0002	4	9
Ga ₂ Ge ₂ Te ₂	509	0.0002	25	64
C ₂	173	0.0003	9	64
F ₂ Se ₂ Tm ₂	195	0.0003	9	25
P ₂	13	0.0003	1	4
LiMnSe ₂	145	0.0004	9	25
Sb ₂	253	0.0004	25	64
Cl ₂ H ₂ Lu ₂	611	0.0005	25	81
Cl ₂ Y ₂	276	0.0005	16	49
CCL ₂ Gd ₂	325	0.0006	16	49
Br ₂ La ₂	381	0.0007	25	64
Br ₂ In ₂ O ₂	817	0.0007	41	102
CoO ₂	192	0.0007	9	49
Br ₂ Zn	227	0.0007	16	49
I ₂ Nd ₂ S ₂	845	0.0008	49	100
Cl ₂ Mg	368	0.0008	25	81
CNb ₂ S ₂	25	0.0008	1	4
Br ₂ Ni	368	0.0008	25	81
HN ₃ OZn	29	0.0009	1	4
Ba ₂ Pt	432	0.0009	39	79
Bi ₂ Te ₃	65	0.0009	4	9
PTe ₂ Ti ₂	530	0.001	25	81
Ge ₂ S ₂	688	0.001	48	112
BiTe	47	0.001	4	9
I ₂ Y ₂	145	0.001	9	25
I ₂ Nd ₂ S ₂	669	0.001	39	79
Te ₂ Ti	227	0.001	16	49
HfSe ₂	227	0.001	16	49
HgI ₂	743	0.0011	70	131
Ag ₂ K ₂ Se ₂	684	0.0011	42	79
H ₂ MnO ₂	485	0.0011	16	81
Br ₂ N ₂ Zr ₂	611	0.0011	25	81
SnTe ₂	317	0.0011	25	64
CBr ₂ Lu ₂	530	0.0012	25	81
Ag ₂	353	0.0012	39	79
Ga ₂ Se ₂	276	0.0012	16	49
I ₂ N ₂ Zr ₂	645	0.0013	33	80
NiO ₂	192	0.0013	9	49
Ga ₂ S ₂	449	0.0013	25	81
N ₃ W ₂	485	0.0013	16	81
N ₃ Na	639	0.0013	51	96
BH ₄ Li	509	0.0014	25	64
CNRb	297	0.0015	30	49
K ₂ O ₄	357	0.0015	33	32
Cl ₂ Tb ₂	145	0.0015	9	25

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

KO₃Br (P3m1 (156))

Structural and electronic properties






	Formula	KO ₃ Br
	Spacegroup	P3m1 (156)
	Prototype	KNO3
	Parent 3D	KO ₃ Br
	Source DB	COD
	DB ID	9015382
DF2-C09	Binding energy [meV/ Å²]	95.26
RVV10	Binding energy [meV/ Å²]	105.26
	Band gap (PBE) [eV]	4.84

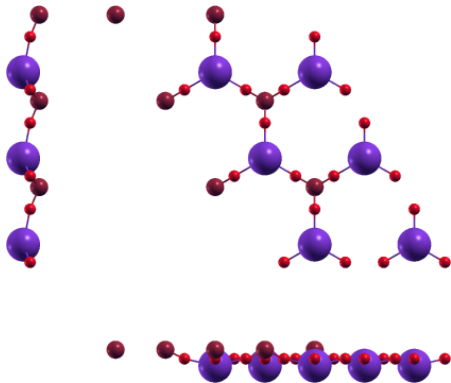


Band structure: Electronic band structure of KO₃Br (P3m1 (156)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of KO₃Br (P3m1 (156)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		7.02383856	0.00000000	0.00000000
a₂		−3.51191928	6.08282263	0.00000000
a₃		0.00000000	0.00000000	22.17629122
		x [Å]	y [Å]	z [Å]
	K	3.51191928	2.02760754	12.12026037
	Br	3.51191928	6.08282263	10.99362200
	O	1.34948372	0.77912479	11.63316116
	O	5.67435484	0.77912479	11.63316116
	O	3.51191928	4.52457305	11.63316116



Orthographic projections: views of KO₃Br (P3m1 (156)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Cl ₂ Rb ₂	9	0.136	1	1
Na	9	0.0049	1	4
I ₃ Sn	9	0.4263	1	1
Hg ₃ N ₂	10	0.0044	1	1
FKO ₂ Se	10	0.1153	1	1
IKO ₃	10	0.0055	1	1
I ₂ Lu ₂ Se ₂	11	0.1205	1	1
Cu ₄ Te ₂	11	0.1449	1	1
Se ₂ Si ₂ Zr ₂	11	0.1631	1	1
Cl ₄ Cu ₂	11	0.1225	1	1
Cl ₄ Mg ₂	11	0.0305	1	1
Cl ₂ Ga ₂ Te ₂	11	0.1203	1	1
Br ₂ Ga ₂ Te ₂	11	0.1198	1	1
CuO ₂	11	0.1417	1	2
In	11	0.1271	1	6
H ₂ Li ₂ O ₂	11	0.1636	1	1
CS ₃ Tl ₂	11	0.1431	1	1
Cl ₄ KTI	11	0.1434	1	1
Sb ₂	12	0.1634	2	1
Pb ₂ Se ₂	13	0.124	1	2
GeI ₂	13	0.1637	2	1
Bi ₂ Se ₂	13	0.1138	1	2
SnTe ₂	13	0.1635	2	1
Se ₂ Yb	13	0.1637	2	1
Mg ₂	13	0.0405	1	4
BiTe ₂	13	0.1637	2	1
AsCuLi ₂	14	0.1636	2	1
Ga ₂ Te ₂	14	0.1636	2	1
Br ₂ La ₂	14	0.1633	2	1
Br ₂ HLa	14	0.1636	2	1
CeLi ₂ P ₂	15	0.1636	2	1
Ba ₂ Ni ₃	15	0.1636	2	1
Sb ₂ Se ₂ Te	15	0.1637	2	1
Li ₂ P ₂ Pr	15	0.1634	2	1
FKO ₂ Se	15	0.1043	1	2
Sb ₂ Se ₂ Te	15	0.1638	2	1
CuGeO ₃	15	0.2702	1	2
Ho ₂ I ₂ S ₂	16	0.1551	2	1
I ₂ Pr ₂ Si ₂	16	0.1636	2	1
BH ₄ Li	16	0.1635	2	1
Ga ₂ Ge ₂ Te ₂	16	0.1634	2	1
Gd ₂ I ₂ S ₂	16	0.1548	2	1
I ₂ S ₂ Tb ₂	16	0.155	2	1
F ₂ Lu ₂ Se ₂	16	0.1632	2	1
Ag ₂ K ₂ Te ₂	16	0.1549	2	1
C ₄ Ca ₂	16	0.1724	2	1
Ce ₂ I ₂ Si ₂	16	0.1638	2	1
Dy ₂ I ₂ S ₂	16	0.155	2	1
Er ₂ I ₂ S ₂	16	0.1552	2	1
I ₂ Lu ₂ Se ₂	17	0.0632	1	2

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

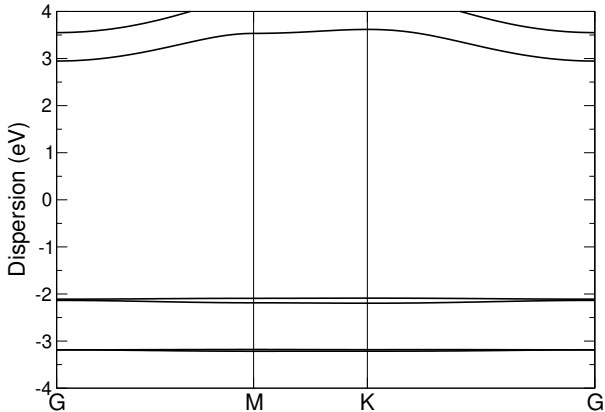
Formula	N° atoms	strain	cell size 1	cell size 2
Bi ₂ Te ₃	445	0.0	25	64
Ga ₂ Se ₂	449	0.0	25	81
BiTe	317	0.0001	25	64
IrTe ₂	368	0.0002	25	81
PdTe ₂	227	0.0002	16	49
Cu ₂ K ₂ Te ₂	675	0.0004	39	80
BaF ₂	120	0.0004	9	25
S ₂	287	0.0005	25	81
CrTe ₂	17	0.0005	1	4
I ₂ Sb ₂ Te ₂	630	0.0005	48	65
STl ₂	120	0.0005	9	25
Cl ₂ Sc ₂	21	0.0006	1	4
Ga ₂ I ₂ Y ₂	195	0.0006	9	25
Ni ₂ SbTe ₂	530	0.0007	25	81
Br ₂ Cd	227	0.0007	16	49
NS ₂ Ta	241	0.0008	9	49
Br ₂ Tb ₂	276	0.0008	16	49
Br ₂ Cr	17	0.0008	1	4
In ₂ S ₃	530	0.0009	25	81
Br ₂ H ₂ Zr ₂	29	0.0009	1	4
Br ₂ PY ₂	325	0.0009	16	49
Br ₂ Dy ₂ S ₂	821	0.001	49	96
Bi ₂ S ₃	325	0.001	16	49
AlLiTe ₂	381	0.001	25	64
LiO ₂	264	0.001	15	63
GeTe	287	0.0011	25	81
Br ₂ Ti	17	0.0011	1	4
Ce ₂ I ₂ S ₂	74	0.0011	4	9
Cl ₄ Mg ₂	435	0.0011	27	50
Ca ₂ Si	47	0.0011	4	9
K ₂ O ₄	796	0.0011	68	76
Ag ₂ K ₂ Te ₂	684	0.0011	42	79
Cr ₂ O ₄	435	0.0011	15	60
Er ₂ I ₂ S ₂	747	0.0011	45	87
FeO ₂	95	0.0012	4	25
GeI ₃ Rb	745	0.0013	100	49
Br ₂ Ho ₂	276	0.0013	16	49
Cu ₂ O ₄	717	0.0013	27	97
I ₂ S ₂ Tm ₂	747	0.0014	45	87
H ₂ Si ₂	449	0.0014	25	81
N ₂ W	192	0.0015	9	49
P ₂ Sn ₂	449	0.0015	25	81
O ₄ PSn	675	0.0015	39	80
F ₂ Se ₂ Yb ₂	611	0.0016	25	81
Cl ₂ Cr ₂ O ₂	943	0.0016	35	128
Cl ₂ H ₂ Sc ₂	29	0.0016	1	4
In ₂ Te ₃	170	0.0017	9	25
Sb ₂ SeTe ₂	170	0.0017	9	25
InSe ₂	368	0.0018	25	81
I ₂ Lu ₂ Se ₂	760	0.0018	50	85

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

KO₃Cl (P3m1 (156))

Structural and electronic properties






	Formula	KO ₃ Cl
	Spacegroup	P3m1 (156)
	Prototype	KNO3
	Parent 3D	KO ₃ Cl
	Source DB	COD
	DB ID	1531970
DF2-C09	Binding energy [meV/ Å²]	86.18
RVV10	Binding energy [meV/ Å²]	95.54
	Band gap (PBE) [eV]	5.03

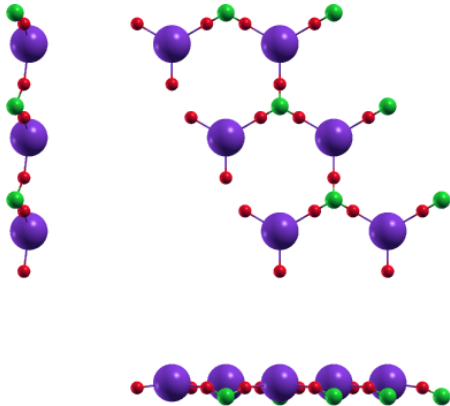


Band structure: Electronic band structure of KO₃Cl (P3m1 (156)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of KO₃Cl (P3m1 (156)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		6.82404734	0.00000000	0.00000000
a₂		−3.41202367	5.90979836	0.00000000
a₃		0.00000000	0.00000000	22.12242602
		x [Å]	y [Å]	z [Å]
	K	−0.00000000	3.93986557	10.17713057
	Cl	3.41202367	5.90979836	11.04290063
	O	2.19971521	5.20987174	10.48931695
	O	−2.19971521	5.20987174	10.48931695
	O	−0.00000000	1.39985323	10.48931695



Orthographic projections: views of KO₃Cl (P3m1 (156)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Cl ₂ Rb ₂	9	0.1478	1	1
Br ₃ Cs	9	0.0033	1	1
Sn	9	0.0418	1	4
In	9	0.0395	1	4
SbSe ₂ Tl	9	0.1234	1	1
I ₃ Sn	9	0.1129	1	1
K ₂ PdS ₂	10	0.5282	1	1
IO ₃ Tl	10	0.007	1	1
Hg ₃ N ₂	10	0.0093	1	1
Hg ₃ S ₂	10	0.4527	1	1
K ₂ PtS ₂	10	0.5248	1	1
Ho ₂ I ₂ S ₂	11	0.1163	1	1
Cl ₄ Cu ₂	11	0.1315	1	1
Gd ₂ I ₂ S ₂	11	0.1151	1	1
I ₂ S ₂ Tb ₂	11	0.1156	1	1
I ₂ S ₂ Yb ₂	11	0.1174	1	1
Cl ₂ Ga ₂ Te ₂	11	0.12	1	1
Cl ₂ Cu	11	0.1069	1	2
Br ₂ Ga ₂ Te ₂	11	0.1197	1	1
Ca ₄ Cu ₂	11	0.118	1	1
Ag ₂ F ₄	11	0.9139	1	1
Dy ₂ I ₂ S ₂	11	0.1159	1	1
Er ₂ I ₂ S ₂	11	0.1167	1	1
I ₂ S ₂ Tm ₂	11	0.1171	1	1
Bi ₂ Te ₂	13	0.2189	1	2
HfTe ₂	13	0.1632	2	1
Pb ₂ Se ₂	13	0.1334	1	2
PdTe ₂	13	0.1636	2	1
CKN	13	0.1549	2	1
Ba ₂ N	13	0.1633	2	1
Te ₂ Zr	13	0.1633	2	1
Bi ₂ Se ₂	13	0.1202	1	2
SbSe ₂ Tl	13	0.0396	1	2
PtTe ₂	13	0.1638	2	1
Br ₂ Cd	13	0.1635	2	1
NaPSn	13	0.1632	2	1
Bi ₂ In ₂	14	0.1549	2	1
Br ₂ Tb ₂	14	0.1637	2	1
Br ₂ Ho ₂	14	0.1637	2	1
Pt ₂ Te ₂	14	0.1632	2	1
Br ₂ PY ₂	15	0.1635	2	1
In ₂ Se ₃	15	0.1632	2	1
FKO ₂ Se	15	0.2834	1	2
Bi ₂ S ₃	15	0.1637	2	1
Cu ₂ Rb ₂ Te ₂	16	0.1549	2	1
Cu ₃ Se ₃	16	0.1633	2	1
F ₂ Ho ₂ Se ₂	16	0.1634	2	1
Er ₂ F ₂ Se ₂	16	0.1632	2	1
Br ₂ Ca ₃ Si	16	0.1632	2	1
Cl ₂ Mn	17	0.0069	1	4

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

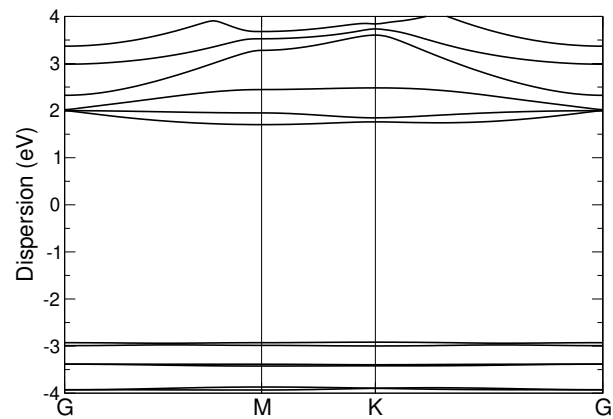
Formula	N° atoms	strain	cell size 1	cell size 2
S ₂ Ti	17	0.0	1	4
LiMnTe ₂	381	0.0001	25	64
IrTe ₂	227	0.0002	16	49
NiTe ₂	368	0.0002	25	81
GeI ₂	317	0.0002	25	64
Cl ₂ Co	17	0.0003	1	4
Ga ₂ Se ₂	276	0.0004	16	49
I ₂ La ₂ Te	65	0.0004	4	9
C ₂ I ₂ La ₂	983	0.0004	49	123
SiTe ₂	368	0.0004	25	81
As ₂ CeLi ₂	445	0.0004	25	64
Bi ₂ Te ₂	511	0.0004	39	79
Bi ₂ STe ₂	445	0.0004	25	64
PbTe	253	0.0004	25	64
CdO ₂	17	0.0005	1	4
Br ₂ Ca ₃ Si	74	0.0005	4	9
H ₂ MnO ₂	290	0.0005	9	49
In ₂ S ₃	325	0.0005	16	49
Cl ₂ Zr	17	0.0006	1	4
Cl ₂ Er ₂ O ₂	611	0.0007	25	81
F ₂ Lu ₂ Se ₂	195	0.0007	9	25
GeTe	178	0.0007	16	49
CaClHO	449	0.0008	25	81
Se ₂ Zr	368	0.0008	25	81
S ₂	178	0.0008	16	49
CdI ₂	317	0.0008	25	64
Br ₂ La ₂	145	0.0009	9	25
FeH ₂ O ₂	485	0.0009	16	81
Cl ₂ O ₂ Tm ₂	611	0.0009	25	81
Br ₂ La ₂ P	445	0.001	25	64
Er ₂ I ₂ S ₂	779	0.001	49	89
Br ₂ Ca ₃ Si	74	0.001	4	9
Ni ₂ SbTe ₂	325	0.001	16	49
ClH ₃ O	745	0.001	49	100
Cl ₂ Fe	17	0.001	1	4
Cu ₂ Rb ₂ Te ₂	684	0.001	42	79
Sb ₂	95	0.0011	9	25
H ₂ Si ₂	276	0.0011	16	49
Bi ₂ In ₂	874	0.0011	70	131
Bi ₂ In ₂	526	0.0011	42	79
Gd ₂ I ₂ S ₂	74	0.0012	4	9
Ho ₂ I ₂ S ₂	779	0.0012	49	89
Gd ₂ I ₂ S ₂	705	0.0012	45	80
Hg ₃ S ₂	1000	0.0012	110	90
Bi ₂ STe ₂	445	0.0013	25	64
CdI ₂	317	0.0013	25	64
Cl ₂ Rh ₂ Te ₂	894	0.0014	60	99
AuI ₄ Li	506	0.0014	40	51
O ₂ Zn	323	0.0014	16	81
Gd ₂ GeI ₂	445	0.0014	25	64

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

KO₃I (P3 (143))

Structural and electronic properties

	Formula	KO ₃ I
	Spacegroup	P3 (143)
	Prototype	IKO3
	Parent 3D	K ₂ O ₆ I ₂
	Source DB	ICSD
	DB ID	247719
DF2-C09	Binding energy [meV/ Å²]	47.43
RVV10	Binding energy [meV/ Å²]	56.0
	Band gap (PBE) [eV]	4.62

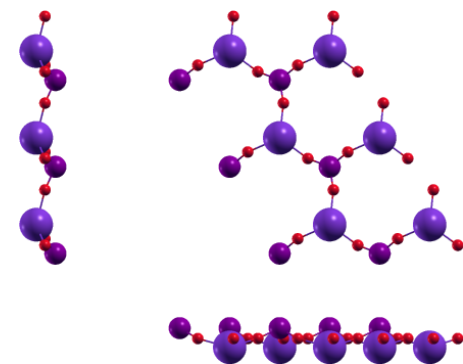


Band structure: Electronic band structure of KO₃I (P3 (143)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of KO₃I (P3 (143)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	7.10557388	−0.00000000	0.00000000
a₂	−3.55278694	6.15360748	0.00000000
a₃	0.00000000	0.00000000	21.29146633
	x [Å]	y [Å]	z [Å]
● I	0.00000000	0.00000000	10.06335119
● O	1.28637268	1.05037377	10.80453044
● O	−3.28632292	4.51438918	10.80453044
● O	1.99995023	6.74245203	10.80453044
● K	3.55278694	2.05120249	11.42764619



Orthographic projections: views of KO₃I (P3 (143)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
CaCl	7	0.1633	1	1
CNRb	8	0.2394	1	1
MnSe ₂	8	0.1633	1	1
Cl ₂ Rb ₂	9	0.1318	1	1
Cu ₂ O ₂	9	0.3026	1	1
Tl	9	0.1253	1	4
Fe ₂ S ₂	9	0.1629	1	1
Na	9	0.0006	1	4
Co ₂ S ₂	9	0.1635	1	1
FKO ₂ Se	10	0.1154	1	1
BrKO ₃	10	0.0054	1	1
I ₂ Lu ₂ Se ₂	11	0.1206	1	1
Cu ₄ Te ₂	11	0.1454	1	1
Cl ₄ Cu ₂	11	0.1195	1	1
LiO ₂	11	0.1367	1	2
Cl ₄ Mg ₂	11	0.0274	1	1
Cl ₄ KTl	11	0.1388	1	1
I ₂ Mg	13	0.1634	2	1
Li ₂ Tl ₂	13	0.2255	1	2
Br ₂ La	13	0.1634	2	1
BrCdI	13	0.1636	2	1
GeI ₂	13	0.1633	2	1
AsKSn	13	0.1638	2	1
PbTe ₂	13	0.1635	2	1
As ₂	13	0.0075	1	4
Se ₂ Yb	13	0.1633	2	1
Mg ₂	13	0.0434	1	4
BiTe ₂	13	0.1633	2	1
MnNaTe ₂	14	0.1636	2	1
AsCuLi ₂	14	0.1632	2	1
Cu ₂ I ₂	14	0.1634	2	1
I ₂ La ₂	14	0.1637	2	1
Gd ₂ I ₂	14	0.1634	2	1
Ga ₂ Te ₂	14	0.1632	2	1
Br ₂ HLa	14	0.1632	2	1
CeLi ₂ P ₂	15	0.1632	2	1
SSb ₂ Te ₂	15	0.1636	2	1
Ba ₂ Ni ₃	15	0.1632	2	1
Sb ₂ Se ₂ Te	15	0.1633	2	1
K	15	2.8061	1	10
Br ₂ Gd ₂ Ge	15	0.1634	2	1
Sb ₂ Se ₂ Te	15	0.1633	2	1
GeI ₃ Rb	15	0.223	2	1
Bi ₂ Se ₃	15	0.1634	2	1
CuGeO ₃	15	0.2625	1	2
I ₂ Pr ₂ Si ₂	16	0.1632	2	1
Gd ₂ I ₂ S ₂	16	0.1552	2	1
Ce ₂ I ₂ Si ₂	16	0.1634	2	1
AgClO ₄	16	0.1548	2	1
Cl ₂ Zn	17	0.0064	1	4

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

Formula	N° atoms	strain	cell size 1	cell size 2
GeI ₂	120	0.0	9	25
NS ₂ Zr	21	0.0002	1	4
As ₂ CeLi ₂	170	0.0002	9	25
Ga ₂ S ₃	25	0.0002	1	4
PbTe	95	0.0003	9	25
Br ₂ CsF	515	0.0003	39	80
LiMnTe ₂	145	0.0003	9	25
In	161	0.0003	16	81
PtS ₂	17	0.0004	1	4
O ₂ Zn	192	0.0005	9	49
Cl ₂ La ₂	276	0.0006	16	49
Na	9	0.0006	1	4
Bi ₂ STe ₂	170	0.0006	9	25
In ₂ Se ₂	276	0.0007	16	49
Ge ₂ I ₂ La ₂	509	0.0007	25	64
F ₂ Se ₂ Tm ₂	611	0.0008	25	81
Br ₂ Hg ₃	745	0.0008	100	49
LiMnSe ₂	449	0.0009	25	81
I ₄ Sr ₂	94	0.0009	8	9
Br ₂ Hg ₃	590	0.001	79	39
Br ₂ Er ₂ S ₂	414	0.001	24	49
CdI ₂	120	0.001	9	25
Br ₂ Lu ₂ S ₂	528	0.0011	30	63
Br ₂ Lu ₂ S ₂	528	0.0011	30	63
Bi ₂ STe ₂	170	0.0011	9	25
Br ₂ La ₂ P	170	0.0012	9	25
Au ₂ K ₂ S ₂	819	0.0012	81	69
O ₂ Pt	323	0.0012	16	81
HfLiS ₂	21	0.0012	1	4
GeNi ₃ Te ₂	611	0.0012	25	81
CdI ₂	120	0.0015	9	25
Au ₂ Br ₂	773	0.0015	53	127
Cu ₂ Rb ₂ Te ₂	675	0.0015	39	80
I ₂ Y ₂	449	0.0015	25	81
Te ₂ Zn	17	0.0015	1	4
Br ₂ Dy ₂ S ₂	816	0.0015	48	96
Gd ₂ GeI ₂	170	0.0016	9	25
As ₂ Sn ₂	276	0.0016	16	49
MoTe ₂	17	0.0017	1	4
Br ₂ Gd ₂	276	0.0017	16	49
AsLi ₃	145	0.0017	9	25
I ₂ Zn	227	0.0018	16	49
Bi ₂ In ₂	515	0.0018	39	80
NaPSn	368	0.0018	25	81
BiClTe	120	0.0018	9	25
Te ₂ W	17	0.0018	1	4
I ₂ Pr	120	0.0019	9	25
Ge ₂ Se ₂	552	0.0019	36	93
AgBrO ₂	565	0.0019	33	100
Br ₂ Ho ₂ S ₂	414	0.002	24	49

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.






KSeO₂F (Pm (6))

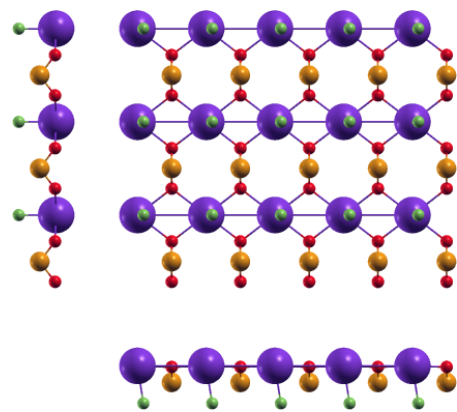
Structural and electronic properties

Formula	KSeO ₂ F
Spacegroup	Pm (6)
Prototype	FKO2Se
Parent 3D	K ₂ Se ₂ O ₄ F ₂
Source DB	ICSD
DB ID	78398
DF2-C09 Binding energy [meV/ Å ²]	115.96
RVV10 Binding energy [meV/ Å ²]	120.84
Band gap (PBE) [eV]	0.05

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of KSeO₂F (Pm (6)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		4.47760691	0.00000000	0.00000000
a₂		0.00000000	6.06169834	0.00000000
a₃		0.00000000	0.00000000	22.75259166
		x [Å]	y [Å]	z [Å]
	K	0.03078507	4.54627376	10.15247151
	Se	2.24757467	1.51542459	11.22518635
	O	2.25988778	2.82855587	10.22166095
	O	2.25988778	0.20229330	10.22166095
	F	0.41434675	4.54627376	12.58941316



Orthographic projections: views of KSeO₂F (Pm (6)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	6	0.2313	1	1
Na	7	0.1401	1	2
Br ₂ Cu	8	0.8407	1	1
CKN	8	0.3052	1	1
Bi ₂ In ₂	9	0.8193	1	1
Au ₂ Br ₂	9	0.2324	1	1
N ₃ Na	9	0.2436	1	1
As ₂	9	0.1451	1	2
S ₂	9	0.5252	1	2
Au ₂ I ₂	9	0.0805	1	1
SbSe ₂ Tl	9	0.144	1	1
Hg ₃ N ₂	10	0.3203	1	1
IKO ₃	10	0.3406	1	1
BrKO ₃	10	0.3293	1	1
Cl ₂ Zn	11	0.1444	1	2
Br ₂ Ho ₂ S ₂	11	0.3205	1	1
I ₂ Lu ₂ Se ₂	11	0.0253	1	1
PSn ₂	11	0.1514	1	2
ReSe ₂	11	0.1334	1	2
Ho ₂ I ₂ S ₂	11	0.3272	1	1
HfS ₂	11	0.1469	1	2
GeTe ₂	11	0.5153	1	2
Br ₂ Co	11	0.1448	1	2
Ca ₂ N	11	0.1454	1	2
K ₂ O ₂ Tl ₂	11	0.1529	1	1
S ₂ Ti	11	0.1307	1	2
Br ₂ S ₂ Y ₂	11	0.3254	1	1
I ₄ Zr ₂	11	0.543	1	1
Gd ₂ I ₂ S ₂	11	0.3334	1	1
C ₂ Br ₂ Gd ₂	11	0.4909	1	1
Br ₂ Mn	11	0.3357	1	2
Cl ₂ Ni	11	0.1339	1	2
Cl ₂ Co	11	0.1306	1	2
CrTe ₂	11	0.137	1	2
CoTe ₂	11	0.1472	1	2
Br ₂ V	11	0.1331	1	2
ClN ₂ Zr	11	0.1321	1	2
Cl ₂ Fe	11	0.1303	1	2
I ₂ S ₂ Tb ₂	11	0.3307	1	1
Te ₄ TiZr	11	0.5155	1	1
Se ₂ Ti	11	0.1391	1	2
I ₂ S ₂ Yb ₂	11	0.3237	1	1
Br ₂ Ti	11	0.1367	1	2
Cu ₂ Rb ₂ Te ₂	11	0.2749	1	1
Br ₂ Dy ₂ S ₂	11	0.3233	1	1
AsSe ₂	11	0.1346	1	2
Cl ₂ Ga ₂ Te ₂	11	0.0285	1	1
S ₂ Sn	11	0.151	1	2
Ag ₂ K ₂ Te ₂	11	0.8762	1	1
Br ₂ Ga ₂ Te ₂	11	0.0249	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

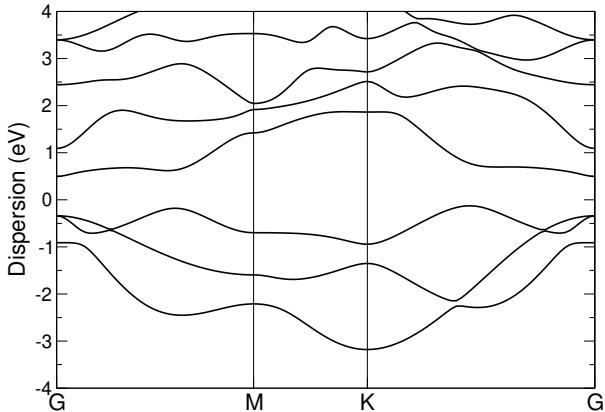
Formula	N° atoms	strain	cell size 1	cell size 2
P ₂ Sn ₂	870	0.0004	66	135
S ₂ Zn ₂	870	0.0005	66	135
I ₂ Nd ₂ O ₂	270	0.0007	18	30
Ga ₂ I ₂ Y ₂	750	0.0008	48	85
BaF ₂	495	0.0009	48	85
Br ₂ Dy ₂ S ₂	983	0.0011	79	98
Cl ₂ Er ₂ S ₂	712	0.0012	56	72
Cl ₂ F ₂ Pb ₂	270	0.0012	18	30
Cl ₂ Gd ₂	827	0.0012	63	128
Bi ₂ I ₂ O ₂	270	0.0012	18	30
Cu ₂ Na ₂ Se ₂	270	0.0012	18	30
Br ₂ Cu ₂	540	0.0012	44	80
I ₂ La ₂	510	0.0012	42	75
CdCl ₂	730	0.0013	65	135
I ₂ Mn	730	0.0013	65	135
TaTe ₂	545	0.0013	46	105
Ni ₂ Te ₂	865	0.0013	65	135
Br ₂ F ₂ Yb ₂	700	0.0013	44	80
As ₂ Fe ₂	552	0.0013	40	88
AsKSn	495	0.0013	48	85
GeS ₂	464	0.0013	40	88
InSe ₂	730	0.0013	65	135
F ₂ I ₂ Tm ₂	270	0.0013	18	30
Br ₂ O ₂ Tb ₂	700	0.0013	44	80
Br ₂ S ₂ Yb ₂	795	0.0014	63	80
PbS ₂	411	0.0014	36	77
Ba ₂ N	349	0.0014	32	63
Sm	201	0.0014	21	96
F ₂ Ho ₂ Se ₂	538	0.0014	32	63
H ₂ Si ₂	865	0.0014	65	135
AgClO ₂	794	0.0015	62	121
Br ₂ Ca ₂ F ₂	700	0.0015	44	80
BrCdI	435	0.0015	42	75
I ₂ Y ₂	827	0.0015	63	128
Se ₂ Ta	89	0.0015	7	18
I ₂ Ni	730	0.0015	65	135
Ga ₂ Se ₂	870	0.0015	66	135
SSb ₂ Te ₂	585	0.0015	42	75
Hf ₂ Se ₂ Si ₂	728	0.0015	40	88
Br ₂ Y ₂	488	0.0015	36	77
AsKSn	435	0.0015	42	75
BrNZr	89	0.0015	7	18
Cu ₃ Se ₃	538	0.0016	32	63
C ₂ I ₂ La ₂	895	0.0016	59	100
C ₄ Ca ₂	949	0.0016	65	104
STl ₂	495	0.0016	48	85
Br ₂ S ₂ Y ₂	817	0.0016	65	82
Cl ₂ H ₂ Sc ₂	143	0.0016	7	18
CNNa	275	0.0017	28	45
GeTe	595	0.0017	65	135

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

KSnAs (P3m1 (156))

Structural and electronic properties

	Formula	KSnAs
	Spacegroup	P3m1 (156)
	Prototype	BiTeI
	Parent 3D	K ₂ Sn ₂ As ₂
	Source DB	COD
	DB ID	1008518
DF2-C09	Binding energy [meV/ Å²]	92.03
RVV10	Binding energy [meV/ Å²]	90.76
	Band gap (PBE) [eV]	0.62

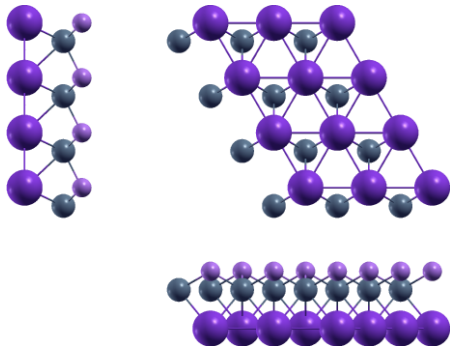


Band structure: Electronic band structure of KSnAs (P3m1 (156)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of KSnAs (P3m1 (156)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.19791941	0.00000000	0.00000000
a₂	−2.09895970	3.63550485	0.00000000
a₃	0.00000000	0.00000000	24.09498029
	x [Å]	y [Å]	z [Å]
●	Sn	0.00000000	0.00000000
●	As	2.09895970	1.21183495
●	K	2.09895970	1.21183495



Orthographic projections: views of KSnAs (P3m1 (156)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
InSe	5	0.0053	1	1
AgTl	5	0.1578	1	1
Ag ₂	5	0.4524	1	1
As ₂	5	1.5568	1	1
PbTe	5	0.0071	1	1
CaCl	5	0.1157	1	1
Cl ₂ Zn	6	1.5492	1	1
I ₂ Mg	6	0.005	1	1
CdI ₂	6	0.0089	1	1
PSn ₂	6	0.25	1	1
Ba ₂ Pt	6	0.4517	1	1
Br ₂ Zn	6	0.2646	1	1
AsSn ₂	6	0.255	1	1
SiTe ₂	6	0.2705	1	1
Te ₂ V	6	1.5297	1	1
I ₂ Pr	6	0.1408	1	1
S ₂ Zr	6	0.249	1	1
Br ₂ La	6	0.0046	1	1
Br ₂ Cu	6	0.7374	1	1
Ca ₂ Si	6	0.4629	1	1
PbS ₂	6	0.2757	1	1
Br ₂ Co	6	1.5537	1	1
BiClTe	6	0.0093	1	1
Ca ₂ N	6	1.5606	1	1
BrCdI	6	0.0019	1	1
Cl ₂ Zn	6	0.1233	1	1
Te ₂ Ti	6	0.265	1	1
BaF ₂	6	0.0014	1	1
RhTe ₂	6	0.2589	1	1
GeI ₂	6	0.0068	1	1
Br ₂ Mn	6	1.5406	1	1
CdClO	6	1.5263	1	1
PbTe ₂	6	0.0028	1	1
I ₂ Nd	6	0.1417	1	1
NiTe ₂	6	0.2697	1	1
Cl ₂ Cu	6	0.066	1	1
S ₂ Sn	6	0.2493	1	1
SnTe ₂	6	0.0089	1	1
I ₂ V	6	0.2725	1	1
GeI ₂	6	0.0074	1	1
Se ₂ Zr	6	0.2711	1	1
I ₂ Pb	6	0.4563	1	1
STl ₂	6	0.0024	1	1
PtSe ₂	6	0.2559	1	1
OTl ₂	6	1.5276	1	1
Br ₂ Fe	6	1.5542	1	1
GeS ₂	6	0.111	1	1
TaTe ₂	6	0.2542	1	1
MnSe ₂	6	0.1156	1	1
Br ₂ Ni	6	1.5912	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

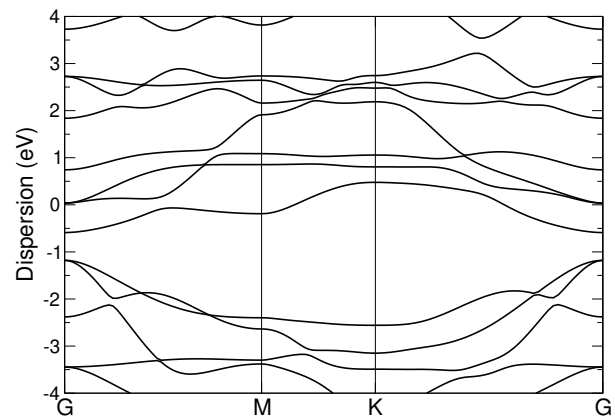
Formula	N° atoms	strain	cell size 1	cell size 2
Se ₂ Ta	183	0.0	25	36
S ₂ Sn	339	0.0	49	64
CCL ₂ Gd ₂	674	0.0001	73	91
Cl ₂ Mg	300	0.0001	43	57
F ₂ Na	543	0.0001	81	100
Bi ₂ Te ₂	388	0.0001	64	49
Br ₂ Ni	300	0.0002	43	57
Cl ₂ O ₂ Yb ₂	843	0.0002	81	100
Br ₂ Zn	492	0.0002	73	91
Cl ₂ H ₂ Sc ₂	291	0.0002	25	36
Cl ₂ H ₂ Lu ₂	471	0.0002	43	57
S ₂ Zr	339	0.0002	49	64
O ₂ Pt	75	0.0002	9	16
PTe ₂ Ti ₂	414	0.0003	43	57
Se ₄ TiZr	339	0.0003	49	32
RhTe ₂	435	0.0003	64	81
AsSn ₂	390	0.0003	57	73
Cl ₂ Zn	255	0.0003	36	49
IO ₃ Tl	317	0.0003	64	25
PtSe ₂	390	0.0003	57	73
NbTe ₂	339	0.0004	49	64
Br ₂ Cu	483	0.0004	76	85
Cl ₂ Mn	123	0.0005	16	25
KS ₂ Ti	304	0.0005	36	49
Te ₂ Ti	492	0.0005	73	91
CBr ₂ Y ₂	674	0.0005	73	91
HfSe ₂	492	0.0005	73	91
I ₂ La ₂	7	0.0005	1	1
As ₂ Cd ₂ K ₂	483	0.0005	65	48
PSn ₂	339	0.0005	49	64
Sb ₂ Te ₂	624	0.0006	100	81
Ga ₂ S ₂	357	0.0006	43	57
AlH ₄ Na	840	0.0006	118	81
O ₄ PSn	483	0.0007	65	48
As ₄	527	0.0007	81	71
Cl ₂ O ₂ Tm ₂	843	0.0007	81	100
Ca ₂ Si	543	0.0007	100	81
Ce ₂ I ₂ S ₂	786	0.0007	100	81
O ₂ Sn ₂	498	0.0007	70	72
Br ₂ Hf ₂ N ₂	675	0.0007	73	76
Br ₂ Ti	183	0.0007	25	36
I ₂ N ₂ Zr ₂	678	0.0008	64	81
CaClHO	643	0.0008	81	100
Br ₂ Mn	255	0.0009	36	49
TaTe ₂	390	0.0009	57	73
Br ₂ Pr ₂	643	0.0009	81	100
Br ₂ H ₂ Zr ₂	291	0.0009	25	36
Br ₂ Co	255	0.0009	36	49
Cl ₂ NSc ₂	173	0.0009	16	25
Br ₂ Fe	255	0.001	36	49

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

KTiS₂ (P3m1 (156))

Structural and electronic properties





	Formula	KTiS ₂
	Spacegroup	P3m1 (156)
	Prototype	LiMnSe2
	Parent 3D	KTiS ₂
	Source DB	ICSD
	DB ID	641335
DF2-C09	Binding energy [meV/ Å²]	N/A
RVV10	Binding energy [meV/ Å²]	124.57
	Band gap (PBE) [eV]	0.0

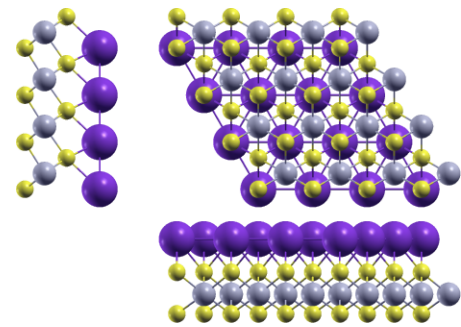


Band structure: Electronic band structure of KTiS₂ (P3m1 (156)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of KTiS₂ (P3m1 (156)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.59453873	−0.00000000	0.00000000
a₂		−1.79726936	3.11296185	0.00000000
a₃		0.00000000	0.00000000	25.06293892
		x [Å]	y [Å]	z [Å]
	Ti	1.79726936	1.03765395	13.68715256
	K	−0.00000000	0.00000000	10.03887197
	S	−0.00000000	0.00000000	14.98438840
	S	0.00000000	2.07530790	12.23043499



Orthographic projections: views of KTiS₂ (P3m1 (156)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.3143	1	1
Tl	5	0.1219	1	1
Sn	5	0.4265	1	1
Na	5	0.006	1	1
In	5	1.6354	1	1
HgO	6	0.1297	1	1
As ₂	6	0.0019	1	1
LiO	6	0.2669	1	1
Mg ₂	6	0.1139	1	1
Sb ₂	6	0.4942	1	1
CrS ₂	7	1.5274	1	1
Cl ₂ Zn	7	0.0008	1	1
S ₂ V	7	0.2566	1	1
MoS ₂	7	0.2576	1	1
MoTe ₂	7	0.0038	1	1
AgTe ₂	7	0.1237	1	1
HfS ₂	7	0.0046	1	1
HfTe ₂	7	0.4542	1	1
Te ₂ V	7	0.0019	1	1
CuTe ₂	7	0.0043	1	1
Br ₂ Co	7	0.0014	1	1
Ca ₂ N	7	0.0024	1	1
AuTe ₂	7	0.4737	1	1
PdTe ₂	7	0.4675	1	1
Mg ₃	7	0.1187	1	1
I ₂ Zn	7	0.4855	1	1
Te ₂ Zn	7	0.004	1	1
S ₂ W	7	0.2577	1	1
Bi ₂ Pd	7	0.1369	1	1
GeI ₂	7	2.9124	1	1
Br ₂ Mn	7	0.0004	1	1
PtS ₂	7	0.005	1	1
CoTe ₂	7	0.005	1	1
CdClO	7	0.0024	1	1
Ba ₂ N	7	0.458	1	1
Se ₂ Ti	7	0.0076	1	1
AsKSn	7	3.0032	1	1
Te ₂ Zr	7	0.4554	1	1
Te ₂ W	7	0.0036	1	1
Cl ₂ Cu	7	0.5854	1	1
SnTe ₂	7	0.4983	1	1
Cl ₂ V	7	0.2633	1	1
STl ₂	7	3.0353	1	1
OTl ₂	7	0.0022	1	1
Br ₂ Fe	7	0.0015	1	1
Br ₂ Ni	7	0.0067	1	1
Se ₂ Yb	7	2.9155	1	1
MoS ₂	7	0.2579	1	1
Cl ₂ Mg	7	0.0067	1	1
BiTe ₂	7	2.919	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

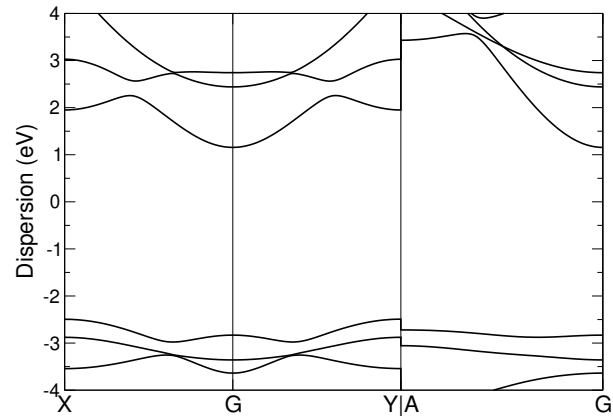
Formula	N° atoms	strain	cell size 1	cell size 2
I ₂ La ₂	340	0.0	49	36
Sb ₂ Te ₃	269	0.0	36	25
H ₂ MgO ₂	593	0.0001	57	73
Se ₂ Yb	357	0.0001	57	43
Li ₂ P ₂ Pr	501	0.0001	64	49
H ₂ NiO ₂	661	0.0001	64	81
GeI ₂	357	0.0002	57	43
Br ₂ Gd ₂	580	0.0002	81	64
Ga ₂ Ge ₂ Te ₂	550	0.0002	64	49
Br ₂ Ca ₃ Si	706	0.0002	91	57
In ₂ Se ₂	520	0.0002	73	57
PdTe ₂	583	0.0002	91	73
As ₂ Sn ₂	580	0.0003	81	64
Br ₂ Er ₂	580	0.0003	81	64
F ₂ Ho ₂ Se ₂	886	0.0003	100	81
Ba ₂ Ni ₃	443	0.0003	57	43
BiTe ₂	357	0.0003	57	43
Ga ₂ Te ₂	400	0.0004	57	43
Br ₂ Mn	7	0.0004	1	1
I ₂ Pr ₂ Si ₂	486	0.0005	57	43
Sb ₂	354	0.0005	64	49
AsKSn	304	0.0005	49	36
LiO	524	0.0005	81	100
CrSe ₂	565	0.0005	73	91
Al ₂ Cl ₂ O ₂	742	0.0005	76	73
Ba ₂ Pt	471	0.0005	81	49
Cu ₄ Te ₂	294	0.0005	36	25
Ge ₂ Se ₂	684	0.0006	103	68
CaI ₂	148	0.0006	25	16
Bi ₂ Te ₂	100	0.0006	16	9
AsCuLi ₂	400	0.0006	57	43
Bi ₂ Cl ₂ O ₂	548	0.0006	65	48
Ni ₂ Se ₂	452	0.0007	65	48
Br ₂ Cd	583	0.0007	91	73
Sb ₂ Se ₂ Te	443	0.0007	57	43
Br ₂ La ₂	452	0.0007	64	49
I ₂ Nd ₂ O ₂	958	0.0007	118	81
Cl ₂ V	565	0.0007	73	91
O ₂ Pt	388	0.0007	49	64
I ₂ Nd ₂ S ₂	466	0.0008	61	37
Ag ₂	422	0.0008	81	49
Cl ₂ Zn	7	0.0008	1	1
Br ₂ Tb ₂	656	0.0008	91	73
S ₂ V	447	0.0008	57	73
Se ₂ Sn ₂	472	0.0008	74	44
Ge ₂ Te ₂	448	0.0009	70	42
Br ₂ PY ₂	729	0.0009	91	73
CeI ₂	404	0.0009	65	48
I ₂ Zn	463	0.0009	73	57
CNRb	426	0.0009	78	38

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Li₂C₂ (C2/m)

Structural and electronic properties

	Formula	Li ₂ C ₂
	Spacegroup	C2/m
	Prototype	CLi
	Parent 3D	C ₄ Li ₄
	Source DB	ICSD
	DB ID	671757
DF2-C09	Binding energy [meV/ Å²]	58.18
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	3.65

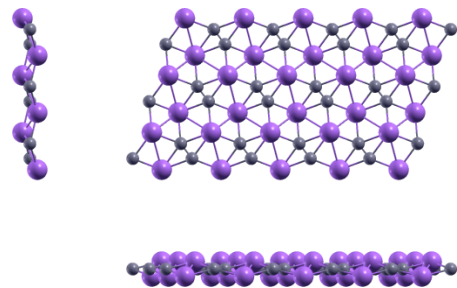


Band structure: Electronic band structure of Li₂C₂ (C2/m) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Li₂C₂ (C2/m) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.19316985	−2.39757675	0.00000000
a₂		3.19243260	2.39673015	0.00000000
a₃		0.00000000	0.00000000	15.40796886
		x [Å]	y [Å]	z [Å]
●	Li	−3.67597398	3.59621558	−0.49799465
●	C	−1.59746443	4.22467862	0.00029532
●	C	−1.59644268	2.96719995	−0.00029532
●	Li	0.48206687	3.59566300	0.49799465



Orthographic projections: views of Li₂C₂ (C2/m) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	5	0.1274	1	1
HgO	6	0.1307	1	1
BN	6	0.2294	1	1
AgTe ₂	7	0.1281	1	1
Mg ₃	7	0.1262	1	1
Cu ₂ Te ₂	8	0.1523	1	1
AgCuTe ₂	8	0.1606	1	1
O ₂ Sn ₂	8	0.7553	1	1
P ₄	8	0.1918	1	1
Mg ₄	8	0.1273	1	1
P ₂	8	0.2946	1	2
Ho ₂ S ₂	8	0.6513	1	1
CuGeO ₃	9	0.2568	1	1
CrS ₂	10	0.2423	1	2
Cl ₂ Mn	10	0.2379	1	2
Cl ₂ O ₂ V ₂	10	0.139	1	1
S ₂ Ta	10	0.2412	1	2
Cu ₄ Te ₂	10	0.3131	1	1
ReS ₂	10	0.251	1	2
Br ₂ Cr ₂ S ₂	10	0.1876	1	1
Cl ₂ Ti	10	0.2948	1	2
NbS ₂	10	0.2405	1	2
Bi ₂ Pd	10	0.4168	1	2
N ₂ W	10	0.1719	1	2
Al ₂ Cl ₂ O ₂	10	0.1353	1	1
Cl ₂ Fe ₂ O ₂	10	0.1362	1	1
Cl ₂ Cr ₂ O ₂	10	0.1364	1	1
Br ₂ Cr ₂ O ₂	10	0.1456	1	1
I ₂ Tm	10	0.9115	1	2
Cl ₂ N ₂ Ti ₂	10	0.1501	1	1
Br ₂ O ₂ V ₂	10	0.1453	1	1
As ₂	10	1.1317	1	3
CdO ₂	10	1.536	1	2
O ₂ Zn	10	0.2375	1	2
Br ₂ O ₂ Ti ₂	10	0.1629	1	1
Cl ₂ O ₂ Ti ₂	10	0.1528	1	1
Br ₂ N ₂ Ti ₂	10	0.6962	1	1
In	10	0.1292	2	2
N ₂ Re	10	0.1481	1	2
HfTe ₂	11	0.1477	2	1
Tl	11	0.0583	2	3
PdTe ₂	11	0.1487	2	1
CNRb	11	0.207	2	1
Ba ₂ N	11	0.148	2	1
Te ₂ Zr	11	0.1478	2	1
F ₂ Ni	11	0.4448	2	1
Br ₂ Cd	11	0.1485	2	1
Cu ₂ I ₂	12	1.0791	1	2
HNiO ₂	12	0.1643	1	2
Ca ₂ O ₂	12	0.4199	1	2

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

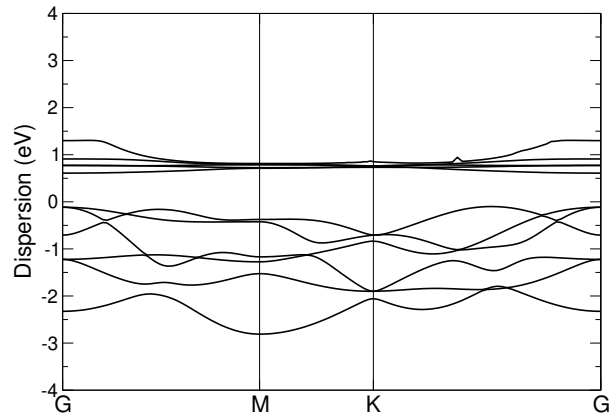
Formula	N° atoms	strain	cell size 1	cell size 2
Ce ₂ I ₂ Si ₂	396	0.0001	39	40
I ₂ Mg	276	0.0003	39	40
Br ₂ Ce ₂ O ₂	244	0.0003	25	24
K ₂ Mn ₂ Sb ₂	244	0.0003	25	24
Br ₂ Ho ₂ O ₂	246	0.0003	24	25
Sb ₂ Se ₂ Te	356	0.0003	39	40
Ca ₂ Mn ₂ Si ₂	246	0.0004	24	25
Au ₂ Br ₂	708	0.0004	96	81
ReSe ₂	548	0.0004	65	96
C ₄ Ca ₂	584	0.0005	62	56
Cl ₂ Ni	548	0.0005	65	96
Gd ₂ I ₂ S ₂	322	0.0005	40	27
Br ₂ N ₂ Zr ₂	832	0.0005	82	84
Ho ₂ I ₂ Se ₂	220	0.0006	28	18
Br ₂ Ca ₂ H ₂	246	0.0006	24	25
Er ₂ I ₂ Se ₂	220	0.0006	28	18
Ir ₂ P ₂	672	0.0006	84	84
Br ₂ La	276	0.0006	39	40
Br ₂ O ₂ Sm ₂	840	0.0006	84	84
I ₂ Nd	588	0.0006	84	84
Eu ₂ I ₂ O ₂	244	0.0007	25	24
Bi ₂ Se ₃	356	0.0007	39	40
I ₂ O ₂ Yb ₂	840	0.0007	84	84
Se ₂ V	633	0.0007	72	115
Sb ₂ Se ₂ Te	356	0.0008	39	40
MnSe ₂	204	0.0008	27	32
NS ₂ Zr	432	0.0008	45	63
Ga ₂ S ₃	495	0.0008	45	63
Bi ₂ Mn ₂	900	0.0008	99	126
Ca ₂ H ₂ I ₂	244	0.0008	25	24
PtS ₂	369	0.0008	45	63
CaCl	172	0.0009	27	32
NbSe ₂	548	0.0009	65	96
I ₂ Pr	588	0.001	84	84
CaI ₂	703	0.001	106	93
Ag ₂ K ₂ Se ₂	784	0.001	91	70
Na	243	0.001	45	63
Cl ₂ Er ₂ S ₂	460	0.001	55	40
Se ₂ Ta	548	0.001	65	96
Ag ₂ Te ₂	352	0.001	43	45
LiMnSe ₂	796	0.001	93	106
Fe ₂ O ₄	950	0.001	74	109
Tl	403	0.0011	72	115
Br ₂ S ₂ Y ₂	560	0.0011	68	48
P ₂ Rh ₂	196	0.0011	24	25
O ₂ Sn ₂	312	0.0011	35	43
BiTe ₂	276	0.0011	39	40
CrS ₂	646	0.0011	67	126
I ₂ Lu ₂ S ₂	460	0.0012	55	40
F ₄ Nb	577	0.0012	68	61

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Li₂CeAs₂ (P-3m1 (164))

Structural and electronic properties

	Formula	Li ₂ CeAs ₂
	Spacegroup	P-3m1 (164)
	Prototype	Bi ₂ Te ₂ S
	Parent 3D	Li ₂ CeAs ₂
	Source DB	ICSD
	DB ID	32042
DF2-C09	Binding energy [meV/ Å²]	54.99
RVV10	Binding energy [meV/ Å²]	58.24
	Band gap (PBE) [eV]	0.71

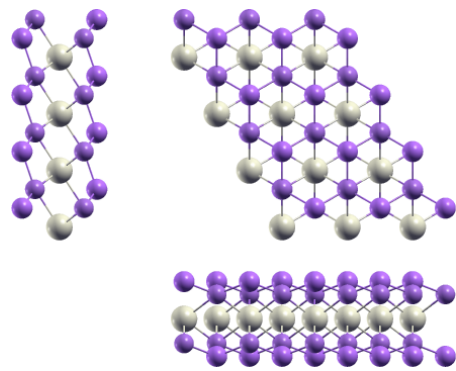


Band structure: Electronic band structure of Li₂CeAs₂ (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Li₂CeAs₂ (P-3m1 (164)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		4.26128504	0.00000000	0.00000000
a₂		-2.13064252	3.69038110	0.00000000
a₃		0.00000000	0.00000000	25.11813245
		x [Å]	y [Å]	z [Å]
●	Li	2.13064252	1.23012703	14.99622285
●	As	0.00000000	2.46025407	14.15749400
●	Li	0.00000000	2.46025407	10.12190960
●	Ce	0.00000000	0.00000000	12.55906622
●	As	2.13064252	1.23012703	10.96063844



Orthographic projections: views of Li₂CeAs₂ (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
InSe	7	0.0018	1	1
AsSb	7	0.2691	1	1
Bi ₂	7	0.004	1	1
AgTl	7	0.1507	1	1
PbTe	7	0.0	1	1
CaCl	7	0.1127	1	1
CdI ₂	8	0.0017	1	1
MoSe ₂	8	4.8797	1	1
Br ₂ Zn	8	0.2548	1	1
Br ₂ Ca	8	0.0029	1	1
HfS ₂	8	1.5257	1	1
AsSn ₂	8	1.5978	1	1
GeTe ₂	8	0.275	1	1
SiTe ₂	8	0.2604	1	1
I ₂ Pr	8	0.135	1	1
S ₂ Zr	8	1.5646	1	1
Br ₂ Cu	8	0.7117	1	1
NSr ₂	8	0.2715	1	1
PbS ₂	8	0.2654	1	1
BiClTe	8	0.0021	1	1
BrCdI	8	0.0088	1	1
Cl ₂ Zn	8	0.1193	1	1
FeI ₂	8	0.2734	1	1
I ₂ Ni	8	0.2753	1	1
HgI ₂	8	0.2061	1	1
Te ₂ Ti	8	0.2552	1	1
CrI ₂	8	0.2727	1	1
BaF ₂	8	0.0056	1	1
BiBrTe	8	0.0077	1	1
RhTe ₂	8	0.2493	1	1
CoTe ₂	8	1.528	1	1
AsKSn	8	0.007	1	1
I ₂ Nd	8	0.1358	1	1
NiTe ₂	8	0.2596	1	1
Cl ₂ Cu	8	0.0681	1	1
S ₂ Sn	8	1.5665	1	1
I ₂ V	8	0.2623	1	1
GeI ₂	8	0.0002	1	1
Se ₂ Zr	8	0.261	1	1
STl ₂	8	0.0046	1	1
PtSe ₂	8	0.2465	1	1
CoI ₂	8	0.2697	1	1
GeS ₂	8	0.4288	1	1
MnSe ₂	8	0.1127	1	1
Br ₂ Ni	8	1.5398	1	1
CeI ₂	8	0.1344	1	1
Br ₂ Mg	8	0.2732	1	1
I ₂ Ti	8	0.2702	1	1
NbTe ₂	8	1.563	1	1
Cl ₂ Mg	8	1.5402	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

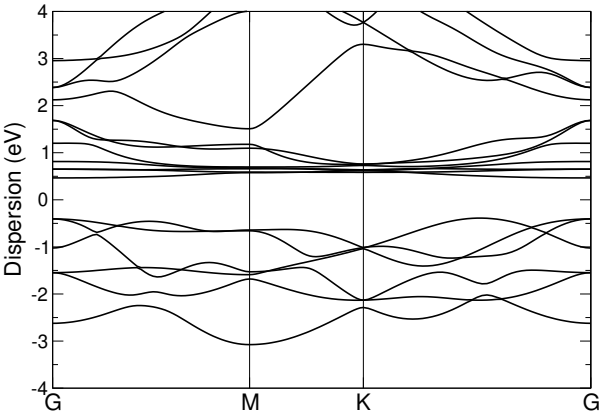
Formula	N° atoms	strain	cell size 1	cell size 2
Ga ₂ S ₃	305	0.0	25	36
H ₂ NiO ₂	125	0.0	9	16
PbTe	7	0.0	1	1
CdO ₂	155	0.0	16	25
NS ₂ Zr	269	0.0001	25	36
RhTe ₂	437	0.0001	49	64
Cl ₂ Co	155	0.0001	16	25
TaTe ₂	386	0.0002	43	57
Ga ₂ Se ₂	729	0.0002	73	91
Br ₂ CsF	517	0.0002	65	48
HfSe ₂	504	0.0002	57	73
GeI ₂	8	0.0002	1	1
Te ₂ Ti	504	0.0002	57	73
MoSe ₂	488	0.0002	49	81
NiTe ₂	563	0.0002	64	81
IKO ₃	170	0.0002	25	9
Cl ₂ Zr	155	0.0002	16	25
Se ₂ W	368	0.0003	37	61
Au ₂ Br ₂	626	0.0003	74	64
O ₂ Zn	272	0.0003	25	49
Tl	246	0.0003	37	61
PTe ₂ Zr ₂	905	0.0003	81	100
Cl ₂ O ₂ Y ₂	911	0.0004	73	91
Na	161	0.0004	25	36
CaClHO	644	0.0004	64	81
Hf ₂ I ₂ N ₂	557	0.0004	43	57
CdClHO	443	0.0004	43	57
ClKO ₃	445	0.0004	64	25
MoSe ₂	368	0.0004	37	61
S ₂ Ti	155	0.0004	16	25
Bi ₂ Te ₂	661	0.0005	81	64
Br ₂ Er ₂ S ₂	949	0.0005	101	74
Br ₂ Zn	504	0.0005	57	73
LiMnTe ₂	9	0.0005	1	1
Cl ₂ O ₂ Tm ₂	806	0.0005	64	81
Br ₂ Y ₂	729	0.0005	73	91
Cl ₂ Fe	155	0.0006	16	25
Cl ₂ H ₂ Lu ₂	474	0.0006	36	49
CCL ₂ Gd ₂	650	0.0006	57	73
PtS ₂	233	0.0007	25	36
Br ₂ Pr ₂	577	0.0007	57	73
CdClHO	501	0.0007	49	64
Br ₂ S ₂ Yb ₂	857	0.0007	91	67
Cl ₂ Er ₂ S ₂	673	0.0007	71	53
H ₄ Ti	865	0.0007	65	108
AsSn ₂	386	0.0007	43	57
PbS ₂	638	0.0007	73	91
Cu ₄ Te ₂	649	0.0008	59	59
SiTe ₂	563	0.0008	64	81
Bi ₂ STe ₂	10	0.0008	1	1

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Li₂CeP₂ (P-3m1 (164))

Structural and electronic properties

	Formula	Li ₂ CeP ₂
	Spacegroup	P-3m1 (164)
	Prototype	Bi2Te2S
	Parent 3D	Li ₂ CeP ₂
	Source DB	ICSD
	DB ID	42016
DF2-C09	Binding energy [meV/ Å²]	59.31
RVV10	Binding energy [meV/ Å²]	63.0
	Band gap (PBE) [eV]	0.85

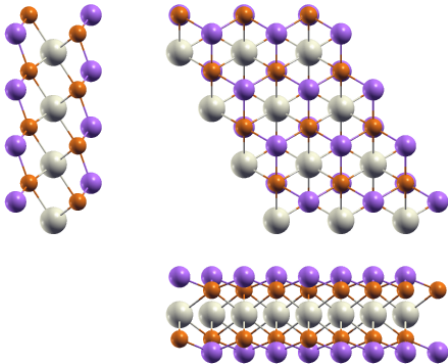


Band structure: Electronic band structure of Li₂CeP₂ (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Li₂CeP₂ (P-3m1 (164)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.12564949	0.00000000	0.00000000
a₂	−2.06282475	3.57291727	0.00000000
a₃	0.00000000	0.00000000	25.05319914
	x [Å]	y [Å]	z [Å]
● Li	0.00000000	2.38194484	10.11943338
● P	2.06282475	1.19097242	10.96738950
● Li	2.06282475	1.19097242	14.93376576
● Ce	0.00000000	0.00000000	12.52659957
● P	0.00000000	2.38194484	14.08580964



Orthographic projections: views of Li₂CeP₂ (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	6	0.4591	1	1
Na	6	1.5585	1	1
Ag ₂	7	0.4729	1	1
As ₂	7	0.249	1	1
Sb ₂	7	0.0025	1	1
CaCl	7	0.1197	1	1
Cl ₂ Zn	8	0.2477	1	1
I ₂ Mg	8	0.0032	1	1
PSn ₂	8	0.2611	1	1
Ba ₂ Pt	8	0.4722	1	1
HfS ₂	8	1.6377	1	1
AsSn ₂	8	0.2665	1	1
Te ₂ V	8	1.5891	1	1
I ₂ Pr	8	0.1482	1	1
S ₂ Zr	8	0.2601	1	1
Br ₂ La	8	0.0035	1	1
Ca ₂ Si	8	0.4838	1	1
Br ₂ Co	8	0.2485	1	1
Ca ₂ N	8	0.2497	1	1
BrCdI	8	0.0064	1	1
Cl ₂ Zn	8	0.1286	1	1
I ₂ Zn	8	0.0057	1	1
RhTe ₂	8	0.2705	1	1
GeI ₂	8	0.0013	1	1
Br ₂ Mn	8	1.6004	1	1
PtS ₂	8	1.566	1	1
CoTe ₂	8	1.6401	1	1
CdClO	8	1.5855	1	1
Se ₂ Ti	8	1.5469	1	1
AsKSn	8	0.0083	1	1
PbTe ₂	8	0.0054	1	1
I ₂ Nd	8	0.1491	1	1
S ₂ Sn	8	0.2604	1	1
SnTe ₂	8	0.0009	1	1
Sn	8	0.6379	1	3
I ₂ Pb	8	0.4769	1	1
PtSe ₂	8	0.2674	1	1
OTl ₂	8	1.5868	1	1
Br ₂ Fe	8	0.2486	1	1
GeS ₂	8	0.114	1	1
TaTe ₂	8	0.2656	1	1
MnSe ₂	8	0.1197	1	1
Br ₂ Ni	8	0.2553	1	1
CeI ₂	8	0.1475	1	1
CuO ₂	8	0.176	1	1
NbTe ₂	8	0.2598	1	1
Se ₂ Yb	8	0.0016	1	1
Cl ₂ Mg	8	0.2554	1	1
BiTe ₂	8	0.0018	1	1
CrSe ₂	8	4.8674	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

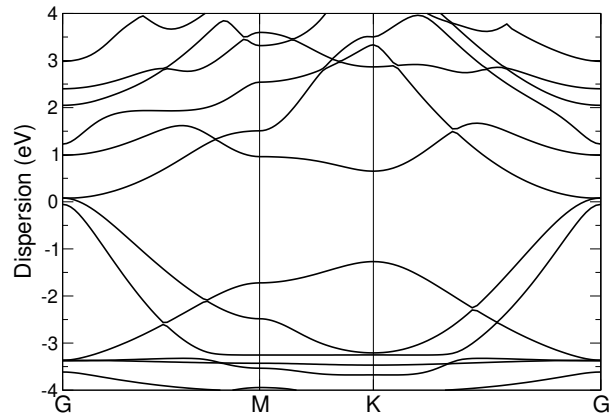
Formula	N° atoms	strain	cell size 1	cell size 2
Se ₂ Ti	327	0.0	36	49
Cl ₂ Mg	504	0.0	57	73
Br ₂ Ni	504	0.0001	57	73
PtSe ₂	705	0.0001	81	100
Br ₂ H ₂ Zr ₂	341	0.0002	25	36
As ₂	373	0.0002	49	64
I ₂ Nd ₂ S ₂	893	0.0002	91	73
Cl ₂ V	368	0.0002	37	61
PTe ₂ Ti ₂	650	0.0002	57	73
CoH ₂ O ₂	125	0.0002	9	16
Ca ₂ Si	536	0.0002	73	57
Ce ₂ I ₂ S ₂	707	0.0002	73	57
FHOZn	569	0.0003	49	81
NaO ₄	205	0.0003	25	16
Cl ₂ H ₂ Lu ₂	723	0.0003	57	73
CCl ₂ Lu ₂	565	0.0003	49	64
Ho ₂ S ₂	356	0.0003	40	39
NbTe ₂	563	0.0003	64	81
CrO ₂	47	0.0004	4	9
I ₂ Pb	597	0.0004	81	64
Ca ₂ N	437	0.0004	49	64
CdClHO	729	0.0004	73	91
CrSe ₂	488	0.0004	49	81
Hf ₂ I ₂ N ₂	911	0.0004	73	91
Br ₂ Zr ₂	376	0.0004	36	49
I ₄ Sr ₂	828	0.0004	114	43
Br ₂ HLa	9	0.0004	1	1
ClNZr	233	0.0004	25	36
Te ₂ V	386	0.0004	43	57
I ₂ La ₂ Sb	905	0.0005	100	81
In	433	0.0005	65	108
I ₂ Pr ₂ S ₂	789	0.0005	81	64
CCl ₂ Sc ₂	305	0.0005	25	36
Br ₂ Fe	437	0.0005	49	64
Cu ₂ Te ₂	827	0.0005	87	98
S ₂ Zr	563	0.0005	64	81
Ga ₂ S ₂	577	0.0006	57	73
Ag ₂ K ₂ Se ₂	613	0.0006	65	48
AgNO ₃	205	0.0006	25	16
I ₂ N ₂ Ti ₂	678	0.0006	60	63
Te ₄ W ₂	756	0.0006	84	56
Br ₂ Co	437	0.0006	49	64
Bi ₂ In ₂	914	0.0006	118	81
BH ₄ Li	11	0.0007	1	1
AgTe ₂	759	0.0007	81	118
Cl ₂ Hf ₂ N ₂	557	0.0007	43	57
OTl ₂	386	0.0007	43	57
AsSn ₂	705	0.0008	81	100
S ₂ Sn	563	0.0008	64	81
K	581	0.0008	100	81

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Li₂CuAs (P-6m2 (187))

Structural and electronic properties





Formula	Li ₂ CuAs
Spacegroup	P-6m2 (187)
Prototype	AsCuLi2
Parent 3D	Li ₄ Cu ₂ As ₂
Source DB	ICSD
DB ID	43938
DF2-C09 Binding energy [meV/ Å²]	62.71
RVV10 Binding energy [meV/ Å²]	62.23
Band gap (PBE) [eV]	0.0

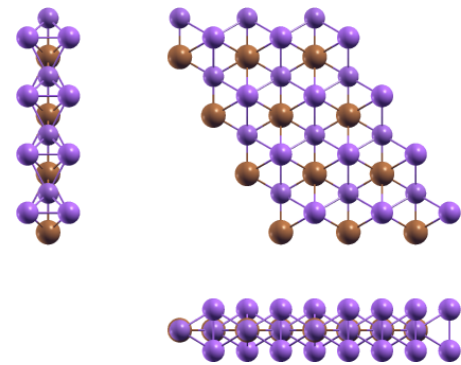


Band structure: Electronic band structure of Li₂CuAs (P-6m2 (187)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Li₂CuAs (P-6m2 (187)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]	
a₁	4.13307947	0.00000000	0.00000000	
a₂	−2.06653973	3.57935181	0.00000000	
a₃	0.00000000	0.00000000	22.61983425	
	x [Å]	y [Å]	z [Å]	
	Li	2.06653973	1.19311727	12.57669733
	Li	2.06653973	1.19311727	10.04313692
	Cu	0.00000000	0.00000000	11.30991713
	As	0.00000000	2.38623454	11.30991713



Orthographic projections: views of Li₂CuAs (P-6m2 (187)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.457	1	1
Na	5	1.5524	1	1
AgTl	6	0.1656	1	1
Ag ₂	6	0.4707	1	1
As ₂	6	0.2479	1	1
Sb ₂	6	0.0033	1	1
CaCl	6	0.1192	1	1
Cl ₂ Zn	7	0.2466	1	1
I ₂ Mg	7	0.0023	1	1
PSn ₂	7	0.2599	1	1
Ba ₂ Pt	7	0.4701	1	1
Br ₂ Zn	7	0.2753	1	1
HfS ₂	7	1.6312	1	1
AsSn ₂	7	0.2653	1	1
Te ₂ V	7	1.5828	1	1
I ₂ Pr	7	0.1474	1	1
S ₂ Zr	7	0.2589	1	1
Br ₂ La	7	0.0027	1	1
Ca ₂ Si	7	0.4816	1	1
Br ₂ Co	7	0.2474	1	1
Ca ₂ N	7	0.2486	1	1
BrCdI	7	0.0055	1	1
Cl ₂ Zn	7	0.128	1	1
Te ₂ Ti	7	0.2757	1	1
I ₂ Zn	7	0.0065	1	1
BaF ₂	7	0.0089	1	1
RhTe ₂	7	0.2693	1	1
GeI ₂	7	0.0005	1	1
Br ₂ Mn	7	1.5941	1	1
PtS ₂	7	1.5598	1	1
CoTe ₂	7	1.6337	1	1
Se ₂ Ti	7	1.5408	1	1
AsKSn	7	0.0075	1	1
PbTe ₂	7	0.0045	1	1
I ₂ Nd	7	0.1483	1	1
S ₂ Sn	7	0.2592	1	1
SnTe ₂	7	0.0018	1	1
Sn	7	0.6351	1	3
Cl ₂ V	7	4.8749	1	1
I ₂ Pb	7	0.4747	1	1
PtSe ₂	7	0.2662	1	1
OTl ₂	7	1.5806	1	1
Br ₂ Fe	7	0.2475	1	1
GeS ₂	7	0.1136	1	1
TaTe ₂	7	0.2644	1	1
MnSe ₂	7	0.1192	1	1
Br ₂ Ni	7	0.2542	1	1
CeI ₂	7	0.1467	1	1
CuO ₂	7	0.1754	1	1
NbTe ₂	7	0.2586	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

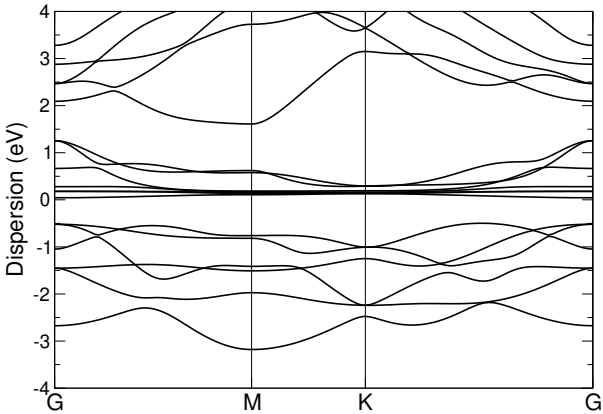
Formula	N° atoms	strain	cell size 1	cell size 2
Cl ₂ V	439	0.0	49	81
S ₂ Sn	499	0.0	64	81
Cl ₂ Zr ₂	244	0.0001	25	36
TaTe ₂	565	0.0001	73	91
Br ₂ Hf ₂ N ₂	580	0.0001	49	64
I ₂ Pr ₂ Si ₂	10	0.0002	1	1
Br ₂ Mn	343	0.0002	43	57
HgI ₂	404	0.0002	65	48
Ga ₂ Te ₂	8	0.0003	1	1
Ba ₂ Ni ₃	9	0.0003	1	1
AgNO ₃	180	0.0003	25	16
S ₂ Zr	499	0.0003	64	81
CCl ₂ Sc ₂	280	0.0003	25	36
ReS ₂	84	0.0004	9	16
CdClHO	724	0.0004	81	100
In	368	0.0004	65	108
Br ₂ HLa	8	0.0005	1	1
PSn ₂	499	0.0005	64	81
GeI ₂	7	0.0005	1	1
Hf ₂ I ₂ N ₂	838	0.0005	73	91
CdClHO	656	0.0005	73	91
Ca ₂ N	388	0.0005	49	64
I ₂ Pb	516	0.0005	81	64
NbTe ₂	499	0.0005	64	81
Cl ₂ H ₂ Lu ₂	666	0.0006	57	73
Ho ₂ S ₂	316	0.0006	40	39
Te ₄ W ₂	672	0.0006	84	56
Ce ₂ I ₂ S ₂	634	0.0006	73	57
Ca ₂ Si	463	0.0006	73	57
CrSe ₂	331	0.0006	37	61
CoH ₂ O ₂	116	0.0006	9	16
KS ₂ Ti	400	0.0006	43	57
Cl ₂ V	331	0.0006	37	61
AsSn ₂	565	0.0007	73	91
Cl ₂ N ₂ Zr ₂	580	0.0007	49	64
I ₂ Nd ₂ S ₂	802	0.0007	91	73
Br ₂ H ₂ Zr ₂	316	0.0007	25	36
Se ₂ Yb	7	0.0007	1	1
Na	193	0.0008	36	49
ClH ₃ O	443	0.0008	57	43
AgTe ₂	678	0.0008	81	118
CeLi ₂ P ₂	9	0.0008	1	1
Se ₂ Ti	291	0.0008	36	49
Br ₂ V	208	0.0009	25	36
AgBrO ₂	332	0.0009	41	42
Cl ₂ Mg	447	0.0009	57	73
Au ₂ I ₂	744	0.0009	105	81
Sb ₂ Te ₂	580	0.0009	81	64
CaH ₂ O ₂	516	0.0009	49	64
Br ₂ Ni	447	0.0009	57	73

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Li₂NdAs₂ (P-3m1 (164))

Structural and electronic properties

	Formula	Li ₂ NdAs ₂
	Spacegroup	P-3m1 (164)
	Prototype	Bi ₂ Te ₂ S
	Parent 3D	Li ₂ NdAs ₂
	Source DB	ICSD
	DB ID	23261
DF2-C09	Binding energy [meV/ Å²]	54.65
RVV10	Binding energy [meV/ Å²]	57.96
	Band gap (PBE) [eV]	0.0

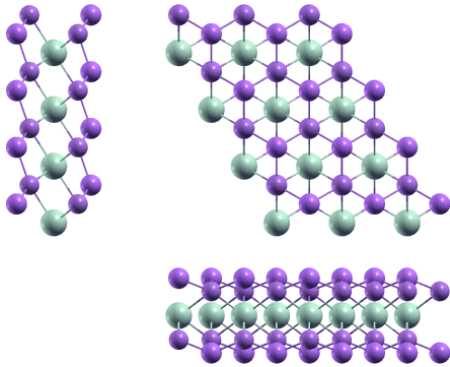


Band structure: Electronic band structure of Li₂NdAs₂ (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Li₂NdAs₂ (P-3m1 (164)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.23909886	0.00000000	0.00000000
a₂	−2.11954943	3.67116730	0.00000000
a₃	0.00000000	0.00000000	25.17297087
	x [Å]	y [Å]	z [Å]
● Li	2.11954943	1.22372243	15.00123422
● As	0.00000000	2.44744487	14.15938130
● Li	0.00000000	2.44744487	10.17173665
● Nd	0.00000000	0.00000000	12.58648543
● As	2.11954943	1.22372243	11.01358957



Orthographic projections: views of Li₂NdAs₂ (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
InSe	7	0.0007	1	1
AsSb	7	0.2727	1	1
Bi ₂	7	0.0065	1	1
AgTl	7	0.1531	1	1
As ₂	7	1.5238	1	1
PbTe	7	0.0024	1	1
CaCl	7	0.1137	1	1
CdI ₂	8	0.0042	1	1
PSn ₂	8	1.5881	1	1
Br ₂ Zn	8	0.2581	1	1
Br ₂ Ca	8	0.0054	1	1
HfS ₂	8	1.5433	1	1
AsSn ₂	8	0.2489	1	1
SiTe ₂	8	0.2639	1	1
I ₂ Pr	8	0.137	1	1
S ₂ Zr	8	1.5825	1	1
Br ₂ La	8	0.0091	1	1
Br ₂ Cu	8	0.7206	1	1
NSr ₂	8	0.2751	1	1
Ca ₂ Si	8	0.4515	1	1
PbS ₂	8	0.2689	1	1
Br ₂ Co	8	1.5208	1	1
BiClTe	8	0.0045	1	1
Ca ₂ N	8	1.5275	1	1
BrCdI	8	0.0064	1	1
Cl ₂ Zn	8	0.1206	1	1
HgI ₂	8	0.2096	1	1
Te ₂ Ti	8	0.2586	1	1
BaF ₂	8	0.0031	1	1
RhTe ₂	8	1.6374	1	1
CoTe ₂	8	1.5456	1	1
AsKSn	8	0.0046	1	1
PbTe ₂	8	0.0073	1	1
I ₂ Nd	8	0.1378	1	1
NiTe ₂	8	0.2631	1	1
Cl ₂ Cu	8	0.0673	1	1
S ₂ Sn	8	1.5845	1	1
I ₂ V	8	0.2658	1	1
GeI ₂	8	0.0027	1	1
Se ₂ Zr	8	0.2645	1	1
STl ₂	8	0.0022	1	1
PtSe ₂	8	0.2497	1	1
CoI ₂	8	0.2734	1	1
Br ₂ Fe	8	1.5212	1	1
GeS ₂	8	0.4344	1	1
TaTe ₂	8	0.2481	1	1
MnSe ₂	8	0.1137	1	1
Br ₂ Ni	8	1.5576	1	1
CeI ₂	8	0.1364	1	1
I ₂ Ti	8	0.2739	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

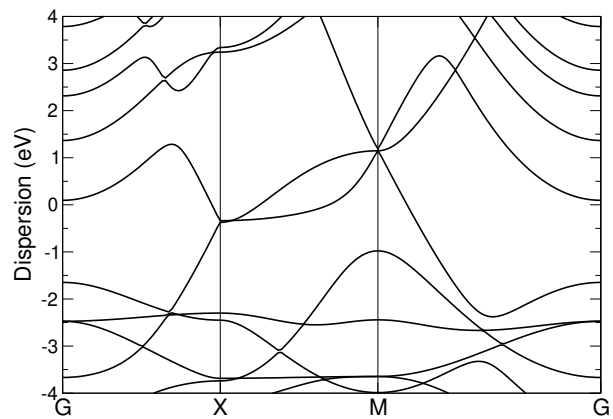
Formula	N° atoms	strain	cell size 1	cell size 2
Ga ₂ Se ₂	577	0.0	57	73
Ga ₂ S ₂	376	0.0	36	49
Cl ₂ Er ₂ O ₂	911	0.0	73	91
Br ₂ Zr ₂	269	0.0001	25	36
FeH ₂ O ₂	370	0.0001	25	49
Se ₂ Zr	638	0.0001	73	91
Bi ₂ Te ₂	593	0.0002	73	57
CoTe ₂	327	0.0002	36	49
Br ₂ O ₂ Ti ₂	470	0.0002	40	45
GeI ₂ Y ₂	10	0.0002	1	1
ClH ₃ O	725	0.0003	81	64
AsSn ₂	437	0.0003	49	64
SiTe ₂	638	0.0003	73	91
NiO ₂	47	0.0003	4	9
Ga ₂ Se ₂	805	0.0003	81	100
Br ₂ Pr ₂	644	0.0004	64	81
PtSe ₂	437	0.0004	49	64
S ₂ V	93	0.0004	9	16
Se ₂ Ti	233	0.0005	25	36
Br ₃ Cs	420	0.0005	64	25
HfS ₂	327	0.0005	36	49
H ₂ MgO ₂	125	0.0005	9	16
HfSe ₂	563	0.0005	64	81
Te ₂ Ti	563	0.0005	64	81
PSn ₂	386	0.0006	43	57
Ho ₂ S ₂	355	0.0006	39	40
Ba ₂ H ₂ I ₂	613	0.0006	65	48
I ₂ La ₂ Si ₂	11	0.0006	1	1
As ₂ Li ₂ Pr	10	0.0006	1	1
InSe	7	0.0007	1	1
HN ₃ OZn	731	0.0007	49	81
F ₂ Se ₂ Y ₂	614	0.0007	64	49
Sn ₂ Te ₂	599	0.0007	75	56
Bi ₂ Se ₂ Te	10	0.0007	1	1
Br ₂ Y ₂	805	0.0007	81	100
Cl ₂ Y ₂	577	0.0007	57	73
Mg ₂	541	0.0007	65	108
Cl ₂ Hg ₂ N ₂	385	0.0008	47	25
HNiO ₂	645	0.0008	49	100
C ₂ Br ₂ Gd ₂	962	0.0008	82	92
Br ₂ Zn	563	0.0008	64	81
CoO ₂	47	0.0008	4	9
Cl ₂ Hf ₂	180	0.0009	16	25
CuTe ₂	327	0.0009	36	49
TaTe ₂	437	0.0009	49	64
Al ₂ Cl ₂ O ₂	39	0.0009	3	4
NiTe ₂	638	0.0009	73	91
C ₂ Br ₂ Tb ₂	962	0.0009	82	92
Cu ₂ O ₂	355	0.0009	39	40
PbS ₂	705	0.0009	81	100

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Li₂PdH₂ (P4/mmm (123))

Structural and electronic properties

Formula	Li ₂ PdH ₂
Spacegroup	P4/mmm (123)
Prototype	Na ₂ HgO ₂
Parent 3D	Li ₂ PdH ₂
Source DB	ICSD
DB ID	108534
DF2-C09 Binding energy [meV/ Å²]	52.71
RVV10 Binding energy [meV/ Å²]	58.91
Band gap (PBE) [eV]	0.0

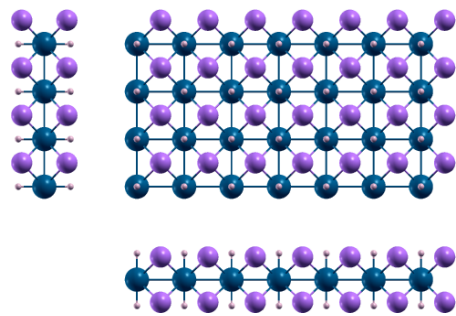


Band structure: Electronic band structure of Li₂PdH₂ (P4/mmm (123)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Li₂PdH₂ (P4/mmm (123)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.06832162	0.00000000	0.00000000
a₂		0.00000000	3.06832162	0.00000000
a₃		0.00000000	0.00000000	23.38431440
		x [Å]	y [Å]	z [Å]
•	H	0.00000000	0.00000000	9.99905899
●	Li	1.53416081	1.53416081	13.15550065
●	Li	1.53416081	1.53416081	10.22881376
•	H	0.00000000	0.00000000	13.38525541
●	Pd	0.00000000	0.00000000	11.69215720



Orthographic projections: views of Li₂PdH₂ (P4/mmm (123)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	6	0.1439	1	1
Na	6	0.1765	1	1
As ₂	7	0.1864	1	1
LiO	7	0.1333	1	1
BN	7	0.1109	1	1
P ₂	7	0.1393	1	1
Mg ₂	7	0.0019	1	1
Cl ₂ Zn	8	0.185	1	1
Cl ₂ Mn	8	0.1491	1	1
MoTe ₂	8	0.1793	1	1
PSn ₂	8	0.7533	1	1
MoSe ₂	8	0.1432	1	1
ReSe ₂	8	0.1624	1	1
S ₂ Ta	8	0.1511	1	1
HfS ₂	8	0.1899	1	1
AsSn ₂	8	0.7677	1	1
Te ₂ V	8	0.1816	1	1
CuTe ₂	8	0.1894	1	1
S ₂ Zr	8	0.1971	1	1
Br ₂ Co	8	0.1858	1	1
Ca ₂ N	8	0.187	1	1
Cl ₂ Ti	8	0.1395	1	1
S ₂ Ti	8	0.1561	1	1
Mg ₃	8	0.0086	1	1
NbS ₂	8	0.1507	1	1
Te ₂ Zn	8	0.1791	1	1
RhTe ₂	8	0.7785	1	1
Br ₂ Mn	8	0.1835	1	1
Cl ₂ Ni	8	0.1634	1	1
Cl ₂ Co	8	0.1557	1	1
CrTe ₂	8	0.1702	1	1
PtS ₂	8	0.1778	1	1
NbS ₂	8	0.1466	1	1
CoTe ₂	8	0.1903	1	1
Br ₂ V	8	0.1616	1	1
ClN ₂ Zr	8	0.1593	1	1
Cl ₂ Fe	8	0.155	1	1
CdClO	8	0.181	1	1
S ₂ Ta	8	0.1458	1	1
Se ₂ V	8	0.1446	1	1
Se ₂ Ti	8	0.1746	1	1
Br ₂ Ti	8	0.1696	1	1
Te ₂ W	8	0.1795	1	1
AsSe ₂	8	0.165	1	1
S ₂ Sn	8	0.1974	1	1
Cl ₂ V	8	0.1314	1	1
PtSe ₂	8	0.7701	1	1
OTl ₂	8	0.1813	1	1
CdO ₂	8	0.1556	1	1
BrN ₂ Zr	8	0.1665	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

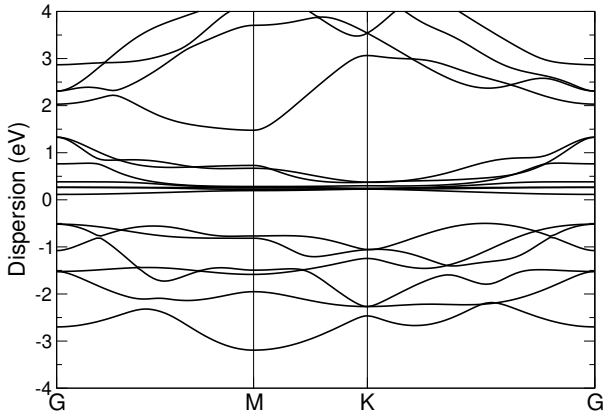
Formula	N° atoms	strain	cell size 1	cell size 2
Cu ₂ I ₂	116	0.0001	16	9
I ₂ S ₂ Tl ₂	330	0.0002	36	25
F ₂ Ni	255	0.0002	36	25
Si ₂ Te ₂ Zr ₂	330	0.0002	36	25
GeS ₂	467	0.0003	64	49
AsLi ₃	800	0.0003	108	65
Ge ₂ Mn ₂ Sr ₂	833	0.0003	97	58
Br ₂ Ho ₂ O ₂	221	0.0004	25	16
H ₂ I ₂ Yb ₂	699	0.0004	81	49
Cu ₂ Se ₂	280	0.0004	36	25
H ₂ I ₂ Sr ₂	395	0.0004	49	25
Br ₂ Nd ₂ O ₂	699	0.0004	81	49
Bi ₂ STe ₂	865	0.0004	108	65
H ₂ Na ₂ Pd	565	0.0005	64	49
I ₂ Nd	725	0.0005	106	65
Br ₂ H ₂ Sr ₂	134	0.0005	16	9
H ₄ Ti	10	0.0005	1	1
Ca ₂ Mn ₂ Si ₂	221	0.0005	25	16
I ₂ O ₂ Tm ₂	920	0.0005	106	65
Br ₂ O ₂ Sm ₂	920	0.0006	106	65
InSe	670	0.0006	108	65
As ₂ Li ₂ Pr	865	0.0006	108	65
Ge ₂ Se ₂	455	0.0006	63	35
I ₂ O ₂ Y ₂	699	0.0006	81	49
Fe ₂ S ₂	389	0.0006	49	36
I ₂ La ₂ Si ₂	930	0.0006	108	65
Ba ₂ H ₂ I ₂	69	0.0006	9	4
Cl ₂ ORu	330	0.0007	42	30
F ₄ Pb	810	0.0007	109	53
Ir ₂ P ₂	790	0.0007	106	65
Fe ₂ Se ₂	280	0.0007	36	25
Br ₂ O ₂ Pr ₂	833	0.0007	97	58
Ge ₂ S ₂	440	0.0008	60	35
Ba ₂ N	833	0.0008	118	81
Br ₂ Ca ₂ H ₂	221	0.0008	25	16
Cu ₂ Se ₂ Tl ₂	134	0.0008	16	9
P ₂ Rh ₂	189	0.0008	25	16
Te ₂ Zr	833	0.0009	118	81
Br ₂ OV	887	0.0009	111	83
DyI ₂	865	0.0009	131	70
F ₂ Tl ₂	189	0.0009	25	16
I ₂ La	552	0.001	81	49
Se ₂ Sn ₂	490	0.001	70	35
I ₂ S ₂ Tb ₂	647	0.0011	79	42
I ₂ O ₂ Yb ₂	920	0.0011	106	65
Cl ₂ S ₂ Tl ₂	649	0.0011	89	34
As ₂ Fe ₂	516	0.0012	64	49
As ₂ Ir ₂	717	0.0012	97	58
Sm	521	0.0012	79	126
Ag ₂ Br ₂	717	0.0012	97	58

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Li₂PrAs₂ (P-3m1 (164))

Structural and electronic properties

	Formula	Li ₂ PrAs ₂
	Spacegroup	P-3m1 (164)
	Prototype	Bi ₂ Te ₂ S
	Parent 3D	Li ₂ PrAs ₂
	Source DB	ICSD
	DB ID	23260
DF2-C09	Binding energy [meV/ Å²]	54.58
RVV10	Binding energy [meV/ Å²]	57.87
	Band gap (PBE) [eV]	0.0

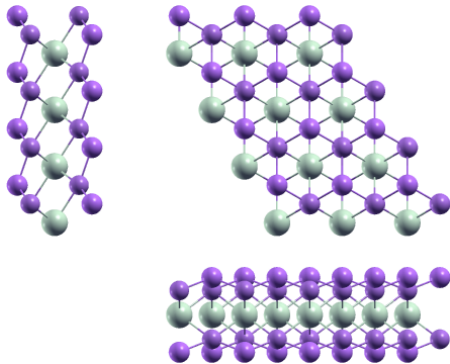


Band structure: Electronic band structure of Li₂PrAs₂ (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Li₂PrAs₂ (P-3m1 (164)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.24489199	0.00000000	0.00000000
a₂	−2.12244599	3.67618430	0.00000000
a₃	0.00000000	0.00000000	25.19146257
	x [Å]	y [Å]	z [Å]
●	Li	2.12244599	1.22539477
●	As	0.00000000	2.45078953
●	Li	0.00000000	2.45078953
●	Pr	0.00000000	12.59573128
●	As	2.12244599	1.22539477



Orthographic projections: views of Li₂PrAs₂ (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
InSe	7	0.0	1	1
AsSb	7	0.2718	1	1
Bi ₂	7	0.0059	1	1
AgTl	7	0.1525	1	1
PbTe	7	0.0018	1	1
CaCl	7	0.1134	1	1
CdI ₂	8	0.0035	1	1
PSn ₂	8	1.5834	1	1
Br ₂ Zn	8	0.2573	1	1
Br ₂ Ca	8	0.0048	1	1
HfS ₂	8	1.5387	1	1
AsSn ₂	8	0.248	1	1
SiTe ₂	8	0.263	1	1
I ₂ Pr	8	0.1365	1	1
Br ₂ Cu	8	0.7183	1	1
NSr ₂	8	0.2742	1	1
Ca ₂ Si	8	0.4499	1	1
PbS ₂	8	0.268	1	1
BiClTe	8	0.0039	1	1
Ca ₂ N	8	1.523	1	1
BrCdI	8	0.007	1	1
Cl ₂ Zn	8	0.1202	1	1
HgI ₂	8	0.2087	1	1
Te ₂ Ti	8	0.2577	1	1
CrI ₂	8	0.2754	1	1
BaF ₂	8	0.0038	1	1
BiBrTe	8	0.0096	1	1
RhTe ₂	8	1.6325	1	1
CoTe ₂	8	1.541	1	1
AsKSn	8	0.0052	1	1
PbTe ₂	8	0.008	1	1
I ₂ Nd	8	0.1373	1	1
NiTe ₂	8	0.2622	1	1
Cl ₂ Cu	8	0.0675	1	1
I ₂ V	8	0.2649	1	1
GeI ₂	8	0.002	1	1
Se ₂ Zr	8	0.2636	1	1
STl ₂	8	0.0028	1	1
PtSe ₂	8	0.2489	1	1
CoI ₂	8	0.2724	1	1
GeS ₂	8	0.4329	1	1
TaTe ₂	8	0.2473	1	1
MnSe ₂	8	0.1134	1	1
Br ₂ Ni	8	1.5529	1	1
CeI ₂	8	0.1359	1	1
Br ₂ Mg	8	0.2759	1	1
I ₂ Ti	8	0.2729	1	1
Cl ₂ Mg	8	1.5533	1	1
F ₂ Ni	8	0.1181	1	1
I ₂ La	8	0.1412	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

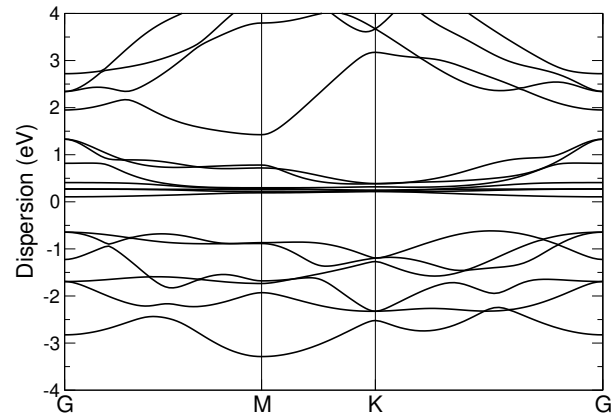
Formula	N° atoms	strain	cell size 1	cell size 2
InSe	7	0.0	1	1
F ₂ Se ₂ Y ₂	614	0.0	64	49
I ₂ La ₂ Si ₂	11	0.0	1	1
Br ₂ Y ₂	805	0.0	81	100
Cl ₂ Y ₂	577	0.0001	57	73
HNiO ₂	645	0.0001	49	100
Se ₂ Ti	233	0.0002	25	36
Ba ₂ H ₂ I ₂	613	0.0002	65	48
S ₂ V	93	0.0003	9	16
PbS ₂	705	0.0003	81	100
PtSe ₂	437	0.0003	49	64
Br ₂ Pr ₂	644	0.0003	64	81
Ga ₂ Se ₂	805	0.0003	81	100
AsLi ₃	9	0.0003	1	1
Ga ₂ S ₂	376	0.0004	36	49
I ₂ V	638	0.0004	73	91
Cl ₂ O ₂ Yb ₂	806	0.0004	64	81
MoS ₂	93	0.0005	9	16
Bi ₂ Te ₂	593	0.0005	73	57
F ₂ Na	563	0.0005	64	81
Br ₂ O ₂ Ti ₂	470	0.0005	40	45
S ₂ W	93	0.0005	9	16
Se ₂ Zr	638	0.0005	73	91
Br ₂ Zr ₂	269	0.0005	25	36
H ₂ Li ₂ Pd	865	0.0006	65	108
CBr ₂ Y ₂	650	0.0006	57	73
C ₂ Br ₂ Gd ₂	962	0.0006	82	92
Ga ₂ Se ₂	577	0.0006	57	73
As ₂ Li ₂ Nd	10	0.0006	1	1
MoS ₂	93	0.0007	9	16
Ge ₂ Se ₂	791	0.0007	91	84
Ga ₂ S ₂	376	0.0007	36	49
Cl ₂ Er ₂ O ₂	911	0.0007	73	91
PTe ₂ Ti ₂	425	0.0007	36	49
Cl ₂ Ho ₂ O ₂	911	0.0008	73	91
FeH ₂ O ₂	370	0.0008	25	49
CoTe ₂	327	0.0008	36	49
Br ₂ Ni	327	0.0008	36	49
GeI ₂ Y ₂	10	0.0009	1	1
Cl ₂ Mg	327	0.0009	36	49
Te ₄ W ₂	785	0.0009	85	60
ClH ₃ O	725	0.0009	81	64
AsSn ₂	437	0.0009	49	64
SiTe ₂	638	0.0009	73	91
NiO ₂	47	0.001	4	9
Bi ₂ STe ₂	10	0.001	1	1
C ₂ Br ₂ Tb ₂	962	0.001	82	92
I ₂ Lu ₂ S ₂	765	0.001	81	60
Br ₂ Lu ₂ S ₂	673	0.0011	71	53
H ₄ Ti	865	0.0011	65	108

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Li₂PrP₂ (P-3m1 (164))

Structural and electronic properties

	Formula	Li ₂ PrP ₂
	Spacegroup	P-3m1 (164)
	Prototype	Bi ₂ Te ₂ S
	Parent 3D	Li ₂ PrP ₂
	Source DB	ICSD
	DB ID	23259
DF2-C09	Binding energy [meV/ Å²]	58.92
RVV10	Binding energy [meV/ Å²]	62.58
	Band gap (PBE) [eV]	0.0

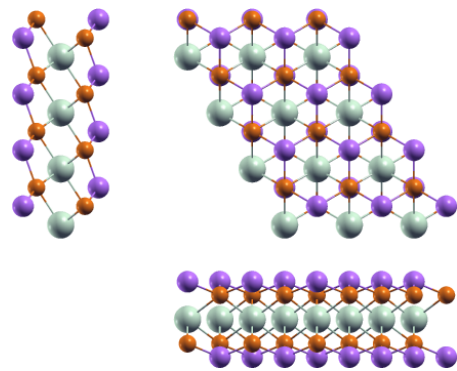


Band structure: Electronic band structure of Li₂PrP₂ (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Li₂PrP₂ (P-3m1 (164)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		4.10885777	0.00000000	0.00000000
a₂		-2.05442889	3.55837521	0.00000000
a₃		0.00000000	0.00000000	25.03930145
		x [Å]	y [Å]	z [Å]
●	Li	0.00000000	2.37225014	10.12629762
●	P	2.05442889	1.18612507	10.97799215
●	Li	2.05442889	1.18612507	14.91300383
●	Pr	0.00000000	0.00000000	12.51965073
●	P	0.00000000	2.37225014	14.06130930



Orthographic projections: views of Li₂PrP₂ (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	6	0.2062	1	1
K	6	0.4639	1	1
Ag ₂	7	0.4778	1	1
As ₂	7	1.6315	1	1
Sb ₂	7	0.0006	1	1
CaCl	7	0.1208	1	1
Cl ₂ Zn	8	0.2502	1	1
I ₂ Mg	8	0.0052	1	1
MoS ₂	8	4.8468	1	1
MoTe ₂	8	1.5891	1	1
PSn ₂	8	0.2638	1	1
Ba ₂ Pt	8	0.4771	1	1
HfS ₂	8	0.2553	1	1
AsSn ₂	8	0.2693	1	1
Te ₂ V	8	0.2466	1	1
I ₂ Pr	8	0.15	1	1
CuTe ₂	8	0.2548	1	1
S ₂ Zr	8	0.2628	1	1
Br ₂ La	8	0.0055	1	1
Ca ₂ Si	8	2.8378	1	1
Br ₂ Co	8	1.6283	1	1
Ca ₂ N	8	1.6355	1	1
AuTe ₂	8	0.0083	1	1
BrCdI	8	0.0084	1	1
Cl ₂ Zn	8	0.1299	1	1
I ₂ Zn	8	0.0038	1	1
RhTe ₂	8	0.2734	1	1
S ₂ W	8	4.8482	1	1
GeI ₂	8	0.0033	1	1
Br ₂ Mn	8	0.2486	1	1
CrTe ₂	8	1.5337	1	1
PtS ₂	8	1.58	1	1
CoTe ₂	8	0.2557	1	1
CdClO	8	1.5997	1	1
Se ₂ Ti	8	1.5608	1	1
Br ₂ Ti	8	1.5295	1	1
Te ₂ W	8	1.5903	1	1
PbTe ₂	8	0.0074	1	1
I ₂ Nd	8	0.1509	1	1
S ₂ Sn	8	0.2631	1	1
SnTe ₂	8	0.001	1	1
I ₂ Pb	8	0.4819	1	1
PtSe ₂	8	0.2702	1	1
OTl ₂	8	0.2462	1	1
Br ₂ Fe	8	1.6288	1	1
GeS ₂	8	0.1148	1	1
TaTe ₂	8	0.2684	1	1
MnSe ₂	8	0.1207	1	1
DyI ₂	8	0.4482	1	1
Br ₂ Ni	8	0.258	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

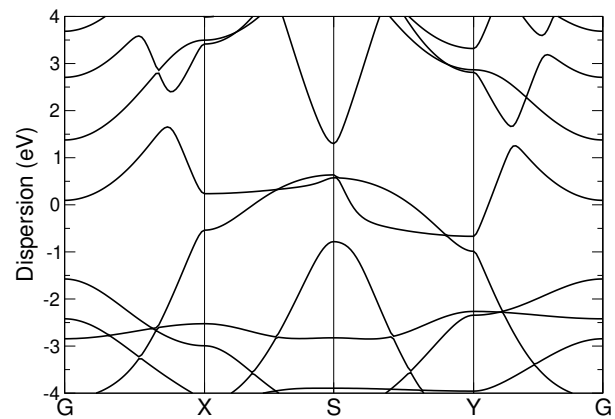
Formula	N° atoms	strain	cell size 1	cell size 2
CdClHO	805	0.0	81	100
H ₂ NiO ₂	650	0.0	49	81
KS ₂ Ti	501	0.0001	49	64
Ga ₂ Ge ₂ Te ₂	11	0.0001	1	1
C ₂	95	0.0001	9	25
KNO ₃	445	0.0001	64	25
HfS ₂	504	0.0001	57	73
CdH ₂ O ₂	500	0.0001	43	57
CS ₂ Ta ₂	205	0.0002	16	25
CoTe ₂	504	0.0002	57	73
Cl ₂ Ti	155	0.0002	16	25
Te ₂ W	386	0.0003	43	57
Ga ₂ S ₂	577	0.0003	57	73
PSn ₂	638	0.0003	73	91
P ₂	130	0.0004	16	25
Ba ₂ Pt	597	0.0004	81	64
MoTe ₂	386	0.0004	43	57
Br ₂ Mn	437	0.0005	49	64
CuTe ₂	504	0.0005	57	73
I ₂ Pb	536	0.0005	73	57
Bi ₂ Te ₂	389	0.0005	49	36
Ge ₂ Se ₂	567	0.0005	67	58
TaTe ₂	705	0.0006	81	100
Sb ₂	7	0.0006	1	1
H ₂ NiO ₂	490	0.0006	37	61
Cl ₂ H ₂ Lu ₂	806	0.0006	64	81
Te ₂ Zn	386	0.0006	43	57
Br ₂ CsF	914	0.0006	118	81
Ag ₂	533	0.0007	81	64
Cl ₂ Zn	437	0.0007	49	64
Cl ₂ Hg ₂ N ₂	240	0.0007	30	15
K ₂ PtSe ₂	265	0.0007	39	14
I ₂ S ₂ Sm ₂	986	0.0007	100	81
HN ₃ OZn	230	0.0008	16	25
P ₄	866	0.0008	98	94
Br ₂ La ₂	9	0.0008	1	1
I ₂ La ₂ Sb	820	0.0008	91	73
S ₂ Sn	638	0.0008	73	91
Sb ₂ Te ₂	593	0.0009	73	57
HfLiS ₂	443	0.0009	43	57
Cl ₂ Mg	563	0.0009	64	81
CNb ₂ S ₂	205	0.0009	16	25
CrSe ₂	368	0.0009	37	61
Tl	523	0.0009	81	118
CaH ₂ O ₂	650	0.001	57	73
Br ₂ Ni	563	0.001	64	81
Ag ₂ Te ₂	576	0.001	64	64
Br ₂ N ₂ Zr ₂	806	0.001	64	81
SnTe ₂	8	0.001	1	1
CdClO	386	0.001	43	57

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Li₂PtH₂ (Pmmm)

Structural and electronic properties

	Formula	Li ₂ PtH ₂
	Spacegroup	Pmmm
	Prototype	Na ₂ HgO ₂
	Parent 3D	H ₂ Li ₂ Pt
	Source DB	MPDS
	DB ID	S1708069
DF2-C09	Binding energy [meV/ Å²]	45.09
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

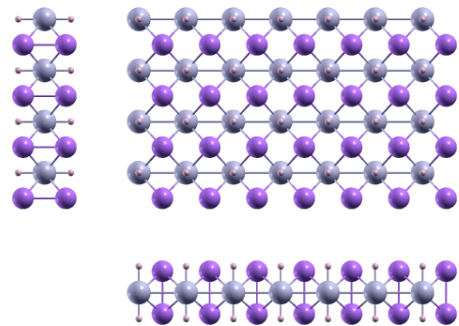


Band structure: Electronic band structure of Li₂PtH₂ (Pmmm) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Li₂PtH₂ (Pmmm) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.00653369	0.00000000	0.00000000
a₂		0.00000000	3.25656175	0.00000000
a₃		0.00000000	0.00000000	18.64870215
		x [Å]	y [Å]	z [Å]
●	Li	1.50326685	0.00000000	-1.36148272
•	H	0.00000000	-1.62828087	-1.67320320
●	Li	1.50326685	0.00000000	1.36148272
•	H	0.00000000	-1.62828087	1.67320320
●	Pt	0.00000000	-1.62828087	0.00000000



Orthographic projections: views of Li₂PtH₂ (Pmmm) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Na	6	0.168	1	1
In	6	0.0271	1	1
HgO	7	0.0274	1	1
AsSb	7	0.217	1	1
Sn	7	0.5884	1	2
Mg ₂	7	0.0207	1	1
Cl ₂ Zn	8	0.6497	1	1
S ₂ V	8	0.1237	1	1
MoS ₂	8	0.1242	1	1
CdCl ₂	8	0.2245	1	1
MoTe ₂	8	0.6344	1	1
PSn ₂	8	0.1882	1	1
Br ₂ Zn	8	0.2024	1	1
HfS ₂	8	0.6623	1	1
AsSn ₂	8	0.1931	1	1
GeTe ₂	8	0.223	1	1
SiTe ₂	8	0.2082	1	1
Te ₂ V	8	0.1728	1	1
I ₂ Mn	8	0.2247	1	1
S ₂ Zr	8	0.1873	1	1
NSr ₂	8	0.2194	1	1
PbS ₂	8	0.2132	1	1
Br ₂ Co	8	0.6517	1	1
FeI ₂	8	0.2213	1	1
I ₂ Ni	8	0.2233	1	1
Te ₂ Ti	8	0.2028	1	1
CrI ₂	8	0.2207	1	1
Te ₂ Zn	8	0.6339	1	1
RhTe ₂	8	0.1969	1	1
S ₂ W	8	0.1242	1	1
Bi ₂ Pd	8	0.036	1	1
Br ₂ Mn	8	0.6457	1	1
PtS ₂	8	0.6304	1	1
CoTe ₂	8	0.6634	1	1
CdClO	8	0.1722	1	1
Se ₂ Ti	8	0.1662	1	1
Te ₂ W	8	0.635	1	1
NiTe ₂	8	0.2073	1	1
S ₂ Sn	8	0.1876	1	1
I ₂ V	8	0.2101	1	1
Cl ₂ V	8	0.1267	1	1
Se ₂ Zr	8	0.2088	1	1
PtSe ₂	8	0.194	1	1
OTl ₂	8	0.1724	1	1
CoI ₂	8	0.2177	1	1
Br ₂ Fe	8	0.6519	1	1
TaTe ₂	8	0.1924	1	1
Br ₂ Ni	8	0.183	1	1
FeSe ₂	8	0.2534	1	1
Br ₂ Mg	8	0.2211	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

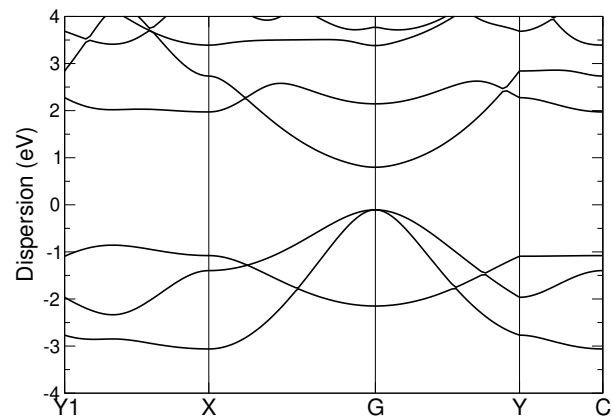
Formula	N° atoms	strain	cell size 1	cell size 2
Bi ₂	498	0.0002	80	49
CCl ₂ Gd ₂	90	0.0002	10	8
NbS ₂	643	0.0002	80	81
Cl ₂ Hf ₂	725	0.0003	81	80
Br ₂ Zn	74	0.0003	10	8
Ga ₂ Gd ₂ I ₂	694	0.0003	80	49
NS ₂ Ta	80	0.0004	8	10
Tl	735	0.0004	122	125
BiBrTe	926	0.0004	136	82
I ₂ La ₂ O ₂	697	0.0004	83	47
Cl ₂ H ₂ Zr ₂	886	0.0004	80	81
CBr ₂ Y ₂	90	0.0004	10	8
Te ₂ Ti	74	0.0006	10	8
BN	172	0.0006	20	36
Ga ₂ I ₂ Tb ₂	694	0.0006	80	49
HfSe ₂	74	0.0006	10	8
Hg ₃ S ₂	515	0.0007	86	17
Bi ₂ SeTe ₂	645	0.0007	80	49
S ₂ Ta	643	0.0007	80	81
Ge ₂ I ₂ La ₂	778	0.0007	92	53
Se ₂ W	985	0.0008	122	125
Se ₂ V	985	0.0008	122	125
LiNbS ₂	725	0.0009	81	80
Au ₂ I ₂	872	0.0009	124	63
MoSe ₂	985	0.0009	122	125
S ₂ Ta	645	0.001	81	80
Br ₂ Ca	547	0.001	80	49
Cl ₂ Y ₂	82	0.001	10	8
Cl ₂ Mn	928	0.001	116	116
LiO	602	0.0011	84	91
Cl ₂ OOs	380	0.0011	48	35
Co ₂ S ₂	489	0.0011	61	46
CaCl	397	0.0012	61	46
Si ₂ Te ₂ Zr ₂	878	0.0012	94	68
STl ₂	435	0.0012	63	40
F ₂ Ni	674	0.0012	94	68
PbS ₂ Sn	901	0.0012	125	69
MnSe ₂	443	0.0012	61	46
Fe ₂ Se ₂	742	0.0012	94	68
Co ₂ S ₂	480	0.0013	60	45
Br ₂ O ₂ Ti ₂	417	0.0013	45	32
Cu ₂ F ₄	715	0.0013	101	35
I ₂ S ₂ Tl ₂	878	0.0013	94	68
Ho ₂ I ₂ Se ₂	783	0.0013	105	43
CrSe ₂	744	0.0013	90	98
LiOS ₂ Ti	805	0.0013	80	81
Cd ₂ I ₃	725	0.0013	92	53
AsI ₂ La ₂	725	0.0014	92	53
Fe ₂ S ₂	539	0.0014	67	51
NbS ₂	645	0.0014	81	80

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Li₃As (P-6m2)

Structural and electronic properties

	Formula	Li ₃ As
	Spacegroup	P-6m2
	Prototype	AsLi3
	Parent 3D	As ₂ Li ₆
	Source DB	COD
	DB ID	1010288
DF2-C09	Binding energy [meV/ Å²]	70.26
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.9

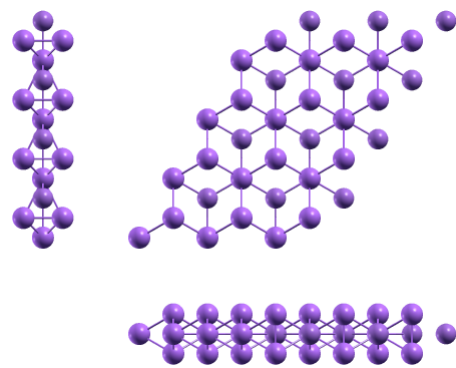


Band structure: Electronic band structure of Li₃As (P-6m2) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Li₃As (P-6m2) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		2.12389248	−3.67868969	0.00000000
a₂		4.24778497	0.00000000	0.00000000
a₃		0.00000000	0.00000000	17.17840741
		x [Å]	y [Å]	z [Å]
●	Li	0.00000000	0.00000000	0.00000000
●	Li	−2.12389248	−1.22622990	−1.22039591
●	Li	−2.12389248	−1.22622990	1.22039591
●	As	−0.00000000	−2.45245979	0.00000000



Orthographic projections: views of Li₃As (P-6m2) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
InSe	6	0.0003	1	1
AsSb	6	0.2713	1	1
Bi ₂	6	0.0055	1	1
AgTl	6	0.1522	1	1
PbTe	6	0.0015	1	1
CaCl	6	0.1133	1	1
CdI ₂	7	0.0032	1	1
PSn ₂	7	1.581	1	1
Br ₂ Zn	7	0.2568	1	1
Br ₂ Ca	7	0.0044	1	1
HfS ₂	7	1.5364	1	1
AsSn ₂	7	0.2476	1	1
SiTe ₂	7	0.2625	1	1
I ₂ Pr	7	0.1362	1	1
Br ₂ Cu	7	0.7171	1	1
NSr ₂	7	0.2737	1	1
Ca ₂ Si	7	0.4492	1	1
PbS ₂	7	0.2675	1	1
BiClTe	7	0.0036	1	1
Ca ₂ N	7	1.5207	1	1
BrCdI	7	0.0073	1	1
Cl ₂ Zn	7	0.1201	1	1
FeI ₂	7	0.2756	1	1
HgI ₂	7	0.2082	1	1
Te ₂ Ti	7	0.2572	1	1
CrI ₂	7	0.2749	1	1
BaF ₂	7	0.0041	1	1
BiBrTe	7	0.0092	1	1
RhTe ₂	7	1.6301	1	1
CoTe ₂	7	1.5387	1	1
AsKSn	7	0.0055	1	1
PbTe ₂	7	0.0083	1	1
I ₂ Nd	7	0.137	1	1
NiTe ₂	7	0.2617	1	1
Cl ₂ Cu	7	0.0676	1	1
I ₂ V	7	0.2644	1	1
GeI ₂	7	0.0017	1	1
Se ₂ Zr	7	0.2631	1	1
STl ₂	7	0.0032	1	1
PtSe ₂	7	0.2485	1	1
CoI ₂	7	0.2719	1	1
GeS ₂	7	0.4322	1	1
TaTe ₂	7	0.2469	1	1
MnSe ₂	7	0.1133	1	1
Br ₂ Ni	7	1.5506	1	1
CeI ₂	7	0.1356	1	1
Br ₂ Mg	7	0.2754	1	1
I ₂ Ti	7	0.2724	1	1
Cl ₂ Mg	7	1.551	1	1
F ₂ Ni	7	0.118	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

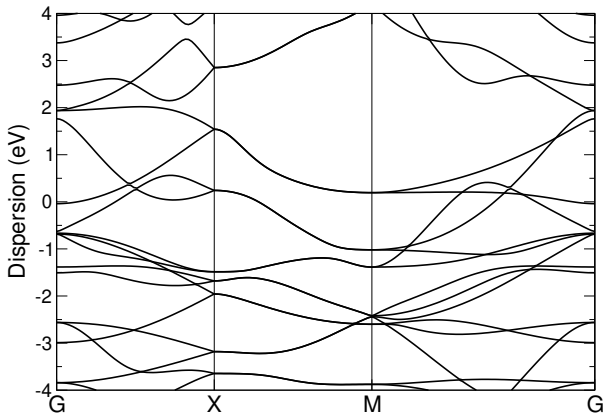
Formula	N° atoms	strain	cell size 1	cell size 2
PbS ₂	624	0.0	81	100
Ga ₂ S ₂	340	0.0	36	49
I ₂ V	565	0.0001	73	91
Cl ₂ O ₂ Yb ₂	742	0.0001	64	81
MoS ₂	84	0.0001	9	16
F ₂ Na	499	0.0002	64	81
HNiO ₂	596	0.0002	49	100
S ₂ W	84	0.0002	9	16
Cl ₂ Y ₂	520	0.0002	57	73
Br ₂ Y ₂	724	0.0003	81	100
F ₂ Se ₂ Y ₂	550	0.0003	64	49
CBr ₂ Y ₂	593	0.0003	57	73
InSe	6	0.0003	1	1
H ₂ Li ₂ Pd	800	0.0003	65	108
As ₂ Li ₂ Pr	9	0.0003	1	1
MoS ₂	84	0.0003	9	16
I ₂ La ₂ Si ₂	10	0.0004	1	1
PTe ₂ Ti ₂	389	0.0004	36	49
Cl ₂ Ho ₂ O ₂	838	0.0004	73	91
Ba ₂ H ₂ I ₂	548	0.0004	65	48
Se ₂ Ti	208	0.0005	25	36
Br ₂ Ni	291	0.0005	36	49
Cl ₂ Mg	291	0.0006	36	49
S ₂ V	84	0.0006	9	16
PtSe ₂	388	0.0006	49	64
Br ₂ Pr ₂	580	0.0006	64	81
Ga ₂ Se ₂	724	0.0006	81	100
Ag ₂ K ₂ Te ₂	958	0.0006	118	81
Bi ₂ STe ₂	9	0.0006	1	1
Ge ₂ Se ₂	700	0.0007	91	84
I ₂ Lu ₂ S ₂	684	0.0007	81	60
C ₂ Br ₂ Gd ₂	880	0.0008	82	92
Te ₄ W ₂	700	0.0008	85	60
CdClHO	452	0.0008	49	64
H ₄ Ti	800	0.0008	65	108
Bi ₂ Te ₂	520	0.0008	73	57
Br ₂ O ₂ Ti ₂	430	0.0008	40	45
Se ₂ Zr	565	0.0008	73	91
Br ₂ Zr ₂	244	0.0009	25	36
Cl ₂ N ₂ Zr ₂	468	0.0009	45	48
CCL ₂ Gd ₂	593	0.0009	57	73
Cl ₂ H ₂ Lu ₂	438	0.0009	36	49
Cl ₂ Fe	139	0.0009	16	25
Ga ₂ Se ₂	520	0.001	57	73
As ₂ Li ₂ Nd	9	0.001	1	1
Cl ₂ O ₂ Tm ₂	742	0.001	64	81
Br ₂ Zn	447	0.001	57	73
Ga ₂ S ₂	340	0.001	36	49
Br ₂ S ₂ Yb ₂	766	0.001	91	67
Cl ₂ Er ₂ O ₂	838	0.001	73	91

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

LiCoAs (P4/nmm (129))

Structural and electronic properties

	Formula	LiCoAs
	Spacegroup	P4/nmm (129)
	Prototype	PbClF
	Parent 3D	Li ₂ Co ₂ As ₂
	Source DB	ICSD
	DB ID	107932
DF2-C09	Binding energy [meV/ Å²]	66.25
RVV10	Binding energy [meV/ Å²]	67.87
	Band gap (PBE) [eV]	0.0

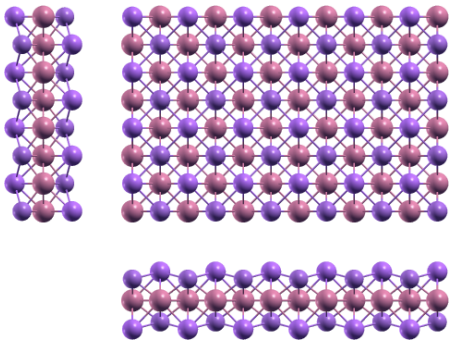


Band structure: Electronic band structure of LiCoAs (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of LiCoAs (P4/nmm (129)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.73582604	0.00000000	0.00000000
a₂		0.00000000	3.73582604	0.00000000
a₃		0.00000000	0.00000000	24.01705966
		x [Å]	y [Å]	z [Å]
●	Li	0.00000000	1.86791302	13.94396047
●	As	1.86791302	0.00000000	13.44989404
●	Li	1.86791302	0.00000000	10.07309919
●	Co	1.86791302	1.86791302	12.00852983
●	Co	0.00000000	0.00000000	12.00852983
●	As	0.00000000	1.86791302	10.56716562



Orthographic projections: views of LiCoAs (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Na	7	0.1088	1	1
InSe	8	0.1669	1	1
HgO	8	0.5844	1	1
Bi ₂	8	0.1736	1	1
GeTe	8	0.1296	1	1
AgTl	8	0.3711	1	1
S ₂	8	0.1307	1	1
PbTe	8	0.1689	1	1
Sb ₂	8	0.1503	1	1
IrTe ₂	9	0.1302	1	1
CrS ₂	9	0.1106	1	1
I ₂ Mg	9	0.1559	1	1
CdI ₂	9	0.1709	1	1
Br ₂ Ca	9	0.1723	1	1
HfTe ₂	9	0.1366	1	1
Br ₂ La	9	0.1563	1	1
Br ₂ Cu	9	0.1174	1	1
I ₂ Yb	9	0.1961	1	1
BiClTe	9	0.1713	1	1
ReS ₂	9	0.1093	1	1
AuTe ₂	9	0.1431	1	1
BrCdI	9	0.1592	1	1
Cl ₂ Zn	9	0.003	1	1
PdTe ₂	9	0.141	1	1
I ₂ Zn	9	0.1472	1	1
BaF ₂	9	0.1627	1	1
BiBrTe	9	0.1778	1	1
Bi ₂ Pd	9	0.2113	1	1
GeI ₂	9	0.1541	1	1
Ba ₂ Hg	9	0.3902	1	1
PtS ₂	9	0.1091	1	1
Ba ₂ N	9	0.1378	1	1
Se ₂ Ti	9	0.1084	1	1
AsKSn	9	0.1612	1	1
Te ₂ Zr	9	0.137	1	1
PbTe ₂	9	0.1582	1	1
Cl ₂ Cu	9	0.1053	1	1
I ₂ Tm	9	0.7529	1	1
SnTe ₂	9	0.1518	1	1
GeI ₂	9	0.1692	1	1
STl ₂	9	0.1637	1	1
BiTe	9	0.186	1	1
DyI ₂	9	0.7682	1	1
Se ₂ Yb	9	0.1543	1	1
BiTe ₂	9	0.1546	1	1
GdI ₂	9	0.1813	1	1
CNNa	9	1.2935	1	1
F ₂ Ni	9	0.0069	1	1
PtTe ₂	9	0.1427	1	1
Br ₂ Cd	9	0.1402	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

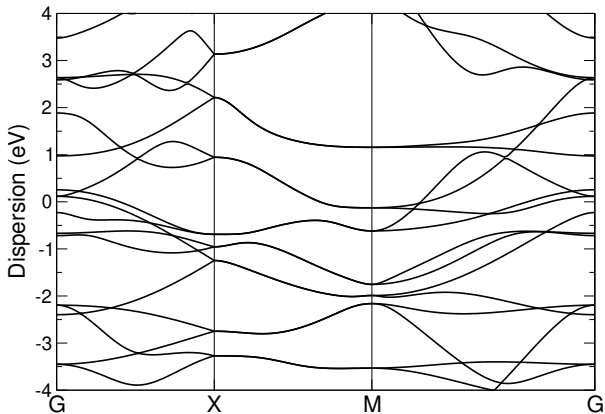
Lattice matching - minimal strain

Formula	N° atoms	strain	cell size 1	cell size 2
Pb ₂ Se ₂	222	0.0	25	18
Ca ₂ O ₂	708	0.0	64	81
Mg ₆	510	0.0	36	49
Br ₂ V	483	0.0002	48	65
Tl	451	0.0002	61	85
Sn	859	0.0003	113	181
F ₄ Pb	815	0.0003	85	61
Ba ₂ Cd	678	0.0004	81	64
Cu ₂ Te ₂	10	0.0004	1	1
Ag ₂ I ₂	316	0.0004	36	25
Cl ₂ S ₂ Tl ₂	150	0.0005	16	9
F ₂ I ₂ Pb ₂	870	0.0005	81	64
Mg ₄	706	0.0006	61	85
Ge ₂ Hf ₂ Te ₂	12	0.0006	1	1
HgI ₂	291	0.0006	36	25
Ho ₂ I ₂ Se ₂	228	0.0006	24	14
Se ₂ V	840	0.0006	81	118
Cl ₂ Zr ₂	548	0.0007	48	65
N ₃ Na	352	0.0007	40	28
HgO	736	0.0008	85	113
Bi ₂ Se ₂	292	0.0009	32	25
ReSe ₂	483	0.0009	48	65
Cu ₂ Na ₂ Te ₂	510	0.0009	49	36
Tl	604	0.0009	81	118
AgNO ₃	973	0.001	108	65
Gd ₂ I ₂ S ₂	774	0.0011	80	49
CCl ₂ Sc ₂	613	0.0011	48	65
CKN	819	0.0011	103	67
K	763	0.0011	113	85
S ₂ V	852	0.0011	79	126
I ₂ S ₂ Tb ₂	846	0.0011	87	54
In	121	0.0011	16	25
Dy ₂ I ₂ S ₂	846	0.0012	87	54
FeSe ₂	537	0.0012	49	81
Br ₂ Ca ₃ Si	882	0.0012	82	65
AgClO ₄	930	0.0013	97	58
Bi ₂ Pd	627	0.0013	64	81
Cl ₄ Mg ₂	942	0.0013	120	37
PbS ₂ Sn	732	0.0013	80	63
I ₂ N ₂ Zr ₂	114	0.0014	10	9
Se ₂ W	840	0.0014	81	118
Br ₂ H ₂ Zr ₂	678	0.0015	48	65
Ba ₂ Hg	687	0.0015	82	65
Cu ₂ O ₄	312	0.0015	24	28
MoSe ₂	840	0.0016	81	118
Sb ₂ Te ₃	919	0.0016	89	77
Cu ₄ Te ₂	996	0.0016	89	77
MoS ₂	852	0.0016	79	126
C	137	0.0016	12	65
Cl ₂ Zn	603	0.0016	62	77

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

LiFeAs (P4/nmm (129))
Structural and electronic properties

	Formula	LiFeAs
	Spacegroup	P4/nmm (129)
	Prototype	PbClF
	Parent 3D	Li ₂ Fe ₂ As ₂
	Source DB	COD
	DB ID	4501852
DF2-C09	Binding energy [meV/ Å²]	62.76
RVV10	Binding energy [meV/ Å²]	65.74
	Band gap (PBE) [eV]	0.0

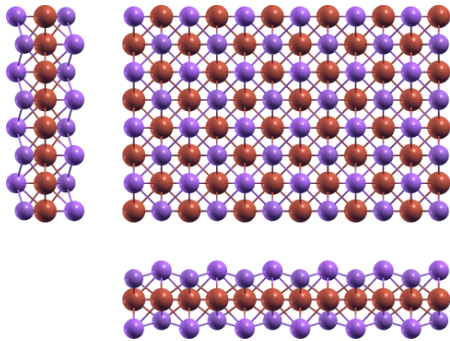


Band structure: Electronic band structure of LiFeAs (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of LiFeAs (P4/nmm (129)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.75498870	0.00000000	0.00000000
a₂		-0.00000000	3.75498870	0.00000000
a₃		0.00000000	0.00000000	24.07574958
		x [Å]	y [Å]	z [Å]
●	Li	-0.00000000	1.87749435	14.00339811
●	As	1.87749435	0.00000000	13.45336839
●	Li	1.87749435	0.00000000	10.07235147
●	Fe	0.00000000	0.00000000	12.03787479
●	Fe	1.87749435	1.87749435	12.03787479
●	As	-0.00000000	1.87749435	10.62238120



Orthographic projections: views of LiFeAs (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	7	1.1251	1	1
K	7	0.7835	1	1
InSe	8	0.1643	1	1
Bi ₂	8	0.1708	1	1
AgTl	8	0.3661	1	1
PbTe	8	0.1662	1	1
Sb ₂	8	0.148	1	1
CrS ₂	9	0.1112	1	1
I ₂ Mg	9	0.1535	1	1
CdI ₂	9	0.1681	1	1
MoTe ₂	9	0.1088	1	1
Br ₂ Ca	9	0.1695	1	1
CaI ₂	9	0.1963	1	1
HfTe ₂	9	0.1347	1	1
Br ₂ La	9	0.1539	1	1
Br ₂ Cu	9	0.1158	1	1
I ₂ Yb	9	0.1929	1	1
BiClTe	9	0.1685	1	1
ReS ₂	9	0.1099	1	1
AuTe ₂	9	0.141	1	1
BrCdI	9	0.1567	1	1
Cl ₂ Zn	9	0.0054	1	1
PdTe ₂	9	0.1389	1	1
I ₂ Zn	9	0.145	1	1
BaF ₂	9	0.1601	1	1
BiBrTe	9	0.175	1	1
Bi ₂ Pd	9	0.2087	1	1
GeI ₂	9	0.1517	1	1
Ba ₂ Hg	9	0.3849	1	1
PtS ₂	9	0.1085	1	1
Ba ₂ N	9	0.1359	1	1
AsKSn	9	0.1586	1	1
Te ₂ Zr	9	0.135	1	1
Te ₂ W	9	0.1088	1	1
PbTe ₂	9	0.1557	1	1
Cl ₂ Cu	9	0.1043	1	1
I ₂ Tm	9	0.1947	1	1
SnTe ₂	9	0.1495	1	1
GeI ₂	9	0.1665	1	1
STl ₂	9	0.1611	1	1
BiTe	9	0.1829	1	1
Se ₂ Yb	9	0.1519	1	1
BiTe ₂	9	0.1522	1	1
GdI ₂	9	0.1784	1	1
PtTe ₂	9	0.1407	1	1
Br ₂ Cd	9	0.1382	1	1
CdI ₂	9	0.1676	1	1
Ba ₂ Cd	9	0.3906	1	1
NaPSn	9	0.134	1	1
I ₂ Pr	9	0.1686	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

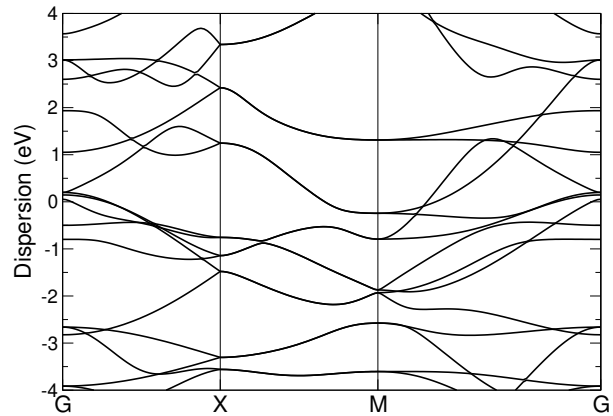
Formula	N° atoms	strain	cell size 1	cell size 2
Br ₂ H ₂ Yb ₂	12	0.0	1	1
H ₂ I ₂ Sr ₂	678	0.0001	64	49
Se ₂ Ta	483	0.0002	48	65
NbSe ₂	483	0.0003	48	65
Fe ₂ SeTe	10	0.0003	1	1
AgTe ₂	621	0.0004	61	85
Cl ₄ Mn	230	0.0004	25	16
C ₂ Br ₂ La ₂	138	0.0004	12	11
Cl ₄ KTl	390	0.0004	49	16
La ₂ S ₂	570	0.0006	63	48
Gd	382	0.0006	46	106
Cl ₂ Ni	483	0.0006	48	65
NbS ₂	840	0.0006	81	118
Se ₂ Sn ₂	504	0.0007	56	42
Mg ₃	258	0.0008	25	36
PbS ₂ Sn	742	0.0008	81	64
LiO ₂	366	0.0008	36	50
AsSe ₂	483	0.0009	48	65
AuI ₄ Li	912	0.001	105	47
Br ₂ Lu ₂ O ₂	12	0.0011	1	1
I ₂ Se ₂ Tb ₂	228	0.0011	24	14
C ₂ Br ₂ Y ₂	888	0.0011	72	76
S ₂ Ta	840	0.0011	81	118
F ₂ I ₂ Pb ₂	882	0.0011	82	65
NbSe ₂	483	0.0011	48	65
AgClO ₄	930	0.0012	97	58
AgCuTe ₂	548	0.0012	54	56
FeSe ₂	537	0.0012	49	81
Ba ₂ Hg	843	0.0012	100	81
Ba ₂ Cd	687	0.0013	82	65
K	763	0.0013	113	85
Ge ₂ Te ₂ Zr ₂	12	0.0013	1	1
PbS ₂ Sn	732	0.0013	80	63
C ₄ Ca ₂	870	0.0014	79	66
Cu ₂ Sr ₂	974	0.0014	103	89
MoS ₂	852	0.0014	79	126
ReSe ₂	483	0.0015	48	65
Cl ₂ Fe	531	0.0015	52	73
CoH ₂ O ₂	929	0.0015	64	109
Cl ₂ Zr	531	0.0015	52	73
S ₂ W	852	0.0015	79	126
Cu ₂ Sr ₂	842	0.0016	89	77
C ₂ Li ₂	862	0.0016	89	82
O ₄ PTl	366	0.0016	36	25
AgClO ₄	780	0.0016	81	49
MoS ₂	852	0.0016	79	126
Cl ₂ N ₂ Zr ₂	834	0.0016	62	77
Sm	403	0.0016	48	115
AgClO ₂	928	0.0016	92	94
HgO	736	0.0016	85	113

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

LiFeP (P4/nmm (129))

Structural and electronic properties

	Formula	LiFeP
	Spacegroup	P4/nmm (129)
	Prototype	PbClF
	Parent 3D	Li ₂ Fe ₂ P ₂
	Source DB	COD
	DB ID	9008322
DF2-C09	Binding energy [meV/ Å²]	72.67
RVV10	Binding energy [meV/ Å²]	76.44
	Band gap (PBE) [eV]	0.0

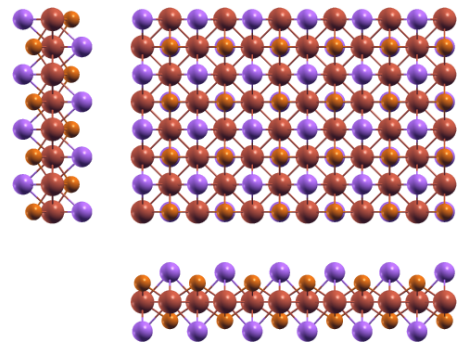


Band structure: Electronic band structure of LiFeP (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of LiFeP (P4/nmm (129)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.66364512	0.00000000	0.00000000
a₂		0.00000000	3.66364512	0.00000000
a₃		0.00000000	0.00000000	24.06761863
		x [Å]	y [Å]	z [Å]
●	Li	0.00000000	1.83182256	13.99698733
●	P	1.83182256	0.00000000	13.28593471
●	Li	1.83182256	0.00000000	10.07063130
●	Fe	0.00000000	0.00000000	12.03380932
●	Fe	1.83182256	1.83182256	12.03380932
●	P	0.00000000	1.83182256	10.78168392



Orthographic projections: views of LiFeP (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
InSe	8	0.1776	1	1
HgO	8	0.2109	1	1
AsSb	8	0.1319	1	1
Bi ₂	8	0.1848	1	1
GeTe	8	0.1365	1	1
AgTl	8	0.3906	1	1
S ₂	8	0.1378	1	1
PbTe	8	0.1798	1	1
Sb ₂	8	0.1596	1	1
CaCl	8	0.0081	1	1
IrTe ₂	9	0.1373	1	1
CrS ₂	9	0.1087	1	1
I ₂ Mg	9	0.1657	1	1
CdCl ₂	9	0.1357	1	1
CdI ₂	9	0.1819	1	1
AgTe ₂	9	0.585	1	1
Br ₂ Ca	9	0.1834	1	1
InSe ₂	9	0.136	1	1
GeTe ₂	9	0.1349	1	1
HfTe ₂	9	0.1444	1	1
I ₂ Mn	9	0.1358	1	1
Br ₂ La	9	0.1661	1	1
Br ₂ Cu	9	0.1242	1	1
NSr ₂	9	0.1331	1	1
I ₂ Yb	9	0.7831	1	1
PbS ₂	9	0.13	1	1
BiClTe	9	0.1824	1	1
AuTe ₂	9	0.1516	1	1
BrCdI	9	0.1693	1	1
Cl ₂ Zn	9	0.0063	1	1
PdTe ₂	9	0.1493	1	1
FeI ₂	9	0.1341	1	1
I ₂ Ni	9	0.135	1	1
Mg ₃	9	0.559	1	1
CrI ₂	9	0.1337	1	1
I ₂ Zn	9	0.1562	1	1
BaF ₂	9	0.1731	1	1
BiBrTe	9	0.1894	1	1
GeI ₂	9	0.1637	1	1
Ba ₂ Hg	9	1.1072	1	1
N ₂ W	9	0.1101	1	1
Ba ₂ N	9	0.1458	1	1
AsKSn	9	0.1714	1	1
Te ₂ Zr	9	0.1448	1	1
PbTe ₂	9	0.1681	1	1
AsSe ₂	9	0.1086	1	1
Cl ₂ Cu	9	0.1098	1	1
I ₂ Tm	9	0.7884	1	1
SnTe ₂	9	0.1613	1	1
GeI ₂	9	0.1801	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

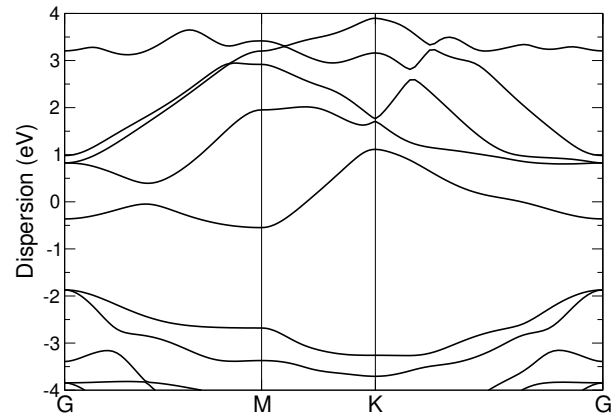
Formula	N° atoms	strain	cell size 1	cell size 2
F ₄ Sn	640	0.0001	65	50
Br ₂ Ca ₃ Si	678	0.0002	64	49
O ₂ Pb ₂	934	0.0003	101	82
Cl ₂ Hf ₂	548	0.0003	48	65
CoO ₂	237	0.0003	20	39
Cu ₂ O ₂	86	0.0004	9	8
F ₄ Nb	806	0.0004	81	64
Mg ₂	222	0.0004	25	36
Bi ₂ O ₂	924	0.0004	100	81
Ba ₂ Hg	531	0.0005	64	49
Mg ₆	678	0.0005	49	64
FeO ₂	237	0.0005	20	39
Bi ₂ Se ₂	874	0.0005	97	73
AlH ₄ Na	780	0.0005	81	49
Ho ₂ S ₂	86	0.0006	9	8
Br ₂ F ₂ Sr ₂	882	0.0006	82	65
I ₂ Lu ₂ Se ₂	414	0.0007	45	24
K	571	0.0008	85	61
Cr ₂ O ₄	54	0.0008	4	5
NiO ₂	237	0.0009	20	39
O ₂ Pb ₂	924	0.0009	100	81
LiNbS ₂	548	0.0009	48	65
AgTe ₂	849	0.0009	85	113
Br ₂ F ₂ Pb ₂	882	0.0009	82	65
S ₂ Ta	483	0.0009	48	65
Bi ₂ Mn ₂	376	0.001	36	40
As ₂ Mg ₂ Na ₂	876	0.0011	85	61
F ₄ Pb	341	0.0011	36	25
Cl ₄ Mn	961	0.0011	106	65
Cl ₄ KTl	636	0.0012	81	25
I ₂ Sb ₂ Te ₂	342	0.0012	40	17
F ₄ Sn	629	0.0012	64	49
Se ₂ Sn ₂	372	0.0013	42	30
Cu ₂ K ₂ Te ₂	246	0.0013	25	16
Hf ₂ Si ₂ Te ₂	12	0.0013	1	1
CKN	441	0.0013	56	35
NbS ₂	483	0.0014	48	65
Br ₂ F ₂ Sr ₂	870	0.0014	81	64
N ₂ W	711	0.0015	64	109
Au ₂ Br ₂	438	0.0015	49	36
Bi ₂ Pd	795	0.0015	82	101
Tl	385	0.0015	52	73
Bi ₂ Se ₂ Te	919	0.0015	89	77
Sb ₂ SeTe ₂	919	0.0016	89	77
In ₂ Te ₃	919	0.0016	89	77
HgO	546	0.0016	64	81
Sn	670	0.0016	89	136
Br ₂ Zr ₂	680	0.0016	62	77
Ag ₂ F ₄	690	0.0016	80	35
Sb ₂ Te ₂	646	0.0016	73	52

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

LiHfS₂ (P3m1)

Structural and electronic properties

	Formula	LiHfS ₂
	Spacegroup	P3m1
	Prototype	LiNbS ₂
	Parent 3D	HfLiS ₂
	Source DB	MPDS
	DB ID	S301113
DF2-C09	Binding energy [meV/ Å²]	112.91
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

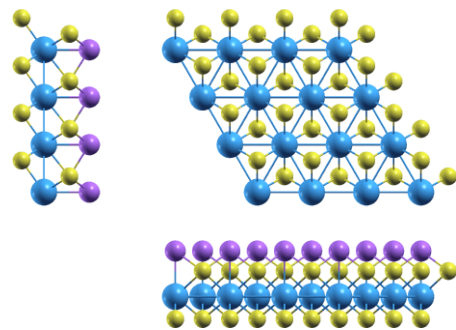


Band structure: Electronic band structure of LiHfS₂ (P3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of LiHfS₂ (P3m1) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	-1.78098432	-3.08475532	0.00000000
a₂	3.56196863	0.00000000	0.00000000
a₃	0.00000000	0.00000000	21.72479617
	x [Å]	y [Å]	z [Å]
● Li	0.00000000	0.00000000	-2.17223761
● S	0.00000000	-2.05650355	-0.87145886
● Hf	0.00000000	0.00000000	0.79242579
● S	1.78098432	-1.02825177	2.25127068



Orthographic projections: views of LiHfS₂ (P3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.3231	1	1
Tl	5	0.1245	1	1
Na	5	0.0018	1	1
In	5	0.1112	1	1
In	5	0.2581	1	1
Gd	5	0.1142	1	1
HgO	6	0.1329	1	1
As ₂	6	0.0062	1	1
LiO	6	0.2731	1	1
Mg ₂	6	0.1157	1	1
Cl ₂ Zn	7	0.0052	1	1
S ₂ V	7	0.2625	1	1
MoS ₂	7	0.2636	1	1
MoTe ₂	7	0.0005	1	1
AgTe ₂	7	0.1264	1	1
HfS ₂	7	0.009	1	1
HfTe ₂	7	0.4649	1	1
Te ₂ V	7	0.0024	1	1
CuTe ₂	7	0.0087	1	1
Br ₂ Co	7	0.0058	1	1
ReS ₂	7	0.2464	1	1
Ca ₂ N	7	0.0068	1	1
AuTe ₂	7	0.4848	1	1
BrCdI	7	3.0357	1	1
PdTe ₂	7	0.4784	1	1
Mg ₃	7	0.121	1	1
I ₂ Zn	7	0.4969	1	1
Te ₂ Zn	7	0.0003	1	1
S ₂ W	7	0.2637	1	1
Bi ₂ Pd	7	0.1405	1	1
Br ₂ Mn	7	0.0039	1	1
CrTe ₂	7	0.0071	1	1
PtS ₂	7	0.0008	1	1
CoTe ₂	7	0.0094	1	1
CdClO	7	0.0019	1	1
Ba ₂ N	7	0.4688	1	1
Se ₂ Ti	7	0.0034	1	1
Br ₂ Ti	7	0.0076	1	1
Te ₂ Zr	7	0.4661	1	1
Te ₂ W	7	0.0006	1	1
Cl ₂ Cu	7	0.5985	1	1
Cl ₂ V	7	0.2695	1	1
OTl ₂	7	0.0021	1	1
Br ₂ Fe	7	0.0059	1	1
Br ₂ Cr	7	0.0074	1	1
FeSe ₂	7	0.4215	1	1
MoS ₂	7	0.2639	1	1
CrSe ₂	7	0.2677	1	1
Se ₂ Ta	7	0.0084	1	1
PtTe ₂	7	0.4837	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

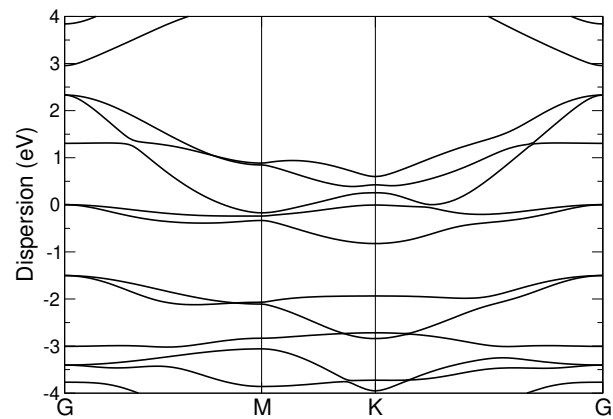
Formula	N° atoms	strain	cell size 1	cell size 2
GeNi ₃ Te ₂	886	0.0	100	81
I ₂ La ₂ Sb	569	0.0	81	49
Br ₂ Cd	516	0.0	81	64
Br ₂ La ₂ P	269	0.0001	36	25
CrSe ₂	624	0.0001	81	100
Br ₂ La	304	0.0001	49	36
Br ₂ La ₂	400	0.0001	57	43
I ₂ S ₂ Sm ₂	466	0.0001	61	37
Br ₂ PY ₂	644	0.0002	81	64
Bi ₂ Se ₃	376	0.0002	49	36
CdI ₂	219	0.0002	36	25
FHOZn	724	0.0002	81	100
PtTe ₂	463	0.0002	73	57
I ₂ Mg	304	0.0002	49	36
CdI ₂	219	0.0002	36	25
K	281	0.0002	61	37
Br ₂ O ₂ Tb ₂	548	0.0003	65	48
Te ₂ Zn	7	0.0003	1	1
Te ₂ Zr	583	0.0003	91	73
CoH ₂ O ₂	457	0.0003	43	57
Cu ₂ Rb ₂ Te ₂	276	0.0003	39	20
C ₄ Ca ₂	852	0.0003	108	70
MoS ₂	565	0.0003	73	91
I ₄ Sr ₂	182	0.0003	32	9
Sb ₂	314	0.0003	57	43
Gd ₂ GeI ₂	269	0.0004	36	25
O ₂ Pt	447	0.0004	57	73
Gd ₂ I ₂	340	0.0004	49	36
MoTe ₂	7	0.0005	1	1
Ce ₂ I ₂ Si ₂	412	0.0005	49	36
S ₂ W	565	0.0005	73	91
Cu ₃ Se ₃	802	0.0005	91	73
Cl ₂ OV	596	0.0005	77	72
MoS ₂	565	0.0005	73	91
I ₂ Zn	403	0.0005	64	49
In ₂ Se ₂	452	0.0006	64	49
AuTe ₂	463	0.0006	73	57
NaPSn	643	0.0006	100	81
BiClTe	219	0.0006	36	25
Bi ₂ In ₂	236	0.0006	39	20
Bi ₂ STe ₂	269	0.0006	36	25
I ₂ La ₂ Sb	429	0.0006	61	37
Te ₂ W	7	0.0006	1	1
HNiO ₂	244	0.0006	25	36
Br ₂ Cu ₂	452	0.0006	65	48
O ₂ Sn ₂	452	0.0007	65	48
I ₂ Pr	219	0.0007	36	25
Eu ₂ I ₂ O ₂	958	0.0007	118	81
Cu ₂ I ₂	340	0.0007	49	36
Br ₂ Gd ₂ Ge	376	0.0007	49	36

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

LiMnSe₂ (P3m1 (156))

Structural and electronic properties

	Formula	LiMnSe ₂
	Spacegroup	P3m1 (156)
	Prototype	LiMnSe ₂
	Parent 3D	LiMnSe ₂
	Source DB	ICSD
	DB ID	50817
DF2-C09	Binding energy [meV/ Å²]	75.52
RVV10	Binding energy [meV/ Å²]	64.44
	Band gap (PBE) [eV]	0.0

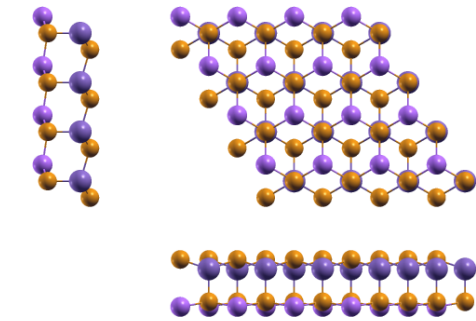


Band structure: Electronic band structure of LiMnSe₂ (P3m1 (156)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of LiMnSe₂ (P3m1 (156)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.94015872	−0.00000000	0.00000000
a₂		−1.97007936	3.41227755	0.00000000
a₃		0.00000000	0.00000000	24.14340306
		x [Å]	y [Å]	z [Å]
●	Mn	1.97007936	1.13742585	10.88285668
●	Se	0.00000000	0.00000000	10.22068492
●	Li	−0.00000000	2.27485170	13.49901700
●	Se	1.97007936	1.13742585	13.14865366



Orthographic projections: views of LiMnSe₂ (P3m1 (156)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	2.9681	1	1
Na	5	0.268	1	1
HgO	6	0.4289	1	1
GeTe	6	0.0056	1	1
S ₂	6	0.004	1	1
CaCl	6	0.1339	1	1
IrTe ₂	7	0.0047	1	1
CrS ₂	7	4.8711	1	1
CdCl ₂	7	0.0066	1	1
Cl ₂ Mn	7	1.5313	1	1
MoTe ₂	7	0.2713	1	1
ReSe ₂	7	1.6273	1	1
S ₂ Ta	7	1.5462	1	1
CaI ₂	7	2.8488	1	1
InSe ₂	7	0.0062	1	1
GeTe ₂	7	0.0076	1	1
HfTe ₂	7	0.0036	1	1
Te ₂ V	7	0.2741	1	1
I ₂ Mn	7	0.0065	1	1
I ₂ Yb	7	0.4845	1	1
LiO ₂	7	0.0698	1	1
Cl ₂ Zn	7	0.146	1	1
PdTe ₂	7	0.0091	1	1
FeI ₂	7	0.0086	1	1
I ₂ Ni	7	0.0074	1	1
S ₂ Ti	7	1.5822	1	1
NbS ₂	7	1.5429	1	1
CrI ₂	7	0.009	1	1
Te ₂ Zn	7	0.2711	1	1
BiBrTe	7	0.4484	1	1
Bi ₂ Pd	7	0.1118	1	1
Cl ₂ Ni	7	1.6341	1	1
CrTe ₂	7	0.2604	1	1
PtS ₂	7	0.2695	1	1
Br ₂ V	7	0.2498	1	1
ClN ₂ Zr	7	0.247	1	1
CdClO	7	0.2734	1	1
Ba ₂ N	7	0.0052	1	1
Se ₂ Ti	7	0.2657	1	1
Br ₂ Ti	7	0.2596	1	1
Te ₂ Zr	7	0.0041	1	1
Te ₂ W	7	0.2715	1	1
AsSe ₂	7	0.254	1	1
I ₂ Tm	7	2.8339	1	1
OTl ₂	7	0.2737	1	1
BiTe	7	0.4646	1	1
BrN ₂ Zr	7	0.2558	1	1
NbSe ₂	7	1.6373	1	1
GeS ₂	7	0.1254	1	1
MnSe ₂	7	0.1338	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

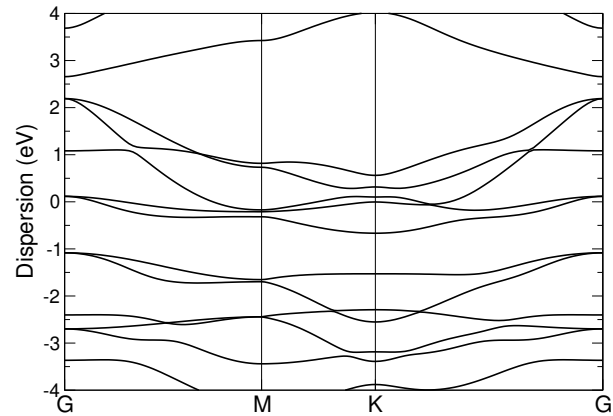
Formula	N° atoms	strain	cell size 1	cell size 2
LiNbS ₂	340	0.0	36	49
S ₂ Ta	291	0.0001	36	49
Gd ₂ I ₂ S ₂	486	0.0001	57	43
P ₂	172	0.0001	25	36
F ₂ Se ₂ Tm ₂	10	0.0001	1	1
Br ₂ Hf ₂	520	0.0002	57	73
Ge ₂ I ₂ La ₂	708	0.0002	81	64
Br ₂ Ti	499	0.0002	64	81
CrS ₂	439	0.0002	49	81
AlLiTe ₂	724	0.0002	100	81
BrN ₂ Zr	447	0.0002	57	73
Cl ₂ Ti	208	0.0003	25	36
Na	424	0.0003	81	100
O ₂ Pt	139	0.0003	16	25
Ba ₂ Cu ₂	520	0.0003	73	57
Cl ₂ H ₂ Sc ₂	742	0.0004	64	81
CS ₂ Ta ₂	280	0.0004	25	36
FeO ₂	247	0.0004	25	49
Br ₂ H ₂ Zr ₂	742	0.0004	64	81
Br ₂ Ca ₃ Si	486	0.0004	57	43
Br ₂ V	388	0.0004	49	64
KNO ₃	145	0.0004	25	9
CNb ₂ S ₂	280	0.0004	25	36
Cl ₂ Zr ₂	452	0.0004	49	64
Br ₂ Cr	499	0.0005	64	81
I ₂ Yb	463	0.0005	73	57
Dy ₂ I ₂ S ₂	550	0.0005	64	49
NbS ₂	291	0.0006	36	49
Se ₂ Ta	499	0.0006	64	81
Br ₂ Zr ₂	656	0.0006	73	91
MnO ₂	496	0.0006	49	100
I ₂ Y ₂	8	0.0006	1	1
C ₂	228	0.0006	25	64
Ga ₂ S ₃	824	0.0007	81	100
Gd	304	0.0007	49	108
Cl ₂ Sc ₂	580	0.0007	64	81
NS ₂ Zr	724	0.0007	81	100
Li ₂ Tl ₂	392	0.0007	61	37
CrTe ₂	499	0.0008	64	81
CCl ₂ Sc ₂	516	0.0008	49	64
NbSe ₂	447	0.0008	57	73
CrS ₂	331	0.0008	37	61
IKO ₃	449	0.0009	81	25
BiTe	583	0.0009	91	73
Se ₂ Ti	565	0.001	73	91
Bi ₂ Te ₃	729	0.001	91	73
C ₂ Li ₂	796	0.001	106	93
Cu ₂ Rb ₂ Te ₂	978	0.001	126	79
AsSe ₂	447	0.0011	57	73
Cl ₂ Hf ₂	340	0.0011	36	49

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

LiMnTe₂ (P3m1 (156))

Structural and electronic properties

	Formula	LiMnTe ₂
	Spacegroup	P3m1 (156)
	Prototype	LiMnSe2
	Parent 3D	LiMnTe ₂
	Source DB	ICSD
	DB ID	110773
DF2-C09	Binding energy [meV/ Å²]	N/A
RVV10	Binding energy [meV/ Å²]	63.36
	Band gap (PBE) [eV]	0.0

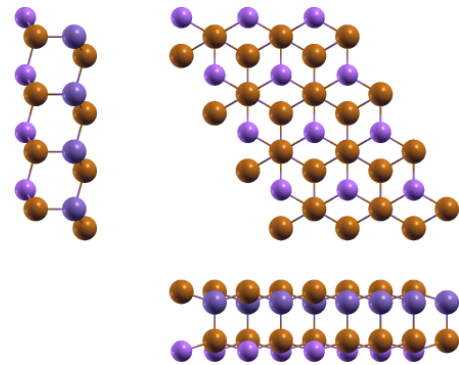


Band structure: Electronic band structure of LiMnTe₂ (P3m1 (156)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of LiMnTe₂ (P3m1 (156)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		4.26588477	0.00000000	0.00000000
a₂		-2.13294238	3.69436458	0.00000000
a₃		0.00000000	0.00000000	24.58275849
		x [Å]	y [Å]	z [Å]
●	Mn	2.13294238	1.23145486	10.85383774
●	Te	0.00000000	0.00000000	10.17261550
●	Li	-0.00000000	2.46290972	13.99267162
●	Te	2.13294238	1.23145486	13.32649816



Orthographic projections: views of LiMnTe₂ (P3m1 (156)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Na	5	1.4481	1	1
InSe	6	0.0023	1	1
AsSb	6	0.2684	1	1
Bi ₂	6	0.0035	1	1
AgTl	6	0.1502	1	1
PbTe	6	0.0005	1	1
CaCl	6	0.1125	1	1
CdCl ₂	7	0.2757	1	1
CdI ₂	7	0.0012	1	1
PSn ₂	7	1.5664	1	1
MoSe ₂	7	4.8688	1	1
Br ₂ Zn	7	0.2541	1	1
Br ₂ Ca	7	0.0024	1	1
HfS ₂	7	1.5221	1	1
AsSn ₂	7	1.5941	1	1
GeTe ₂	7	0.2742	1	1
SiTe ₂	7	0.2597	1	1
I ₂ Pr	7	0.1346	1	1
I ₂ Mn	7	0.2759	1	1
S ₂ Zr	7	1.5609	1	1
Br ₂ Cu	7	0.7099	1	1
NSr ₂	7	0.2707	1	1
PbS ₂	7	0.2647	1	1
BiClTe	7	0.0015	1	1
Cl ₂ Zn	7	0.119	1	1
FeI ₂	7	0.2726	1	1
I ₂ Ni	7	0.2745	1	1
Te ₂ Ti	7	0.2545	1	1
CrI ₂	7	0.2719	1	1
BaF ₂	7	0.0061	1	1
BiBrTe	7	0.0072	1	1
RhTe ₂	7	0.2487	1	1
CoTe ₂	7	1.5244	1	1
AsKSn	7	0.0075	1	1
I ₂ Nd	7	0.1354	1	1
NiTe ₂	7	0.2589	1	1
Cl ₂ Cu	7	0.0683	1	1
S ₂ Sn	7	1.5628	1	1
I ₂ V	7	0.2616	1	1
GeI ₂	7	0.0003	1	1
Se ₂ Zr	7	0.2603	1	1
STl ₂	7	0.0051	1	1
PtSe ₂	7	1.5988	1	1
CoI ₂	7	0.269	1	1
GeS ₂	7	0.4276	1	1
MnSe ₂	7	0.1125	1	1
Br ₂ Ni	7	1.5362	1	1
CeI ₂	7	0.1341	1	1
Br ₂ Mg	7	0.2724	1	1
I ₂ Ti	7	0.2695	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

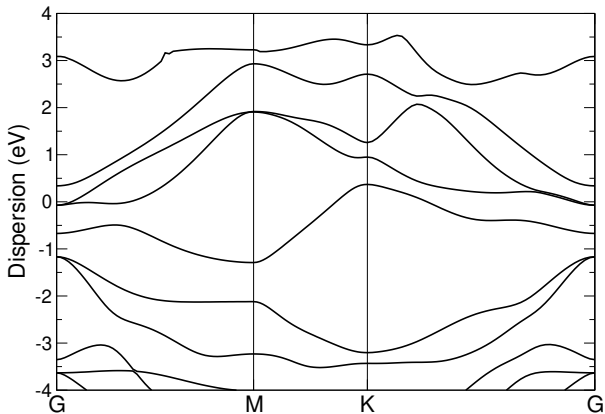
Formula	N° atoms	strain	cell size 1	cell size 2
Br ₂ Y ₂	656	0.0	73	91
Bi ₂ Te ₂	580	0.0	81	64
S ₂ Ti	139	0.0001	16	25
ClKO ₃	381	0.0001	64	25
Se ₂ W	439	0.0001	49	81
PtS ₂	208	0.0002	25	36
PTe ₂ Zr ₂	824	0.0002	81	100
Br ₂ Pr ₂	520	0.0002	57	73
Tl	209	0.0002	37	61
AsSn ₂	343	0.0002	43	57
PbS ₂	565	0.0002	73	91
IKO ₃	145	0.0003	25	9
NiTe ₂	499	0.0003	64	81
MoSe ₂	439	0.0003	49	81
GeI ₂	7	0.0003	1	1
SiTe ₂	499	0.0003	64	81
Bi ₂ STe ₂	9	0.0003	1	1
Ga ₂ Se ₂	656	0.0003	73	91
ClH ₃ O	729	0.0003	91	73
TaTe ₂	343	0.0004	43	57
Br ₂ Er ₂ S ₂	848	0.0004	101	74
Cl ₂ Co	139	0.0004	16	25
Br ₂ N ₂ Zr ₂	438	0.0004	36	49
RhTe ₂	388	0.0004	49	64
NS ₂ Zr	244	0.0005	25	36
CB ₂ Lu ₂	389	0.0005	36	49
H ₂ NiO ₂	116	0.0005	9	16
As ₂ CeLi ₂	9	0.0005	1	1
Ga ₂ S ₃	280	0.0005	25	36
Br ₂ CsF	452	0.0005	65	48
AsSb	524	0.0005	81	100
PbTe	6	0.0005	1	1
CdO ₂	139	0.0005	16	25
Cl ₂ Er ₂ O ₂	742	0.0006	64	81
I ₂ N ₂ Zr ₂	580	0.0007	49	64
Se ₂ V	331	0.0007	37	61
HfSe ₂	447	0.0007	57	73
Te ₂ Ti	447	0.0007	57	73
Au ₂ Br ₂	552	0.0007	74	64
Se ₂ Zr	499	0.0007	64	81
Cl ₂ Zr	139	0.0007	16	25
CdI ₂	7	0.0007	1	1
Se ₂ W	331	0.0008	37	61
Au ₂ Br ₂	508	0.0008	68	59
Pb ₂ Se ₂	624	0.0008	86	70
O ₂ Zn	247	0.0008	25	49
Cu ₂ O ₄	930	0.0009	78	103
Cl ₂ O ₂ Y ₂	838	0.0009	73	91
Na	136	0.0009	25	36
Br ₂ La ₂ P	9	0.0009	1	1

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

LiNbS₂ (P3m1)

Structural and electronic properties





	Formula	LiNbS ₂
	Spacegroup	P3m1
	Prototype	LiNbS ₂
	Parent 3D	LiNbS ₂
	Source DB	MPDS
	DB ID	S301114
DF2-C09	Binding energy [meV/ Å²]	120.63
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

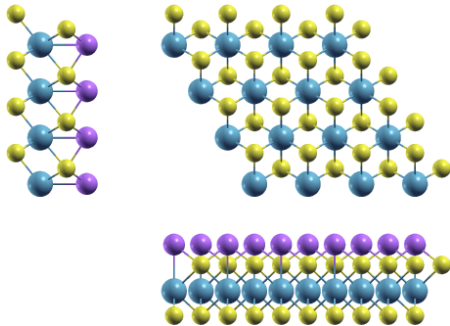


Band structure: Electronic band structure of LiNbS₂ (P3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of LiNbS₂ (P3m1) in Cartesian coordinates.

		<i>x</i> [Å]	<i>y</i> [Å]	<i>z</i> [Å]
a₁		−1.68853408	−2.92462681	0.00000000
a₂		3.37706816	0.00000000	0.00000000
a₃		0.00000000	0.00000000	21.79824406
		<i>x</i> [Å]	<i>y</i> [Å]	<i>z</i> [Å]
	Li	0.00000000	0.00000000	−2.17730963
	S	0.00000000	−1.94975121	−0.88820643
	Nb	0.00000000	0.00000000	0.76096537
	S	1.68853408	−0.97487560	2.30455069



Orthographic projections: views of LiNbS₂ (P3m1) as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	5	0.1436	1	1
Tl	5	0.0078	1	1
Sn	5	0.1203	1	1
In	5	0.1228	1	1
AsSb	6	2.8445	1	1
Mg ₂	6	0.1305	1	1
CrS ₂	7	0.273	1	1
Cl ₂ Mn	7	0.0021	1	1
AgTe ₂	7	0.1463	1	1
MoSe ₂	7	0.0085	1	1
S ₂ Ta	7	0.0001	1	1
Br ₂ Zn	7	0.464	1	1
GeTe ₂	7	0.5009	1	1
SiTe ₂	7	0.4745	1	1
NSr ₂	7	0.4946	1	1
PbS ₂	7	0.4835	1	1
LiO ₂	7	0.3192	1	1
FeI ₂	7	0.498	1	1
I ₂ Ni	7	0.5014	1	1
S ₂ Ti	7	0.0049	1	1
Mg ₃	7	0.1385	1	1
Te ₂ Ti	7	0.4648	1	1
NbS ₂	7	0.0005	1	1
CrI ₂	7	0.4968	1	1
RhTe ₂	7	0.4539	1	1
N ₂ W	7	0.2632	1	1
Cl ₂ Co	7	0.0046	1	1
NbS ₂	7	0.0048	1	1
ClN ₂ Zr	7	0.0082	1	1
Cl ₂ Fe	7	0.0038	1	1
S ₂ Ta	7	0.0056	1	1
Se ₂ V	7	0.0069	1	1
NiTe ₂	7	0.4729	1	1
Cl ₂ Cu	7	0.113	1	1
I ₂ V	7	0.4779	1	1
Se ₂ Zr	7	0.4755	1	1
PtSe ₂	7	0.4486	1	1
CdO ₂	7	0.0044	1	1
O ₂ Zn	7	0.2681	1	1
Cl ₂ Zr	7	0.0042	1	1
FeSe ₂	7	0.1169	1	1
Br ₂ Mg	7	0.4976	1	1
F ₂ Na	7	0.469	1	1
Se ₂ Sn	7	0.4939	1	1
HfSe ₂	7	0.4648	1	1
Se ₂ W	7	0.0083	1	1
Cu ₂ I ₂	8	0.3228	1	1
Br ₂ Pr ₂	8	0.467	1	1
HNiO ₂	8	1.6391	1	1
Cl ₂ Hf ₂	8	0.0011	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

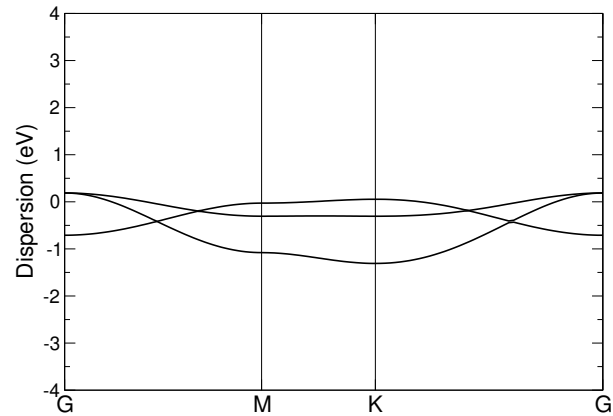
Formula	N° atoms	strain	cell size 1	cell size 2
LiMnSe ₂	340	0.0	49	36
Br ₂ Pr ₂	656	0.0	91	73
InSe ₂	357	0.0001	57	43
S ₂ Ta	7	0.0001	1	1
Cl ₂ Y ₂	724	0.0001	100	81
PbS ₂	463	0.0001	73	57
Br ₂ Hg ₃	41	0.0001	9	1
Br ₂ Y ₂	520	0.0001	73	57
F ₂ Se ₂ Tm ₂	412	0.0002	49	36
Se ₂ Zr	516	0.0002	81	64
Cl ₂ Er ₂ H ₂	486	0.0002	57	43
STl ₂	148	0.0002	25	16
H ₂ Si ₂	400	0.0002	57	43
Cu ₂ Sr ₂	520	0.0003	81	49
NSr ₂	403	0.0003	64	49
I ₂ Mn	357	0.0003	57	43
Cl ₂ La ₂	244	0.0003	36	25
Cl ₂ Er ₂ O ₂	708	0.0004	81	64
O ₂ Zn	624	0.0004	81	100
Cu ₂ Sr ₂	392	0.0004	61	37
FeO ₂	208	0.0004	25	36
FeH ₂ O ₂	747	0.0004	73	91
SbSe ₂ Tl	104	0.0004	18	8
CdCl ₂	357	0.0004	57	43
CBr ₂ Y ₂	805	0.0005	100	81
Ga ₂ Se ₂	520	0.0005	73	57
C ₂ Br ₂ Y ₂	878	0.0005	104	77
Hf ₂ Si ₂ Te ₂	548	0.0005	65	48
NbS ₂	7	0.0005	1	1
NS ₂ Ta	580	0.0005	64	81
Se ₂ Sn	403	0.0006	64	49
I ₂ Y ₂	340	0.0006	49	36
Dy ₂ I ₂ S ₂	118	0.0006	16	9
CrI ₂	403	0.0006	64	49
SiTe ₂	516	0.0006	81	64
I ₂ Sb ₂ Te ₂	676	0.0006	115	36
GeTe	314	0.0006	57	43
BiBrTe	355	0.0006	61	37
Ni ₂ Te ₂	400	0.0006	57	43
I ₂ La ₂ P	569	0.0007	81	49
PbS ₂ Sn	932	0.0007	150	83
La ₂ S ₂	92	0.0007	15	8
As ₂ Sn ₂	244	0.0007	36	25
Cl ₂ Y ₂	501	0.0007	64	49
Bi ₂ Te ₂	472	0.0007	79	39
I ₂ V	516	0.0007	81	64
Cl ₂ O ₂ Yb ₂	802	0.0008	91	73
Ga ₂ Se ₂	724	0.0008	100	81
Br ₂ Gd ₂	244	0.0008	36	25
N ₂ W	565	0.0008	73	91

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

LiO (P3m1)

Structural and electronic properties

	Formula	LiO
	Spacegroup	P3m1
	Prototype	GeTe
	Parent 3D	Li ₃ O ₃ S ₆ Ti ₃
	Source DB	MPDS
	DB ID	S2050313
DF2-C09	Binding energy [meV/ Å²]	36.62
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

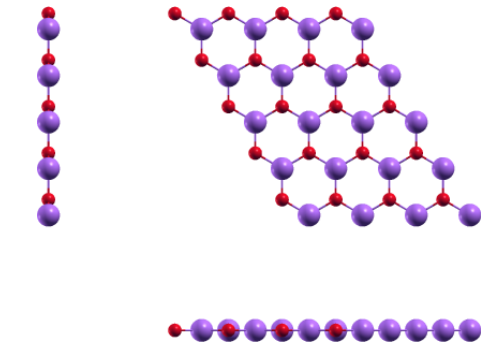


Band structure: Electronic band structure of LiO (P3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of LiO (P3m1) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	-1.61586562	-2.79876136	0.00000000
a₂	3.23173125	0.00000000	0.00000000
a₃	0.00000000	0.00000000	12.14858370
	x [Å]	y [Å]	z [Å]
● Li	0.00000000	-1.86584090	0.00001431
● O	1.61586562	-0.93292045	-0.00001431



Orthographic projections: views of LiO (P3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Sn	3	0.134	1	1
Na	3	0.4474	1	1
In	3	0.1375	1	1
As ₂	4	0.467	1	1
P ₂	4	0.0077	1	1
Mg ₂	4	0.1476	1	1
Cl ₂ Zn	5	0.4644	1	1
S ₂ V	5	0.0072	1	1
MoS ₂	5	0.0065	1	1
MoTe ₂	5	0.4529	1	1
HfS ₂	5	0.474	1	1
FeO ₂	5	0.2468	1	1
AsSn ₂	5	0.5	1	1
Te ₂ V	5	0.4576	1	1
I ₂ Pr	5	0.3203	1	1
CuTe ₂	5	0.4731	1	1
NiO ₂	5	0.2485	1	1
Br ₂ Co	5	0.466	1	1
Tl	5	0.2306	2	1
Ca ₂ N	5	0.4684	1	1
Cl ₂ Ti	5	0.0079	1	1
K	5	0.223	2	1
Te ₂ Zn	5	0.4525	1	1
S ₂ W	5	0.0065	1	1
Br ₂ Mn	5	0.4614	1	1
PtS ₂	5	0.4499	1	1
CoTe ₂	5	0.4748	1	1
CdClO	5	0.4564	1	1
Te ₂ W	5	0.4533	1	1
I ₂ Nd	5	0.3223	1	1
Cl ₂ V	5	0.0025	1	1
OTl ₂	5	0.4569	1	1
Br ₂ Fe	5	0.4661	1	1
TaTe ₂	5	0.4985	1	1
Br ₂ Ni	5	0.4791	1	1
CeI ₂	5	0.3188	1	1
FeSe ₂	5	0.1292	1	1
NbTe ₂	5	0.4874	1	1
MoS ₂	5	0.0063	1	1
Cl ₂ Mg	5	0.4792	1	1
CrSe ₂	5	0.0037	1	1
I ₂ La	5	0.3322	1	1
CrSe ₂	5	0.0013	1	1
N ₂ Re	5	0.2566	1	1
F ₂ Zn	5	0.3123	1	1
CoO ₂	5	0.2478	1	1
CdClHO	6	0.497	1	1
NS ₂ Zr	6	0.4484	1	1
Ir ₂ P ₂	6	0.3219	1	1
Ag ₂ Br ₂	6	0.3333	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

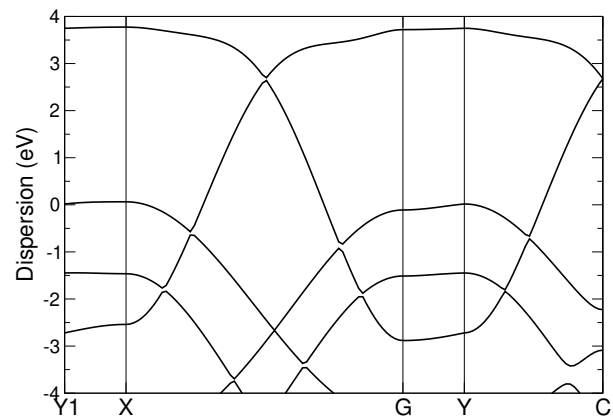
Formula	N° atoms	strain	cell size 1	cell size 2
I ₂ Ni	147	0.0	36	25
As ₂	328	0.0001	91	73
Br ₂ Pr ₂	242	0.0001	49	36
CCL ₂ Lu ₂	547	0.0001	91	73
Br ₂ Mn	443	0.0001	100	81
Sb ₂ Se ₂ Te	307	0.0001	61	37
Br ₂ Er ₂	114	0.0001	25	16
Br ₂ La	309	0.0002	81	49
I ₂ Mg	309	0.0002	81	49
GeTe ₂	147	0.0002	36	25
Bi ₂ Se ₃	407	0.0002	81	49
Ce ₂ I ₂ Si ₂	344	0.0002	61	37
CdClHO	286	0.0003	57	43
Br ₂ Fe	401	0.0003	91	73
Ga ₂ S ₂	418	0.0003	81	64
Br ₂ N ₂ Zr ₂	488	0.0003	73	57
Br ₂ Co	401	0.0004	91	73
CBr ₂ Lu ₂	431	0.0004	73	57
F ₂ Se ₂ Y ₂	42	0.0004	9	4
AuTe ₂	98	0.0004	25	16
Sb ₂ Te ₃	77	0.0005	16	9
I ₂ Mg	233	0.0005	61	37
CoTe ₂	354	0.0005	81	64
Gd ₂ I ₂	358	0.0005	81	49
H ₂ Na ₂ Pd	370	0.0005	65	48
Cl ₂ O ₂ Sc ₂	408	0.0005	69	45
KS ₂ Ti	524	0.0005	100	81
Sb ₂ Se ₂ Te	307	0.0006	61	37
Ni ₂ Te ₂	172	0.0006	36	25
I ₂ S ₂ Tb ₂	248	0.0006	49	25
Ca ₂ N	401	0.0006	91	73
CdClHO	324	0.0006	64	49
NiO ₂	290	0.0006	49	64
AgBrO ₂	418	0.0006	93	58
Hf ₂ I ₂ N ₂	422	0.0006	64	49
Bi ₂ SeTe ₂	77	0.0007	16	9
Br ₂ Gd ₂	114	0.0007	25	16
AgNO ₃	253	0.0007	64	25
N ₃ W ₂	662	0.0007	81	100
Ga ₂ S ₂	418	0.0007	81	64
Ge ₂ Se ₂ Zr ₂	722	0.0007	118	81
Ca ₂ Cl ₂	560	0.0007	118	81
Ba ₂ Cd	138	0.0008	39	20
Cu ₂ I ₂	358	0.0008	81	49
Br ₂ Gd ₂ Ge	407	0.0008	81	49
As ₂ Sn ₂	114	0.0008	25	16
HfS ₂	354	0.0008	81	64
CdCl ₂	147	0.0008	36	25
Cl ₂ O ₂ Yb ₂	314	0.0008	49	36
Br ₂ La	233	0.0008	61	37

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

LiO₂ (P-3m1)

Structural and electronic properties

	Formula	LiO ₂
	Spacegroup	P-3m1
	Prototype	CdI2
	Parent 3D	LiO ₂ S ₂ Ti
	Source DB	ICSD
	DB ID	60533
DF2-C09	Binding energy [meV/ Å²]	64.09
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

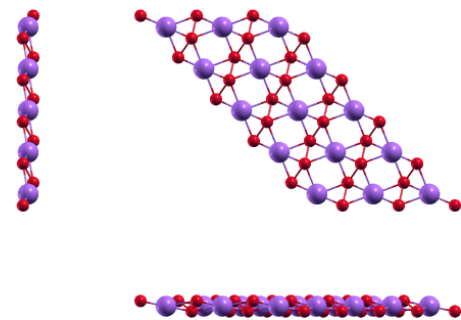


Band structure: Electronic band structure of LiO₂ (P-3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of LiO₂ (P-3m1) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		1.50236066	−3.38797814	0.00000000
a₂		1.50236066	3.38797814	0.00000000
a₃		0.00000000	0.00000000	15.18064725
		x [Å]	y [Å]	z [Å]
●	Li	−1.50236066	−0.00000000	0.00000000
●	O	0.00000000	1.54580962	0.34006988
●	O	−0.00000000	−1.54580962	−0.34006988



Orthographic projections: views of LiO₂ (P-3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	4	0.1182	1	1
Gd	4	0.1101	1	1
HgO	5	0.1273	1	1
GeTe	5	0.1132	1	1
S ₂	5	0.115	1	1
Na	5	0.7045	1	2
CaCl	5	0.637	1	1
IrTe ₂	6	0.1142	1	1
CdCl ₂	6	0.1119	1	1
AgTe ₂	6	0.1203	1	1
S ₂ Ta	6	0.2945	1	1
InSe ₂	6	0.1124	1	1
GeTe ₂	6	0.1108	1	1
I ₂ Mn	6	0.1121	1	1
NSr ₂	6	0.1081	1	1
FeI ₂	6	0.1095	1	1
I ₂ Ni	6	0.111	1	1
CrI ₂	6	0.109	1	1
Bi ₂ Pd	6	0.1358	1	1
Cl ₂ Cu	6	0.3778	1	1
CdO ₂	6	2.7436	1	1
O ₂ Zn	6	8.3026	1	1
MnSe ₂	6	0.6368	1	1
Br ₂ Mg	6	0.1094	1	1
I ₂ Ti	6	0.1071	1	1
Se ₂ Sn	6	1.1054	1	1
H ₂ Si ₂	7	0.1127	1	1
Li ₂ Tl ₂	7	1.2485	1	1
Cl ₂ Gd ₂	7	0.1177	1	1
Cl ₂ OOs	7	0.6524	1	1
Cl ₂ Hf ₂	7	0.2965	1	1
Ca ₂ O ₂	7	0.1371	1	1
Cl ₂ OV	7	0.1411	1	1
Br ₂ Hf ₂	7	2.8667	1	1
Tl	7	0.1367	2	1
S ₂ Zn ₂	7	0.1166	1	1
Ge ₂ S ₂	7	0.4438	1	1
Cl ₂ Zr ₂	7	0.3105	1	1
P ₂ Sn ₂	7	0.1162	1	1
LiMnSe ₂	7	0.12	1	1
Mg ₄	7	0.118	1	1
Sn	7	0.2293	2	1
Ga ₂ Se ₂	7	0.1145	1	1
Fe ₂ S ₂	7	0.6303	1	1
Co ₂ S ₂	7	0.6392	1	1
Ni ₂ Te ₂	7	0.1117	1	1
LiNbS ₂	7	0.2946	1	1
I ₂ Y ₂	7	0.1192	1	1
Cl ₂ Tb ₂	7	0.1186	1	1
Ca ₂ Cl ₂	7	0.6512	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

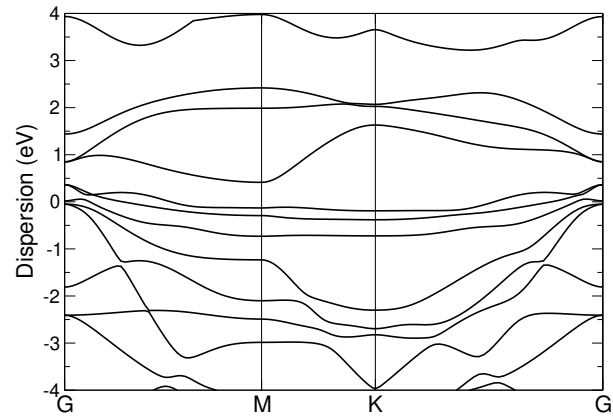
Formula	N° atoms	strain	cell size 1	cell size 2
N ₄	562	0.0003	74	85
Se ₂ Ta ₄	75	0.0005	9	8
Br ₂ F ₂ Yb ₂	510	0.0005	72	49
I ₂ Lu ₂ Se ₂	537	0.0006	99	40
Fe ₂ SeTe	294	0.0006	50	36
Br ₂ Ca ₂ F ₂	510	0.0006	72	49
Br ₂ Cr ₂ O ₂	777	0.0007	99	80
Br ₂ Lu ₂ O ₂	366	0.0007	50	36
CdO ₂	705	0.0007	117	118
I ₂ N ₂ Zr ₂	381	0.0008	55	36
I ₂ Lu ₂ S ₂	330	0.0008	56	27
Br ₂ H ₂ Yb ₂	366	0.0008	50	36
Br ₂ Cu ₂	412	0.0008	72	49
As ₂ Fe ₂ Li ₂	366	0.0008	50	36
O ₄ PTl	72	0.0008	12	6
Ge ₂ Te ₂ Zr ₂	366	0.0008	50	36
F ₂ Zn	363	0.0009	72	49
Br ₂ N ₂ Ti ₂	477	0.001	63	48
BiBrTe	327	0.001	67	42
Te ₂ Zn	387	0.001	67	62
BrKO ₃	264	0.001	63	15
Cl ₂ H ₂ Zr ₂	558	0.001	60	63
AgNO ₂	433	0.0011	79	49
S ₂ Zn ₂	103	0.0011	17	13
Br ₂ Gd ₂ O ₂	510	0.0011	72	49
Ag ₂ Te ₂	232	0.0011	40	28
NbS ₂	369	0.0011	60	63
Cl ₂ Gd ₂	103	0.0011	17	13
Br ₂ O ₂ Tb ₂	510	0.0012	72	49
Ba ₂ F ₂ I ₂	72	0.0012	12	6
F ₄ Nb	551	0.0012	92	55
Br ₂ Cr ₂ S ₂	282	0.0012	40	27
Nd	373	0.0012	81	130
F ₂ Se ₂ Yb ₂	129	0.0012	17	13
Cl ₂ Hf ₂	831	0.0012	117	120
CrTe ₂	369	0.0012	63	60
SSb ₂ Te ₂	350	0.0012	55	37
LiOS ₂ Ti	495	0.0012	60	63
Cl ₂ Sc ₂	429	0.0013	63	60
P ₂ Sn ₂	103	0.0013	17	13
Ca ₄ Cu ₂	534	0.0013	98	40
AgTl	335	0.0013	79	49
HN ₃ OZn	588	0.0013	62	67
Br ₂ O ₂ Sc ₂	468	0.0014	64	46
Au ₂ Se ₂	307	0.0014	65	28
Br ₂ Cr	369	0.0014	63	60
Cl ₂ N ₂ Ti ₂	648	0.0014	84	66
Cu ₂ Sr ₂	369	0.0015	67	42
Bi ₂	470	0.0015	110	70
Br ₂ H ₂ Zr ₂	549	0.0015	63	60

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

LiTiS₂O (P3m1)

Structural and electronic properties

	Formula	LiTiS ₂ O
	Spacegroup	P3m1
	Prototype	LiOS2Ti
	Parent 3D	Li ₃ O ₃ S ₆ Ti ₃
	Source DB	MPDS
	DB ID	S2050313
DF2-C09	Binding energy [meV/ Å²]	36.62
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

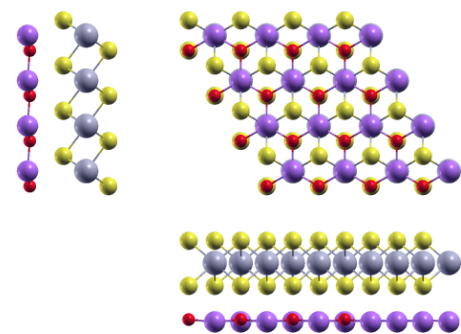


Band structure: Electronic band structure of LiTiS₂O (P3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of LiTiS₂O (P3m1) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		-1.67540786	-2.90189154	0.00000000
a₂		3.35081572	0.00000000	0.00000000
a₃		0.00000000	0.00000000	22.13054544
		x [Å]	y [Å]	z [Å]
●	Li	0.00000000	-1.93459436	2.28580195
●	Ti	0.00000000	-1.93459436	-1.48992981
●	S	0.00000000	0.00000000	-2.91550895
●	S	1.67540786	-0.96729718	-0.01846809
●	O	0.00000000	0.00000000	2.13810490



Orthographic projections: views of LiTiS₂O (P3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	6	0.1469	1	1
Tl	6	0.0042	1	1
Sn	6	0.1224	1	1
In	6	0.1251	1	1
AsSb	7	0.5001	1	1
Mg ₂	7	0.1332	1	1
Cl ₂ Mn	8	0.0015	1	1
AgTe ₂	8	0.1497	1	1
MoSe ₂	8	0.0049	1	1
S ₂ Ta	8	0.0036	1	1
Br ₂ Zn	8	0.4734	1	1
AsSn ₂	8	0.4561	1	1
SiTe ₂	8	0.484	1	1
PbS ₂	8	0.4932	1	1
Cl ₂ Ti	8	0.0091	1	1
S ₂ Ti	8	0.0087	1	1
Mg ₃	8	0.1416	1	1
Te ₂ Ti	8	0.4741	1	1
NbS ₂	8	0.0032	1	1
CrI ₂	8	2.9238	1	1
RhTe ₂	8	0.4631	1	1
N ₂ W	8	0.2684	1	1
Cl ₂ Co	8	0.0084	1	1
NbS ₂	8	0.0012	1	1
Cl ₂ Fe	8	0.0076	1	1
S ₂ Ta	8	0.002	1	1
Se ₂ V	8	0.0033	1	1
NiTe ₂	8	0.4824	1	1
Cl ₂ Cu	8	0.1172	1	1
Se ₂ Zr	8	0.4851	1	1
PtSe ₂	8	0.4577	1	1
CdO ₂	8	0.0082	1	1
CoI ₂	8	0.5012	1	1
O ₂ Zn	8	0.2735	1	1
TaTe ₂	8	0.4546	1	1
Cl ₂ Zr	8	0.008	1	1
FeSe ₂	8	0.1188	1	1
F ₂ Na	8	0.4784	1	1
HfSe ₂	8	0.4742	1	1
Se ₂ W	8	0.0047	1	1
Cu ₂ I ₂	9	0.3305	1	1
CdClHO	9	0.4533	1	1
Br ₂ Pr ₂	9	0.4764	1	1
HNiO ₂	9	0.2579	1	1
Cl ₂ Hf ₂	9	0.0049	1	1
Bi ₂ Mn ₂	9	0.2381	1	1
CdClHO	9	0.4612	1	1
Cl ₂ Y ₂	9	0.4702	1	1
O ₂ Pb ₂	9	0.3235	1	1
As ₄	9	0.3813	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

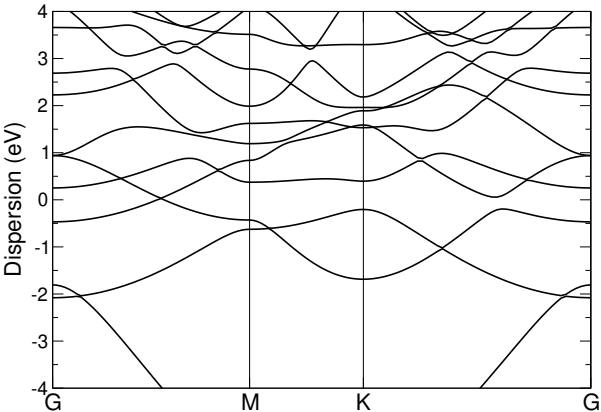
Formula	N° atoms	strain	cell size 1	cell size 2
CdClHO	824	0.0	100	81
Bi ₂ SeTe ₂	490	0.0	61	37
Br ₂ Tb ₂	280	0.0001	36	25
NSr ₂	414	0.0001	57	43
C ₂ F ₂	569	0.0001	49	81
Br ₂ Pr ₂	661	0.0002	81	64
Bi ₂ S ₃	305	0.0002	36	25
Ni ₂ SbTe ₂	425	0.0002	49	36
ClH ₃ O	590	0.0003	79	39
SiTe ₂	536	0.0003	73	57
NiTe ₂	536	0.0003	73	57
Se ₂ Sn	414	0.0004	57	43
S ₂	317	0.0004	49	36
GeI ₃ Rb	50	0.0004	9	1
I ₂ N ₂ Zr ₂	893	0.0004	91	73
Br ₂ Ho ₂	280	0.0004	36	25
I ₂ Yb	107	0.0004	16	9
N ₃ W ₂	500	0.0004	43	57
Cu ₂ Na ₂ Te ₂	315	0.0005	39	20
Cl ₂ Y ₂	500	0.0005	57	43
Cl ₂ Er ₂ O ₂	707	0.0005	73	57
Sb ₂ Te ₃	650	0.0005	81	49
I ₂ La ₂	189	0.0005	25	16
Bi ₂	379	0.0005	61	37
Ge ₂ Se ₂ Zr ₂	613	0.0006	65	48
Ca ₂ Cl ₂	517	0.0006	65	48
N ₂ W	705	0.0006	81	100
P ₂ Sn ₂	389	0.0006	49	36
Ga ₂ Se ₂	747	0.0006	91	73
Ba ₂ Cu ₂	116	0.0006	16	9
AgClO ₄	974	0.0006	130	54
NS ₂ Ta	729	0.0007	73	91
H ₂ MnO ₂	565	0.0007	49	64
PdTe ₂	255	0.0007	36	25
GeI ₂ La ₂	125	0.0007	16	9
Se ₂ Zr	536	0.0007	73	57
HfSe ₂	597	0.0007	81	64
BN	77	0.0007	9	16
F ₂ Se ₂ Yb ₂	461	0.0007	49	36
Te ₂ Ti	597	0.0007	81	64
C ₂ F ₂	429	0.0008	37	61
RhTe ₂	743	0.0008	100	81
Sm	246	0.0008	37	61
CrI ₂	414	0.0008	57	43
BrCdI	173	0.0008	25	16
Ga ₂ Se ₂	389	0.0008	49	36
PbS ₂	467	0.0008	64	49
SSb ₂ Te ₂	205	0.0009	25	16
Cl ₂ O ₂ Yb ₂	789	0.0009	81	64
Cl ₂ H ₂ Zr ₂	11	0.0009	1	1

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

LiTl (P3m1 (156))

Structural and electronic properties

	Formula	LiTl
	Spacegroup	P3m1 (156)
	Prototype	LiTl
	Parent 3D	Li ₄ Tl ₄
	Source DB	ICSD
	DB ID	262070
DF2-C09	Binding energy [meV/ Å²]	117.26
RVV10	Binding energy [meV/ Å²]	108.18
	Band gap (PBE) [eV]	0.01

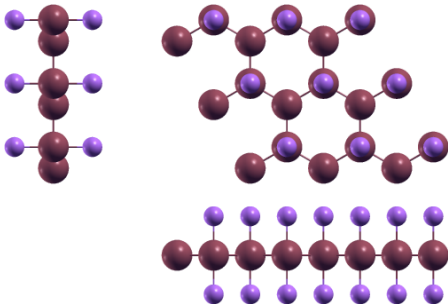


Band structure: Electronic band structure of LiTl (P3m1 (156)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of LiTl (P3m1 (156)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	5.05118348	0.00000000	0.00000000
a₂	-2.52559174	4.37445322	0.00000000
a₃	0.00000000	0.00000000	25.76469504
	x [Å]	y [Å]	z [Å]
● Li	2.52559174	1.45815107	15.57076124
● Tl	2.52559174	1.45815107	12.88272470
● Tl	0.00000000	0.00000000	12.87898188
● Li	2.52559174	1.45815107	10.19461230



Orthographic projections: views of LiTl (P3m1 (156)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.115	1	1
K	5	0.2721	1	1
Bi ₂	6	1.5218	1	1
CaI ₂	7	0.259	1	1
I ₂ Yb	7	0.2555	1	1
LiO ₂	7	0.1984	1	1
HgI ₂	7	0.124	1	1
Ba ₂ Hg	7	0.4349	1	1
CNRb	7	0.1933	1	1
I ₂ Tm	7	0.2574	1	1
BiTe	7	1.5951	1	1
DyI ₂	7	0.2629	1	1
Bi ₂ In ₂	8	0.1354	1	1
Cu ₂ Sr ₂	8	1.5548	1	1
In ₂ Se ₂	8	0.6598	1	1
S ₂ Sn ₂	8	0.11	1	1
Au ₂ Br ₂	8	0.1183	1	1
AlLiTe ₂	8	1.5867	1	1
N ₃ Na	8	0.125	1	1
S ₂ Zn ₂	8	4.8458	1	1
Ge ₂ S ₂	8	0.1105	1	1
Ge ₂ Se ₂	8	0.109	1	1
La ₂ S ₂	8	0.1148	1	1
PbS ₂ Sn	8	0.1111	1	1
Ba ₂ Cu ₂	8	0.2553	1	1
Ag ₂ I ₂	8	0.1246	1	1
Se ₂ Sn ₂	8	0.1158	1	1
Br ₂ CsF	8	0.1338	1	1
Sn ₂ Te ₂	8	0.1297	1	1
Cl ₂ Tb ₂	8	4.8804	1	1
F ₄ Pb	9	0.1197	1	1
F ₄ Sn	9	0.4331	1	1
AsI ₂ La ₂	9	0.2491	1	1
Bi ₂ Te ₃	9	1.5946	1	1
GeI ₂ La ₂	9	0.257	1	1
I ₂ La ₂ P	9	1.5614	1	1
Cd ₂ I ₃	9	0.2491	1	1
Sb ₂ Te ₃	9	1.534	1	1
Bi ₂ SeTe ₂	9	1.5259	1	1
I ₂ La ₂ Sb	9	0.2726	1	1
Cl ₄ Mn	9	0.14	1	1
I ₂ La ₂ Te	9	0.2686	1	1
Ba ₂ H ₂ I ₂	10	0.1324	1	1
MoTe ₂	10	0.2211	1	2
Gd ₂ I ₂ S ₂	10	0.2663	1	1
Cl ₂ O ₂ V ₂	10	0.117	1	1
C ₂ Br ₂ Y ₂	10	0.2065	1	1
Cu ₄ Te ₂	10	1.5382	1	1
AlH ₄ Na	10	0.1422	1	1
Te ₂ V	10	0.2236	1	2

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

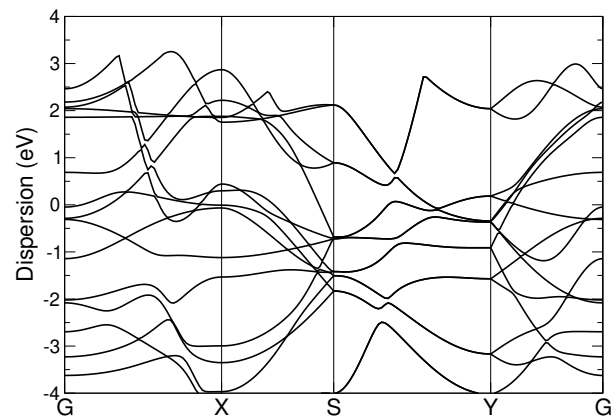
Formula	N° atoms	strain	cell size 1	cell size 2
Br ₂ Er ₂	164	0.0	16	25
I ₂ Yb	447	0.0	57	73
CCL ₂ Lu ₂	345	0.0	25	49
Se ₂ Ti	496	0.0001	49	100
Ga ₂ I ₂ Y ₂	316	0.0001	25	36
BiBrTe	291	0.0001	36	49
As ₂	198	0.0001	25	49
Na	235	0.0001	39	79
Br ₂ Ca ₃ Si	324	0.0001	36	30
Cd ₂ I ₃	516	0.0001	49	64
Ba ₂ Cu ₂	520	0.0001	57	73
I ₂ Y ₂	392	0.0001	37	61
AsI ₂ La ₂	516	0.0001	49	64
NiTe ₂	84	0.0002	9	16
BaF ₂	208	0.0002	25	36
CaI ₂	499	0.0002	64	81
Cl ₂ Tb ₂	520	0.0002	49	81
Ga ₂ S ₃	551	0.0003	39	79
Br ₂ Fe	247	0.0003	25	49
Bi ₂ Te ₃	457	0.0003	43	57
Co ₂ Se ₂	692	0.0003	65	108
NS ₂ Zr	472	0.0003	39	79
Br ₂ Zr ₂	596	0.0003	49	100
Cl ₂ NSc ₂	61	0.0003	4	9
Br ₂ Co	247	0.0003	25	49
BiTe	343	0.0004	43	57
Cl ₂ Tb ₂	392	0.0004	37	61
CaClHO	100	0.0005	9	16
Cl ₂ Gd ₂	520	0.0005	49	81
In	164	0.0005	25	64
Br ₂ Gd ₂	164	0.0005	16	25
FeH ₂ O ₂	161	0.0005	9	25
I ₂ S ₂ Tb ₂	838	0.0005	73	91
AuTe ₂	139	0.0006	16	25
Cl ₂ O ₂ Tm ₂	132	0.0006	9	16
Ca ₂ N	247	0.0006	25	49
As ₂ Sn ₂	164	0.0006	16	25
CNRb	551	0.0006	80	77
Br ₂ Ca ₃ Si	924	0.0006	81	100
I ₂ La ₂ Te	824	0.0007	81	100
Ni ₂ Se ₂	796	0.0007	81	118
LiMnSe ₂	392	0.0007	37	61
SiTe ₂	84	0.0007	9	16
AlLiTe ₂	400	0.0008	43	57
Cl ₂ Mn	43	0.0008	4	9
Te ₄ W ₂	700	0.0008	70	70
NbS ₂	43	0.0008	4	9
Br ₂ Ca ₃ Si	924	0.0008	81	100
F ₂ Se ₂ Tm ₂	514	0.0009	37	61
Hf ₂ Si ₂ Te ₂	908	0.0009	65	108

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Mn₂Bi₂ (Pmma)

Structural and electronic properties

	Formula	Mn ₂ Bi ₂
	Spacegroup	Pmma
	Prototype	FeSe
	Parent 3D	Bi ₂ Mn ₂
	Source DB	MPDS
	DB ID	S1831446
DF2-C09	Binding energy [meV/ Å²]	30.7
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

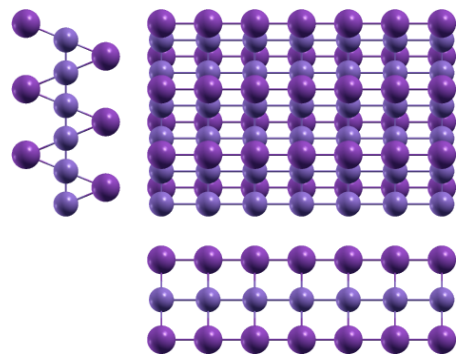


Band structure: Electronic band structure of Mn₂Bi₂ (Pmma) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Mn₂Bi₂ (Pmma) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		0.00000000	-2.93552187	0.00000000
a₂		4.11100168	0.00000000	0.00000000
a₃		0.00000000	0.00000000	22.01023714
		x [Å]	y [Å]	z [Å]
●	Bi	-1.02775042	0.00000000	-8.50283500
●	Mn	-2.05550084	0.00000000	-11.00511857
●	Mn	0.00000000	0.00000000	-11.00511857
●	Bi	1.02775042	0.00000000	-13.50740215



Orthographic projections: views of Mn₂Bi₂ (Pmma) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	5	0.1309	1	1
Na	5	0.1511	1	1
Sm	5	0.4533	1	1
HgO	6	0.9477	1	1
AsSb	6	0.1882	1	1
GeTe	6	0.1955	1	1
AgTl	6	0.4084	1	1
As ₂	6	0.1578	1	1
S ₂	6	0.1974	1	1
IrTe ₂	7	0.1966	1	1
Cl ₂ Zn	7	0.1569	1	1
CdCl ₂	7	0.1942	1	1
Cl ₂ Mn	7	0.1339	1	1
MoTe ₂	7	0.1529	1	1
PSn ₂	7	0.166	1	1
MoSe ₂	7	0.1305	1	1
ReSe ₂	7	0.1419	1	1
S ₂ Ta	7	0.135	1	1
Br ₂ Zn	7	0.1768	1	1
HfS ₂	7	0.1602	1	1
InSe ₂	7	0.1946	1	1
AsSn ₂	7	0.1697	1	1
GeTe ₂	7	0.193	1	1
SiTe ₂	7	0.1813	1	1
Te ₂ V	7	0.1545	1	1
I ₂ Mn	7	0.1943	1	1
CuTe ₂	7	0.1599	1	1
S ₂ Zr	7	0.1653	1	1
Br ₂ Cu	7	0.1354	1	1
NSr ₂	7	0.1901	1	1
PbS ₂	7	0.1853	1	1
Br ₂ Co	7	0.1574	1	1
Ca ₂ N	7	0.1582	1	1
FeI ₂	7	0.1917	1	1
I ₂ Ni	7	0.1932	1	1
S ₂ Ti	7	0.138	1	1
Te ₂ Ti	7	0.1772	1	1
NbS ₂	7	0.1348	1	1
CrI ₂	7	0.1911	1	1
Te ₂ Zn	7	0.1528	1	1
RhTe ₂	7	0.1726	1	1
Ba ₂ Hg	7	0.4221	1	1
N ₂ W	7	0.1179	1	1
Br ₂ Mn	7	0.1558	1	1
Cl ₂ Ni	7	0.1425	1	1
Cl ₂ Co	7	0.1378	1	1
CrTe ₂	7	0.1469	1	1
PtS ₂	7	0.1519	1	1
NbS ₂	7	0.1324	1	1
CoTe ₂	7	0.1605	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

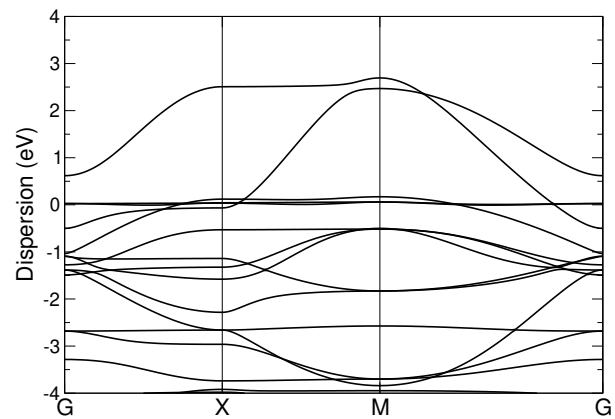
Formula	N° atoms	strain	cell size 1	cell size 2
Br ₂ F ₂ Sr ₂	58	0.0001	7	5
Br ₂ F ₂ Pb ₂	58	0.0004	7	5
Cl ₂ Hf ₂	124	0.0004	14	17
Hf ₂ Se ₂ Si ₂	354	0.0006	36	35
Cl ₄ Mn	431	0.0008	64	35
C ₂ Li ₂	900	0.0008	126	99
RhTe ₂	378	0.0009	54	54
I ₂ N ₂ Zr ₂	540	0.001	54	54
I ₂ Pb	285	0.001	48	31
Fe ₂ Li ₂ P ₂	376	0.001	40	36
BiTe	616	0.0011	100	72
PbS ₂	425	0.0011	62	59
As ₂ Fe ₂	284	0.0011	36	35
AuI ₄ Li	692	0.0011	110	42
Bi ₂ Te ₃	760	0.0011	100	72
Br ₂ Y ₂	484	0.0012	62	59
Ga ₂ Se ₂	892	0.0012	114	109
As ₄	468	0.0012	69	48
NS ₂ Ta	316	0.0013	31	48
I ₂ Pr ₂ S ₂	378	0.0013	48	31
Br ₂ CsF	640	0.0013	102	58
Cl ₄ KTI	408	0.0014	72	20
Ga ₂ Se ₂	484	0.0014	62	59
CdClHO	432	0.0014	54	54
Cl ₂ Rh ₂ Te ₂	564	0.0014	81	40
HfSe ₂	764	0.0014	110	108
Te ₂ Ti	764	0.0014	110	108
Hf ₂ Si ₂ Te ₂	376	0.0015	40	36
Bi ₂ Te ₂	372	0.0015	58	35
LiNbS ₂	124	0.0015	14	17
Ba ₂ H ₂ I ₂	756	0.0015	102	58
S ₂ Ta	107	0.0016	14	17
Br ₂ Zn	764	0.0016	110	108
Fe ₂ Se ₂	636	0.0016	84	75
Cr ₂ O ₄	268	0.0016	25	28
N ₂ W	757	0.0016	88	135
F ₄ Nb	53	0.0016	7	5
Si ₂ Te ₂ Zr ₂	786	0.0017	84	75
F ₂ Ni	561	0.0017	84	75
Cl ₂ Rh ₂ Te ₂	550	0.0017	79	39
Br ₂ Dy ₂ S ₂	66	0.0017	9	5
PTe ₂ Zr ₂	543	0.0017	62	59
Sb ₂ Te ₂	316	0.0017	48	31
Br ₂ H ₂ Sr ₂	58	0.0017	7	5
AgCuTe ₂	620	0.0017	82	73
Cu ₂ Se ₂	672	0.0018	89	79
Ca ₂ Cl ₂	936	0.0018	122	112
CNRb	446	0.0018	80	42
I ₂ N ₂ Zr ₂	634	0.0018	73	57
Ga ₂ Se ₂	432	0.0018	54	54

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

MnCl₄ (P4/mmm)

Structural and electronic properties

	Formula	MnCl ₄
	Spacegroup	P4/mmm
	Prototype	SnF4
	Parent 3D	Cl ₄ MnN ₂
	Source DB	MPDS
	DB ID	S1100446
DF2-C09	Binding energy [meV/ Å²]	38.6
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

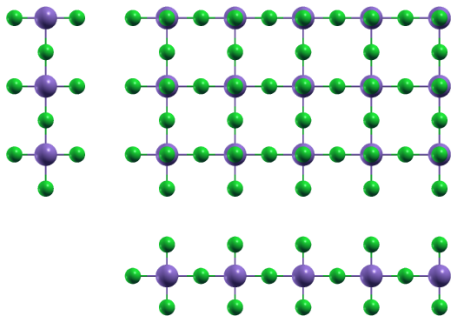


Band structure: Electronic band structure of MnCl₄ (P4/mmm) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of MnCl₄ (P4/mmm) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		4.68985167	0.00000000	0.00000000
a₂		0.00000000	4.68985167	0.00000000
a₃		0.00000000	0.00000000	20.34120020
		x [Å]	y [Å]	z [Å]
●	Cl	2.34492583	-2.34492583	-2.15529952
●	Mn	2.34492583	-2.34492583	0.00000000
●	Cl	2.34492583	-2.34492583	2.15529952
●	Cl	2.34492583	0.00000000	0.00000000
●	Cl	0.00000000	-2.34492583	0.00000000



Orthographic projections: views of MnCl₄ (P4/mmm) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
AsSb	7	0.1107	1	1
GeTe	7	0.1094	1	1
Gd	7	0.1441	1	2
IrTe ₂	8	0.1092	1	1
CdCl ₂	8	0.1096	1	1
InSe ₂	8	0.1095	1	1
I ₂ Mn	8	0.1096	1	1
Br ₂ Cu	8	0.1028	1	1
NSr ₂	8	0.1103	1	1
I ₂ Yb	8	0.109	1	1
FeI ₂	8	0.11	1	1
I ₂ Ni	8	0.1098	1	1
CrI ₂	8	0.1101	1	1
Ba ₂ Hg	8	0.2145	1	1
CNRb	8	0.0373	1	1
CKN	8	0.251	1	1
CoI ₂	8	0.1106	1	1
Br ₂ Mg	8	0.1101	1	1
CNNa	8	0.4784	1	1
Se ₂ Sn	8	0.1104	1	1
Ba ₂ Cd	8	0.2175	1	1
H ₂ Si ₂	9	0.1095	1	1
Li ₂ Tl ₂	9	0.1418	1	1
Bi ₂ In ₂	9	0.0055	1	1
Cu ₂ I ₂	9	0.5909	1	1
Nd	9	0.0554	1	4
S ₂ Sn ₂	9	0.2059	1	1
Au ₂ Br ₂	9	0.6369	1	1
Ge ₂ Te ₂	9	0.2249	1	1
N ₃ Na	9	0.0292	1	1
S ₂ Zn ₂	9	0.1088	1	1
As ₄	9	0.1911	1	1
Ga ₂ Se ₂	9	0.1114	1	1
P ₄	9	0.1635	1	1
P ₂ Sn ₂	9	0.1089	1	1
Ga ₂ Se ₂	9	0.1092	1	1
Ni ₂ Te ₂	9	0.1096	1	1
Bi ₂ O ₂	9	0.5848	1	1
La ₂ S ₂	9	0.2256	1	1
PbS ₂ Sn	9	0.215	1	1
Ba ₂ Cu ₂	9	0.109	1	1
Br ₂ CsF	9	0.0075	1	1
As ₂ O ₃	10	0.1771	1	1
F ₄ Sn	10	0.2136	1	1
PTe ₂ Zr ₂	10	0.1109	1	1
F ₄ Nb	10	0.2073	1	1
NaO ₄	10	0.1505	1	1
AgNO ₃	10	0.1513	1	1
In ₂ S ₃	10	0.1093	1	1
Ni ₂ SbTe ₂	10	0.109	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

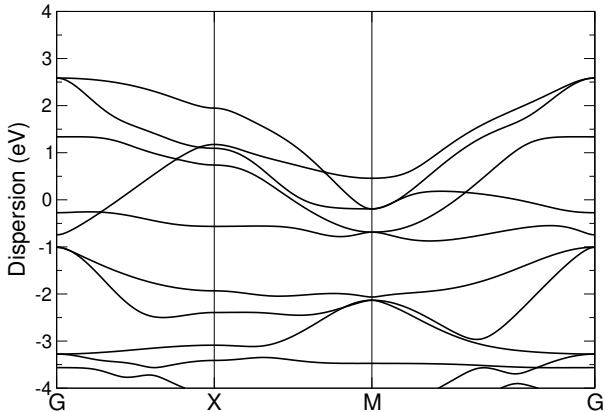
Formula	N° atoms	strain	cell size 1	cell size 2
F ₄ Sn	735	0.0	65	82
I ₂ O ₂ Yb ₂	341	0.0001	25	36
Co ₂ Se ₂	569	0.0001	49	81
As ₂	178	0.0002	20	39
BiBrTe	435	0.0002	48	65
Hf ₂ Se ₂ Si ₂	141	0.0002	9	16
CCl ₂ Lu ₂	295	0.0002	20	39
Ge ₂ Mn ₂ Sr ₂	815	0.0003	61	85
I ₂ Pr	233	0.0003	25	36
C ₂ Br ₂ La ₂	760	0.0003	56	80
As ₂ Fe ₂	109	0.0003	9	16
As ₂ Fe ₂ Li ₂	230	0.0004	16	25
Mg ₃	47	0.0004	4	9
Br ₂ F ₂ Pb ₂	629	0.0004	49	64
Br ₂ H ₂ Yb ₂	230	0.0004	16	25
Br ₂ Fe	217	0.0004	20	39
Br ₂ F ₂ Sr ₂	640	0.0004	50	65
O ₂ Pb ₂	877	0.0005	85	113
Fe ₂ Se ₂	749	0.0005	65	106
Br ₂ Co	217	0.0005	20	39
Ir ₂ P ₂	269	0.0005	25	36
Ca ₂ N	217	0.0005	20	39
Ba ₂ Ge ₂ Mn ₂	474	0.0006	36	49
As ₂ Ir ₂	645	0.0006	61	85
Br ₂ O ₂ Sm ₂	341	0.0006	25	36
Br ₂ F ₂ Sr ₂	629	0.0007	49	64
F ₂ I ₂ Tm ₂	474	0.0007	36	49
MnNaTe ₂	877	0.0007	81	118
Fe ₂ SeTe	180	0.0007	16	25
CBr ₂ Y ₂	505	0.0007	36	65
I ₂ Nd	233	0.0007	25	36
Hf ₂ Si ₂ Te ₂	731	0.0007	49	81
Bi ₂ Mn ₂	431	0.0008	35	64
Cu ₂ Na ₂ Se ₂	474	0.0008	36	49
Bi ₂ I ₂ O ₂	474	0.0008	36	49
F ₄ Sn	725	0.0008	64	81
Bi ₂ O ₂	877	0.0008	85	113
Ge ₂ Se ₂ Zr ₂	872	0.0008	58	97
Cl ₄ KTI	395	0.0008	49	25
Ca ₂ Cl ₂	678	0.0008	58	97
Ba ₂ Hg	571	0.0008	65	82
Cl ₂ F ₂ Pb ₂	474	0.0009	36	49
F ₂ I ₂ Yb ₂	474	0.0009	36	49
C ₄ Ca ₂	907	0.0009	71	92
I ₂ La ₂ O ₂	806	0.0009	64	81
BrCdI	759	0.0009	81	118
Br ₂ H ₂ Sr ₂	629	0.0009	49	64
Br ₂ Eu ₂ O ₂	341	0.0009	25	36
Bi ₂ Pd	817	0.0009	74	149
Cu ₂ Sr ₂	500	0.001	48	65

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

MnSe₂ (P-4m2)

Structural and electronic properties

	Formula	MnSe ₂
	Spacegroup	P-4m2
	Prototype	HgI2
	Parent 3D	KMnSe ₂
	Source DB	ICSD
	DB ID	672265
DF2-C09	Binding energy [meV/ Å²]	93.05
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

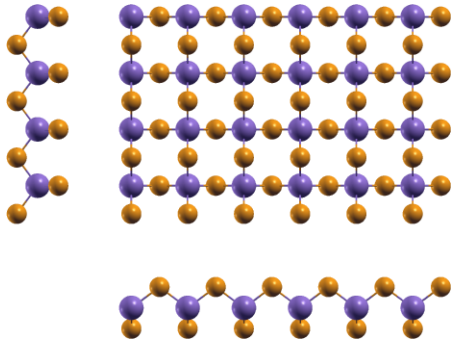


Band structure: Electronic band structure of MnSe₂ (P-4m2) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of MnSe₂ (P-4m2) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.59936198	0.00000000	0.00000000
a₂	0.00000000	3.59936198	0.00000000
a₃	0.00000000	0.00000000	16.76349095
	x [Å]	y [Å]	z [Å]
● Mn	0.00000000	-1.79968099	0.00000000
● Se	0.00000000	-3.59936198	1.33236158
● Se	1.79968099	-1.79968099	-1.33236158



Orthographic projections: views of MnSe₂ (P-4m2) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	4	0.2069	1	1
InSe	5	0.1881	1	1
HgO	5	0.2203	1	1
AsSb	5	0.1384	1	1
Bi ₂	5	0.1957	1	1
GeTe	5	0.1436	1	1
AgTl	5	0.4092	1	1
S ₂	5	0.145	1	1
PbTe	5	0.1903	1	1
Sb ₂	5	0.1687	1	1
CaCl	5	0.0001	1	1
IrTe ₂	6	0.1444	1	1
I ₂ Mg	6	0.1753	1	1
CdCl ₂	6	0.1427	1	1
CdI ₂	6	0.1926	1	1
AgTe ₂	6	0.2101	1	1
Br ₂ Zn	6	0.1305	1	1
Br ₂ Ca	6	0.1942	1	1
InSe ₂	6	0.143	1	1
GeTe ₂	6	0.1418	1	1
SiTe ₂	6	0.1336	1	1
HfTe ₂	6	0.1522	1	1
I ₂ Mn	6	0.1428	1	1
Br ₂ La	6	0.1757	1	1
Br ₂ Cu	6	0.1311	1	1
NSr ₂	6	0.1398	1	1
PbS ₂	6	0.1363	1	1
BiClTe	6	0.1931	1	1
AuTe ₂	6	0.1601	1	1
BrCdI	6	0.1791	1	1
LiO ₂	6	0.3493	1	1
PdTe ₂	6	0.1576	1	1
FeI ₂	6	0.1408	1	1
I ₂ Ni	6	0.1419	1	1
S ₂ Ti	6	0.1086	1	1
Mg ₃	6	0.5834	1	1
Te ₂ Ti	6	0.1307	1	1
CrI ₂	6	0.1404	1	1
I ₂ Zn	6	0.1651	1	1
BaF ₂	6	0.1832	1	1
GeI ₂	6	0.1731	1	1
Cl ₂ Co	6	0.1085	1	1
Ba ₂ N	6	0.1537	1	1
AsKSn	6	0.1814	1	1
Te ₂ Zr	6	0.1527	1	1
PbTe ₂	6	0.1779	1	1
NiTe ₂	6	0.1331	1	1
SnTe ₂	6	0.1705	1	1
I ₂ V	6	0.1346	1	1
GeI ₂	6	0.1906	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

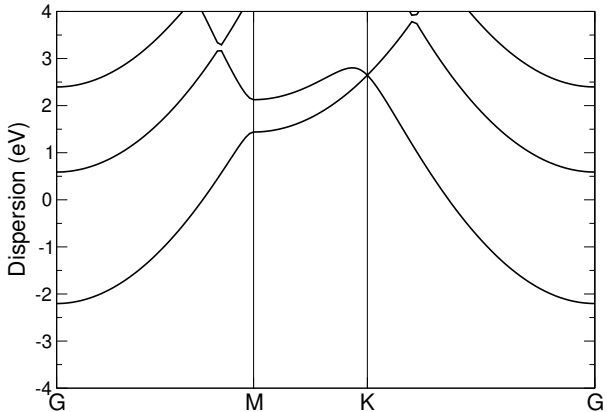
Formula	N° atoms	strain	cell size 1	cell size 2
Ba ₂ H ₂ I ₂	708	0.0	106	65
K ₂ Mn ₂ Sb ₂	795	0.0001	101	82
CaCl	5	0.0001	1	1
Br ₂ Ce ₂ O ₂	795	0.0001	101	82
Eu ₂ I ₂ O ₂	786	0.0001	100	81
K	133	0.0002	36	25
FeSe ₂	675	0.0002	89	136
Mg ₆	687	0.0003	65	82
Bi ₂ O ₂	887	0.0003	145	113
Mg ₃	594	0.0003	85	113
I ₂ O ₂ Pr ₂	627	0.0004	81	64
Cu ₂ Rb ₂ Te ₂	537	0.0004	81	49
Br ₂ F ₂ Pb ₂	495	0.0004	65	50
HgO	448	0.0004	82	101
Tl	209	0.0004	48	65
Mg ₆	678	0.0004	64	81
Br ₂ F ₂ Sr ₂	486	0.0005	64	49
As ₂ Mg ₂ Na ₂	258	0.0005	36	25
Au ₂ Br ₂	492	0.0005	84	60
Se ₂ V	339	0.0005	48	65
Mg ₄	410	0.0006	50	65
K ₂ Mn ₂ Sb ₂	786	0.0006	100	81
Br ₂ Ce ₂ O ₂	786	0.0006	100	81
CrSe ₂	597	0.0007	81	118
Bi ₂ In ₂	439	0.0007	81	49
Ca ₂ Si	597	0.0007	118	81
Ce ₂ I ₂ S ₂	840	0.0007	118	81
FHOZn	715	0.0007	81	118
Co ₂ S ₂	7	0.0007	1	1
Br ₂ F ₂ Pb ₂	486	0.0007	64	49
C ₂ Li ₂	204	0.0008	32	27
Ba ₂ Cd	255	0.0008	49	36
Cu ₄ Te ₂	954	0.0008	120	99
I ₂ O ₂ Sm ₂	786	0.0008	100	81
Sn ₂ Te ₂	748	0.0008	136	85
AgTe ₂	774	0.0009	113	145
I ₃ Sn	292	0.0009	64	25
F ₂ I ₂ Pb ₂	363	0.0009	49	36
HgO	443	0.0009	81	100
I ₂ Nd ₂ O ₂	636	0.0009	82	65
Tl	215	0.001	50	65
Br ₂ H ₂ Sr ₂	495	0.001	65	50
Ca ₂ H ₂ I ₂	795	0.001	101	82
Se ₂ W	339	0.001	48	65
Mg ₂	353	0.001	61	85
CrS ₂	615	0.001	79	126
Cl ₄ Mn	860	0.0011	145	85
MoSe ₂	339	0.0011	48	65
Sb ₂ Te ₂	678	0.0012	118	81
Eu ₂ H ₂ I ₂	786	0.0012	100	81

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Na (P6/mmm (191))

Structural and electronic properties

	Formula	Na
	Spacegroup	P6/mmm (191)
	Prototype	In
	Parent 3D	NaCrSe ₂
	Source DB	COD
	DB ID	9012110
DF2-C09	Binding energy [meV/ Å²]	87.04
RVV10	Binding energy [meV/ Å²]	98.59
	Band gap (PBE) [eV]	0.0

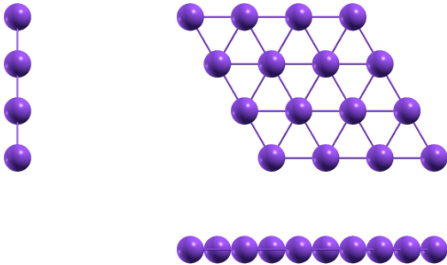


Band structure: Electronic band structure of Na (P6/mmm (191)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Na (P6/mmm (191)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.54835685	0.00000000	0.00000000
a₂	−1.77417843	3.07296718	0.00000000
a₃	0.00000000	0.00000000	20.00000000
	x [Å]	y [Å]	z [Å]
● Na	1.77417843	3.07296718	10.00000000



Orthographic projections: views of Na (P6/mmm (191)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	2	0.3269	1	1
Tl	2	0.1257	1	1
K	2	13.6876	1	1
In	2	0.1118	1	1
In	2	0.2606	1	1
Gd	2	0.1138	1	1
HgO	3	0.1343	1	1
As ₂	3	0.0081	1	1
S ₂	3	0.4504	1	1
LiO	3	0.2758	1	1
Mg ₂	3	0.1166	1	1
IrTe ₂	4	0.4488	1	1
Cl ₂ Zn	4	0.007	1	1
I ₂ Mg	4	3.0178	1	1
S ₂ V	4	0.2651	1	1
MoS ₂	4	0.2661	1	1
MoTe ₂	4	0.0023	1	1
AgTe ₂	4	0.1276	1	1
HfTe ₂	4	0.4695	1	1
Te ₂ V	4	0.0042	1	1
Br ₂ La	4	3.0224	1	1
Br ₂ Cu	4	1.0874	1	1
Br ₂ Co	4	0.0076	1	1
ReS ₂	4	0.2488	1	1
Ca ₂ N	4	0.0086	1	1
AuTe ₂	4	2.8408	1	1
PdTe ₂	4	0.4831	1	1
Mg ₃	4	0.122	1	1
I ₂ Zn	4	0.5017	1	1
Te ₂ Zn	4	0.0021	1	1
S ₂ W	4	0.2662	1	1
Bi ₂ Pd	4	0.1421	1	1
GeI ₂	4	2.9929	1	1
N ₂ W	4	1.5225	1	1
Br ₂ Mn	4	0.0058	1	1
CrTe ₂	4	0.0053	1	1
PtS ₂	4	0.001	1	1
CdClO	4	0.0037	1	1
Ba ₂ N	4	0.4734	1	1
Se ₂ Ti	4	0.0016	1	1
Br ₂ Ti	4	0.0059	1	1
Te ₂ Zr	4	0.4707	1	1
Te ₂ W	4	0.0024	1	1
Cl ₂ V	4	0.2721	1	1
OTl ₂	4	0.0039	1	1
BrNZr	4	0.0085	1	1
Br ₂ Fe	4	0.0077	1	1
Br ₂ Cr	4	0.0056	1	1
FeSe ₂	4	0.4256	1	1
Se ₂ Yb	4	2.9961	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

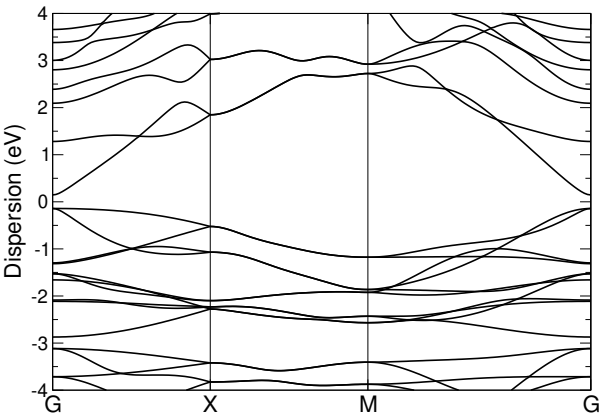
Formula	N° atoms	strain	cell size 1	cell size 2
Cl ₂ La ₂	260	0.0	64	49
PdTe ₂	244	0.0	73	57
O ₂ Zn	183	0.0	36	49
Se ₂ Yb	157	0.0001	49	36
Li ₂ Tl ₂	235	0.0001	79	39
Ge ₂ I ₂ La ₂	121	0.0001	25	16
NaPSn	310	0.0001	91	73
F ₂ Se ₂ Tm ₂	586	0.0002	100	81
F ₂ Tl ₂	257	0.0002	65	48
P ₂ Rh ₂	257	0.0002	65	48
BiTe ₂	157	0.0002	49	36
Br ₂ Ca ₃ Si	283	0.0003	61	37
GeI ₂	157	0.0003	49	36
LiMnSe ₂	424	0.0003	100	81
MnO ₂	292	0.0003	49	81
Pt ₂ Te ₂	383	0.0003	91	73
PbTe	86	0.0003	36	25
H ₂ MgO ₂	528	0.0003	73	91
MnO ₂	220	0.0003	37	61
I ₂ La ₂ Te	246	0.0003	61	37
Ga ₂ S ₃	6	0.0004	1	1
F ₂ Lu ₂ Se ₂	315	0.0004	57	43
As ₂ CeLi ₂	161	0.0004	36	25
ReS ₂	241	0.0004	49	64
H ₂ NiO ₂	581	0.0004	81	100
NS ₂ Zr	5	0.0004	1	1
Br ₂ CsF	119	0.0004	39	20
GeNi ₃ Te ₂	529	0.0005	91	73
H ₂ Na ₂ O ₂	749	0.0005	113	106
Ba ₂ Ni ₃	229	0.0005	49	36
Bi ₂ STe ₂	161	0.0005	36	25
Ga ₂ Te ₂	193	0.0005	49	36
Br ₂ Dy ₂ O ₂	353	0.0005	65	48
Br ₂ O ₂ Y ₂	353	0.0005	65	48
Br ₂ Tb ₂	301	0.0005	73	57
S ₂ V	346	0.0006	73	91
Sb ₂ Se ₂ Te	229	0.0006	49	36
GeI ₂	111	0.0006	36	25
F ₂ Ho ₂ Se ₂	465	0.0006	81	64
IKO ₃	9	0.0006	4	1
I ₂ Pr ₂ Si ₂	265	0.0006	49	36
O ₂ Pt	307	0.0006	64	81
Cu ₂ S ₂	257	0.0006	65	48
Ca ₂ H ₂ I ₂	604	0.0006	118	81
AsCuLi ₂	193	0.0008	49	36
Er ₂ F ₂ Se ₂	529	0.0008	91	73
MoS ₂	381	0.0008	81	100
Bi ₂ S ₃	358	0.0008	73	57
LiMnTe ₂	136	0.0009	36	25
I ₂ Y ₂	424	0.0009	100	81

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

NaCuSe (P4/nmm (129))

Structural and electronic properties

Formula	NaCuSe
Spacegroup	P4/nmm (129)
Prototype	PbClF
Parent 3D	Na ₂ Cu ₂ Se ₂
Source DB	COD
DB ID	7221370
DF2-C09 Binding energy [meV/ Å²]	35.98
RVV10 Binding energy [meV/ Å²]	42.58
Band gap (PBE) [eV]	0.29

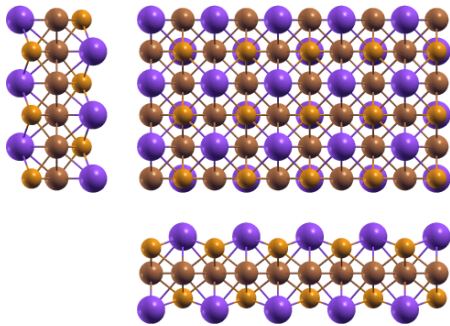


Band structure: Electronic band structure of NaCuSe (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NaCuSe (P4/nmm (129)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.02667279	-0.00000000	0.00000000
a₂	0.00000000	4.02667279	0.00000000
a₃	0.00000000	0.00000000	24.62805102
	x [Å]	y [Å]	z [Å]
Na	0.00000000	2.01333640	14.62887137
Na	2.01333640	-0.00000000	9.99917965
Cu	0.00000000	0.00000000	12.31402551
Cu	2.01333640	2.01333640	12.31402551
Se	0.00000000	2.01333640	10.72664664
Se	2.01333640	-0.00000000	13.90140438



Orthographic projections: views of NaCuSe (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	7	0.167	1	1
Tl	7	0.11	1	1
InSe	8	0.1336	1	1
Bi ₂	8	0.1382	1	1
Ag ₂	8	0.1732	1	1
P ₂	8	0.1112	1	1
PbTe	8	0.1349	1	1
CaCl	8	0.2158	1	1
Cl ₂ Mn	9	0.1088	1	1
CdI ₂	9	0.1363	1	1
Nd	9	0.1804	1	3
MoSe ₂	9	0.1102	1	1
Ba ₂ Pt	9	0.1729	1	1
Br ₂ Ca	9	0.1373	1	1
CaI ₂	9	0.1571	1	1
Br ₂ Cu	9	0.1002	1	1
Ca ₂ Si	9	0.1783	1	1
I ₂ Yb	9	0.1545	1	1
BiClTe	9	0.1366	1	1
Cl ₂ Ti	9	0.1112	1	1
HgI ₂	9	0.383	1	1
BaF ₂	9	0.1307	1	1
BiBrTe	9	0.1412	1	1
NbS ₂	9	0.1094	1	1
S ₂ Ta	9	0.1096	1	1
CKN	9	0.4867	1	1
Se ₂ V	9	0.1098	1	1
AsKSn	9	0.1297	1	1
Cl ₂ Cu	9	0.0966	1	1
I ₂ Tm	9	0.1559	1	1
GeI ₂	9	0.1351	1	1
I ₂ Pb	9	0.1751	1	1
STl ₂	9	0.1314	1	1
BiTe	9	0.147	1	1
GeS ₂	9	0.5891	1	1
MnSe ₂	9	0.2157	1	1
DyI ₂	9	0.1601	1	1
GdI ₂	9	0.1437	1	1
I ₂ La	9	0.0085	1	1
CdI ₂	9	0.136	1	1
Sm	9	0.1615	1	3
I ₂ Pr	9	0.1367	1	1
Se ₂ W	9	0.1102	1	1
Bi ₂ Te ₂	10	0.1945	1	1
Bi ₂ In ₂	10	1.1275	1	1
Cu ₂ I ₂	10	0.0077	1	1
Cu ₂ Sr ₂	10	0.1421	1	1
Cl ₂ OOs	10	0.2221	1	1
LiMnTe ₂	10	0.1354	1	1
Cu ₂ Te ₂	10	0.0575	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

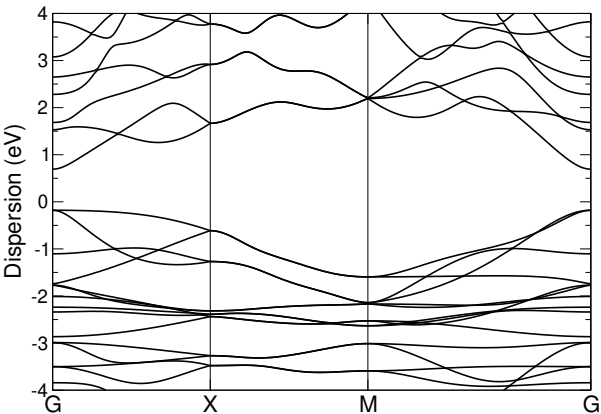
Formula	N° atoms	strain	cell size 1	cell size 2
Bi ₂ I ₂ O ₂	12	0.0	1	1
Cl ₂ F ₂ Pb ₂	12	0.0001	1	1
Ba ₂ F ₂ I ₂	882	0.0001	82	65
Fe ₂ S ₂	718	0.0001	65	82
F ₂ I ₂ Tm ₂	12	0.0001	1	1
HgI ₂	843	0.0003	100	81
I ₃ Sn	866	0.0004	109	53
CoH ₂ O ₂	315	0.0005	20	39
Ba ₂ H ₂ I ₂	690	0.0005	65	50
Ba ₂ H ₂ I ₂	678	0.0006	64	49
Hf ₂ Se ₂ Si ₂	678	0.0006	49	64
O ₄ PTl	882	0.0006	82	65
Ca ₂ Cl ₂	896	0.0006	82	101
ReS ₂	237	0.0006	20	39
CdClHO	548	0.0006	48	65
Fe ₂ S ₂	708	0.0007	64	81
Cl ₄ Mn	474	0.0008	49	36
PtSe ₂	483	0.0008	48	65
Ba ₂ F ₂ I ₂	870	0.0008	81	64
Cl ₂ Rb ₂	484	0.0009	64	25
Te ₂ V	840	0.0009	81	118
I ₂ Nd ₂ O ₂	12	0.0009	1	1
Br ₂ Mn	840	0.0011	81	118
As ₂ Fe ₂	550	0.0011	49	64
AgClO ₂	384	0.0011	36	42
OTl ₂	840	0.0011	81	118
O ₄ PTl	870	0.0012	81	64
Ca ₂ Cl ₂	886	0.0012	81	100
As ₂ Cd ₂ K ₂	870	0.0012	81	64
Mg ₄	814	0.0012	65	106
AgClO ₄	366	0.0012	36	25
Mg ₃	537	0.0012	49	81
O ₂ Sn ₂	740	0.0012	66	86
FKO ₂ Se	270	0.0012	30	18
As ₂ Co ₂	896	0.0013	82	101
CdClO	840	0.0013	81	118
H ₂ Na ₂ O ₂	876	0.0013	61	85
Br ₂ CsF	580	0.0013	64	49
Ba ₂ Ge ₂ Mn ₂	12	0.0014	1	1
Ag ₂ I ₂	924	0.0014	100	81
RhTe ₂	483	0.0014	48	65
MoSe ₂	711	0.0014	64	109
KS ₂ Ti	958	0.0014	81	118
Se ₂ W	711	0.0014	64	109
I ₃ Sn	796	0.0014	100	49
AsSn ₂	483	0.0014	48	65
CNNa	489	0.0015	55	53
Tl	496	0.0015	65	106
Ni ₂ Te ₂	680	0.0016	62	77
Cl ₂ H ₂ Lu ₂	750	0.0016	52	73

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

NaCuTe (P4/nmm (129))

Structural and electronic properties

	Formula	NaCuTe
	Spacegroup	P4/nmm (129)
	Prototype	PbClF
	Parent 3D	Na ₂ Cu ₂ Te ₂
	Source DB	COD
	DB ID	7221371
DF2-C09	Binding energy [meV/ Å²]	32.71
RVV10	Binding energy [meV/ Å²]	38.04
	Band gap (PBE) [eV]	0.87

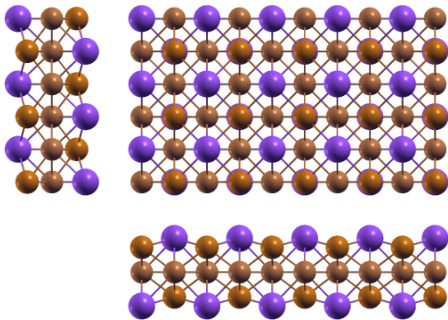


Band structure: Electronic band structure of NaCuTe (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NaCuTe (P4/nmm (129)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.34991788	0.00000000	0.00000000
a₂	0.00000000	4.34991788	0.00000000
a₃	0.00000000	0.00000000	24.61712485
	x [Å]	y [Å]	z [Å]
● Na	2.17495894	0.00000000	10.05894824
● Na	0.00000000	2.17495894	14.55817661
● Cu	0.00000000	0.00000000	12.30856243
● Cu	2.17495894	2.17495894	12.30856243
● Te	2.17495894	0.00000000	13.96066169
● Te	0.00000000	2.17495894	10.65646316



Orthographic projections: views of NaCuTe (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	7	0.0035	1	1
K	7	0.1328	1	1
Na	7	0.1112	1	1
Ag ₂	8	0.1371	1	1
As ₂	8	0.1094	1	1
Cl ₂ Zn	9	0.1097	1	1
MoTe ₂	9	0.1107	1	1
Nd	9	0.1421	1	3
Ba ₂ Pt	9	0.1369	1	1
HfS ₂	9	0.1089	1	1
Te ₂ V	9	0.1103	1	1
I ₂ Pr	9	0.2182	1	1
Ca ₂ Si	9	0.1406	1	1
Br ₂ Co	9	0.1095	1	1
Ca ₂ N	9	0.1093	1	1
Cl ₂ Zn	9	0.56	1	1
GeI ₂	9	0.109	1	1
Br ₂ Mn	9	0.1099	1	1
PtS ₂	9	0.111	1	1
CoTe ₂	9	0.1088	1	1
CdClO	9	0.1104	1	1
CKN	9	0.3991	1	1
Te ₂ W	9	0.1107	1	1
I ₂ Nd	9	0.2193	1	1
Cl ₂ Cu	9	0.1468	1	1
I ₂ Pb	9	0.1384	1	1
OTl ₂	9	0.1103	1	1
Br ₂ Fe	9	0.1095	1	1
CeI ₂	9	0.2173	1	1
Se ₂ Yb	9	0.109	1	1
BiTe ₂	9	0.1091	1	1
F ₂ Zn	9	0.2137	1	1
Bi ₂ Te ₂	10	0.1523	1	1
Fe ₂ Te ₂	10	0.5934	1	1
Li ₂ Tl ₂	10	0.1789	1	1
Ca ₂ Cl ₂	10	0.5947	1	1
NS ₂ Zr	10	0.1111	1	1
Ir ₂ P ₂	10	0.219	1	1
S ₂ Sn ₂	10	0.0222	1	1
Cu ₂ S ₂	10	0.2102	1	1
Au ₂ Br ₂	10	0.0111	1	1
Br ₂ Cu ₂	10	0.2122	1	1
Cu ₂ Te ₂	10	0.5675	1	1
AgBrO ₂	10	0.1257	1	1
Ge ₂ S ₂	10	0.0476	1	1
O ₂ Sn ₂	10	0.6123	1	1
AsCuLi ₂	10	0.1088	1	1
KS ₂ Ti	10	0.1098	1	1
Ga ₂ S ₂	10	0.1088	1	1
P ₂ Rh ₂	10	0.2095	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

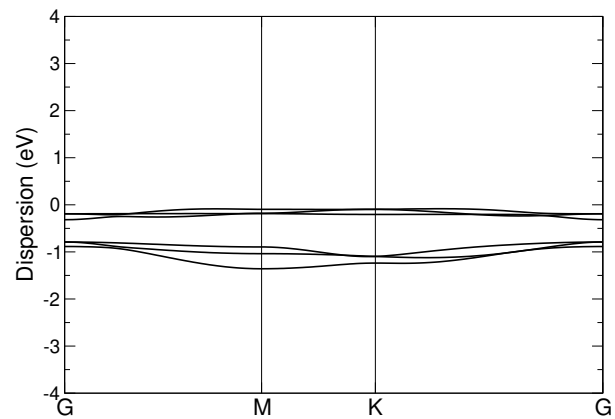
Formula	N° atoms	strain	cell size 1	cell size 2
Cu ₂ Se ₂	706	0.0	61	85
Br ₂ F ₂ Yb ₂	870	0.0	64	81
H ₂ Li ₂ O ₂	612	0.0001	41	61
F ₂ Zn	636	0.0001	65	82
Ca ₂ Cl ₂	550	0.0001	49	64
Cu ₂ F ₄	612	0.0001	61	41
I ₂ Nd	786	0.0001	81	100
As ₂ Ru ₂	550	0.0001	49	64
Se ₂ Ta ₄	780	0.0001	49	81
I ₂ S ₂ Tl ₂	876	0.0002	61	85
PdTe ₂	483	0.0002	48	65
Br ₂ Hf ₂	476	0.0003	36	65
Br ₂ Ca ₂ F ₂	882	0.0003	65	82
Ir ₂ P ₂	886	0.0003	81	100
Br ₂ Gd ₂ O ₂	882	0.0003	65	82
Br ₂ O ₂ Tm ₂	678	0.0004	49	64
Cl ₂ H ₂ Zr ₂	354	0.0004	20	39
Cl ₂ S ₂ Tl ₂	678	0.0004	64	49
Br ₂ Tb ₂	548	0.0004	48	65
Br ₂ Ca ₂ F ₂	870	0.0005	64	81
Fe ₂ Te ₂	550	0.0005	49	64
Cu ₂ Te ₂	412	0.0005	36	49
Br ₂ Cu ₂	708	0.0005	64	81
LiOS ₂ Ti	315	0.0005	20	39
F ₂ Ni	621	0.0006	61	85
Si ₂ Te ₂ Zr ₂	876	0.0006	61	85
Al ₂ Cl ₂ O ₂	678	0.0007	43	70
Bi ₂ S ₃	613	0.0007	48	65
NbS ₂	237	0.0007	20	39
F ₂ Zn	627	0.0008	64	81
I ₂ Ni	840	0.0009	81	118
FeI ₂	840	0.0009	81	118
Br ₂ Er ₂ O ₂	690	0.0009	50	65
Br ₂ O ₂ Tb ₂	870	0.0009	64	81
Br ₂ Ho ₂	548	0.0009	48	65
As ₂ Co ₂ Li ₂	510	0.0009	36	49
Br ₂ O ₂ Yb ₂	678	0.0009	49	64
Pb ₂ Se ₂	496	0.0009	50	49
Cl ₂ ORu	588	0.0009	50	72
AgClO ₂	780	0.001	68	93
N ₂ W	633	0.001	48	115
I ₂ Lu ₂ O ₂	882	0.001	65	82
Br ₂ Mg	840	0.001	81	118
Ge ₂ Se ₂ Zr ₂	366	0.001	25	36
Ca ₂ Cl ₂	294	0.001	25	36
Br ₂ F ₂ Tm ₂	882	0.0011	65	82
I ₂ Pr	786	0.0011	81	100
Fe ₂ Se ₂	706	0.0011	61	85
Br ₂ Gd ₂ O ₂	870	0.0011	64	81
CdClHO	978	0.0011	79	126

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

NaF₂ (P-3m1)

Structural and electronic properties

	Formula	NaF ₂
	Spacegroup	P-3m1
	Prototype	CdI2
	Parent 3D	F ₂ Na
	Source DB	MPDS
	DB ID	S1718698
DF2-C09	Binding energy [meV/ Å²]	50.73
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

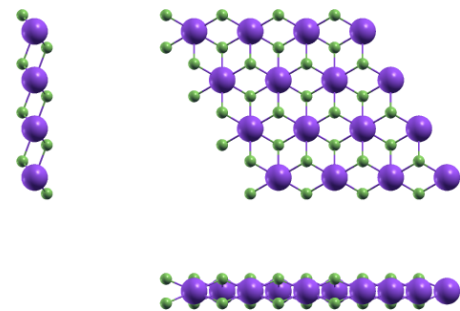


Band structure: Electronic band structure of NaF₂ (P-3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NaF₂ (P-3m1) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		1.88856886	−3.27110663	0.00000000
a₂		1.88857701	3.27111133	0.00000000
a₃		0.00000000	0.00000000	15.88252676
		x [Å]	y [Å]	z [Å]
•	F	0.94428519	−0.54518331	−0.82207248
•	F	2.83286068	0.54518801	0.82207248
●	Na	0.94428850	1.63555566	0.00000000



Orthographic projections: views of NaF₂ (P-3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	4	0.1113	1	1
InSe	5	0.4748	1	1
HgO	5	0.1161	1	1
AsSb	5	0.0084	1	1
PbTe	5	0.4793	1	1
CaCl	5	0.1512	1	1
I ₂ Mg	6	0.4491	1	1
Cl ₂ Mn	6	0.2601	1	1
CdI ₂	6	0.4838	1	1
AgTe ₂	6	0.1123	1	1
S ₂ Ta	6	0.263	1	1
Br ₂ Zn	6	0.002	1	1
Br ₂ Ca	6	0.487	1	1
AsSn ₂	6	0.0087	1	1
SiTe ₂	6	0.0022	1	1
Br ₂ La	6	0.4499	1	1
PbS ₂	6	0.0057	1	1
BiClTe	6	0.4847	1	1
BrCdI	6	0.4568	1	1
S ₂ Ti	6	0.2702	1	1
Mg ₃	6	0.4335	1	1
Te ₂ Ti	6	0.0017	1	1
NbS ₂	6	0.2624	1	1
BaF ₂	6	0.4651	1	1
BiBrTe	6	0.4994	1	1
RhTe ₂	6	0.006	1	1
Bi ₂ Pd	6	0.1209	1	1
Cl ₂ Co	6	0.2697	1	1
NbS ₂	6	0.2564	1	1
ClN ₂ Zr	6	0.2748	1	1
Cl ₂ Fe	6	0.2686	1	1
S ₂ Ta	6	0.2553	1	1
Se ₂ V	6	0.2534	1	1
AsKSn	6	0.4615	1	1
PbTe ₂	6	0.4544	1	1
NiTe ₂	6	0.0016	1	1
I ₂ V	6	0.0035	1	1
GeI ₂	6	0.4799	1	1
Se ₂ Zr	6	0.0026	1	1
STl ₂	6	0.4675	1	1
PtSe ₂	6	0.0081	1	1
CdO ₂	6	0.2695	1	1
CoI ₂	6	0.0088	1	1
GeS ₂	6	0.1402	1	1
TaTe ₂	6	0.0092	1	1
MnSe ₂	6	0.1511	1	1
Cl ₂ Zr	6	0.2692	1	1
I ₂ Ti	6	0.0092	1	1
CdI ₂	6	0.4827	1	1
I ₂ Pr	6	0.485	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

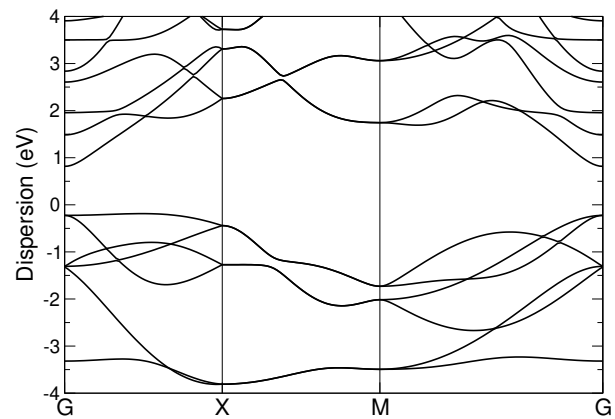
Formula	N° atoms	strain	cell size 1	cell size 2
CNb ₂ S ₂	414	0.0	43	57
Cl ₂ O ₂ Yb ₂	9	0.0001	1	1
I ₂ La ₂ P	386	0.0001	57	43
Br ₂ La ₂ P	504	0.0001	73	57
AsKSn	543	0.0001	100	81
S ₂ Ta	390	0.0002	57	73
AsLi ₃	499	0.0002	81	64
F ₂ Se ₂ Y ₂	405	0.0002	61	37
Cu ₄ Te ₂	486	0.0002	64	49
CdI ₂	390	0.0002	73	57
CdI ₂	390	0.0002	73	57
STl ₂	492	0.0002	91	73
Cu ₂ I ₂	387	0.0003	65	48
Cl ₂ Hf ₂	583	0.0003	73	91
Gd ₂ GeI ₂	504	0.0003	73	57
N ₂ W	123	0.0004	16	25
O ₂ Pt	183	0.0004	25	36
I ₂ La ₂	624	0.0004	100	81
Sb ₂ Te ₃	437	0.0004	64	49
InSe	371	0.0005	81	64
Bi ₂ STe ₂	563	0.0005	81	64
As ₂ Li ₂ Pr	563	0.0005	81	64
Gd ₂ I ₂ S ₂	258	0.0005	36	25
P ₂	243	0.0005	43	57
I ₂ La ₂ Si ₂	627	0.0005	81	64
GeI ₃ Rb	237	0.0005	64	9
BiClTe	390	0.0006	73	57
Cl ₂ Mn	435	0.0006	64	81
Br ₂ H ₂ Sr ₂	483	0.0006	65	48
Bi ₂ STe ₂	504	0.0006	73	57
FeSe ₂	597	0.0006	81	118
I ₂ Pr	390	0.0007	73	57
Sn ₂ Te ₂	452	0.0007	84	50
Cl ₂ Ti	300	0.0007	43	57
NbS ₂	390	0.0007	57	73
Cl ₂ Fe	543	0.0007	81	100
BaF ₂	492	0.0007	91	73
Cu ₂ Se ₂ Tl ₂	483	0.0007	65	48
Er ₂ I ₂ Se ₂	660	0.0007	108	56
CS ₂ Ta ₂	414	0.0008	43	57
Br ₂ Ca ₃ Si	258	0.0008	36	25
Br ₂ Pr ₂	7	0.0008	1	1
AlH ₄ Na	411	0.0008	65	36
Cl ₂ O ₂ Tm ₂	9	0.0008	1	1
LiNbS ₂	583	0.0008	73	91
GdI ₂	300	0.0008	57	43
LiO	206	0.0008	36	49
FeH ₂ O ₂	173	0.0009	16	25
C ₂ Br ₂ Gd ₂	768	0.0009	92	82
S ₂ Ta	492	0.0009	73	91

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

NaMgAs (P4/nmm (129))

Structural and electronic properties

Formula	NaMgAs
Spacegroup	P4/nmm (129)
Prototype	PbClF
Parent 3D	Na ₂ Mg ₂ As ₂
Source DB	COD
DB ID	9008321
DF2-C09 Binding energy [meV/ Å²]	43.37
RVV10 Binding energy [meV/ Å²]	47.82
Band gap (PBE) [eV]	1.0

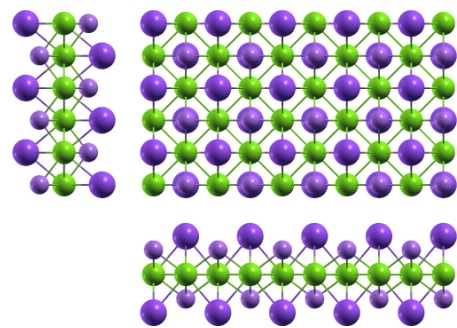


Band structure: Electronic band structure of NaMgAs (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NaMgAs (P4/nmm (129)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.31487734	0.00000000	0.00000000
a₂	0.00000000	4.31487734	0.00000000
a₃	0.00000000	0.00000000	25.25091732
	x [Å]	y [Å]	z [Å]
Na	0.00000000	2.15743867	15.18150050
As	2.15743867	0.00000000	14.26667287
Na	2.15743867	0.00000000	10.06941682
Mg	0.00000000	0.00000000	12.62545866
Mg	2.15743867	2.15743867	12.62545866
As	0.00000000	2.15743867	10.98424445



Orthographic projections: views of NaMgAs (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	7	0.0003	1	1
K	7	0.1358	1	1
Na	7	0.1103	1	1
Ag ₂	8	0.1403	1	1
As ₂	8	0.1087	1	1
Sb ₂	8	0.109	1	1
Cl ₂ Zn	9	0.1089	1	1
MoTe ₂	9	0.1098	1	1
Nd	9	0.1455	1	3
Ba ₂ Pt	9	0.14	1	1
Te ₂ V	9	0.1094	1	1
Ca ₂ Si	9	0.144	1	1
Br ₂ Co	9	0.1088	1	1
Br ₂ Mn	9	0.1091	1	1
PtS ₂	9	0.1101	1	1
CdClO	9	0.1095	1	1
CKN	9	0.4076	1	1
Se ₂ Ti	9	0.1107	1	1
Te ₂ W	9	0.1098	1	1
I ₂ Pb	9	0.1416	1	1
OTl ₂	9	0.1095	1	1
Br ₂ Fe	9	0.1088	1	1
DyI ₂	9	0.1309	1	1
F ₂ Ni	9	0.5595	1	1
F ₂ Zn	9	0.218	1	1
Bi ₂ Te ₂	10	0.1561	1	1
Fe ₂ Te ₂	10	0.2083	1	1
Li ₂ Tl ₂	10	0.1836	1	1
Ca ₂ Cl ₂	10	0.2087	1	1
Cl ₂ OOS	10	0.5677	1	1
NS ₂ Zr	10	0.1102	1	1
S ₂ Sn ₂	10	0.0195	1	1
Cu ₂ S ₂	10	0.2144	1	1
Au ₂ Br ₂	10	0.0084	1	1
Br ₂ Cu ₂	10	0.2165	1	1
N ₃ Na	10	0.0289	1	1
AgBrO ₂	10	0.1273	1	1
Br ₂ Zr ₂	10	0.1108	1	1
O ₂ Sn ₂	10	0.215	1	1
KS ₂ Ti	10	0.109	1	1
P ₂ Rh ₂	10	0.2136	1	1
F ₂ Tl ₂	10	0.2138	1	1
BN	10	0.1482	1	2
Au ₂ I ₂	10	0.0187	1	1
Sb ₂ Te ₂	10	0.1428	1	1
Ge ₂ Se ₂	10	0.0279	1	1
Cu ₂ Se ₂	10	0.5611	1	1
Ag ₂ Te ₂	10	0.6301	1	1
As ₂ Ru ₂	10	0.2089	1	1
AgClO ₂	10	0.1211	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

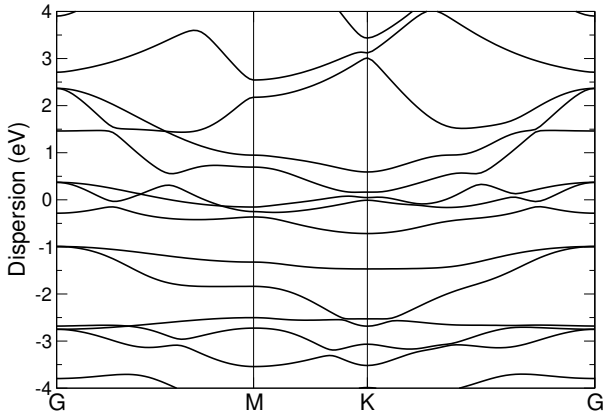
Formula	N° atoms	strain	cell size 1	cell size 2
P ₂ Rh ₂	718	0.0001	65	82
F ₂ Tl ₂	718	0.0002	65	82
Tl	159	0.0002	20	39
AgClO ₄	882	0.0002	82	65
Ba ₂ N	483	0.0002	48	65
Ca ₂ Cl ₂ F ₂	678	0.0002	49	64
Hf ₂ Si ₂ Te ₂	876	0.0003	61	85
K	7	0.0003	1	1
Br ₂ Ho ₂ O ₂	870	0.0004	64	81
Bi ₂ Se ₂	866	0.0004	85	89
Cu ₃ Se ₃	678	0.0004	48	65
Br ₂ O ₂ V ₂	402	0.0004	27	40
MnSe ₂	258	0.0005	25	36
Cl ₄ Cu ₂	972	0.0005	109	53
Se ₂ W	237	0.0005	20	39
Ca ₂ Mn ₂ Si ₂	870	0.0005	64	81
CaCl	222	0.0006	25	36
Br ₂ Dy ₂ O ₂	882	0.0006	65	82
Br ₂ O ₂ Y ₂	882	0.0006	65	82
Hf ₃ Te ₂	461	0.0007	36	49
MoSe ₂	237	0.0007	20	39
AsSb	722	0.0007	81	118
Ho ₂ S ₂	578	0.0007	53	65
Cu ₂ S ₂	718	0.0007	65	82
Br ₂ Ca ₂ H ₂	870	0.0008	64	81
I ₄ Zr ₂	576	0.0008	56	40
P ₂ Rh ₂	708	0.0008	64	81
Co ₂ Se ₂	706	0.0008	61	85
F ₂ Tl ₂	708	0.0009	64	81
CoI ₂	840	0.0009	81	118
Cl ₂ O ₂ V ₂	690	0.0009	45	70
Se ₂ V	237	0.001	20	39
AgClO ₄	870	0.001	81	64
S ₂ Zr	852	0.001	79	126
NbTe ₂	852	0.0011	79	126
S ₂ Sn	852	0.0011	79	126
Fe ₂ Li ₂ P ₂	876	0.0011	61	85
Bi ₂ Pd	945	0.0011	85	145
Br ₂ Cu	636	0.0012	63	86
Te ₂ Zr	483	0.0012	48	65
Ni ₂ Se ₂	896	0.0012	82	101
F ₂ Zn	786	0.0012	81	100
Co ₂ S ₂	294	0.0012	25	36
Ca ₂ Cl ₂ H ₂	510	0.0012	36	49
Cu ₂ Te ₂	962	0.0012	85	113
Ag ₂ Te ₂	698	0.0012	63	80
C ₂ Br ₂ Gd ₂	630	0.0013	45	60
Ge ₂ Te ₂ Zr ₂	678	0.0013	49	64
O ₂ Sn ₂	718	0.0013	65	82
Cl ₂ Rb ₂	70	0.0013	9	4

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

NaMnTe₂ (P3m1 (156))

Structural and electronic properties





	Formula	NaMnTe ₂
	Spacegroup	P3m1 (156)
	Prototype	LiMnSe2
	Parent 3D	NaMnTe ₂
	Source DB	ICSD
	DB ID	110774
DF2-C09	Binding energy [meV/ Å²]	74.04
RVV10	Binding energy [meV/ Å²]	71.12
	Band gap (PBE) [eV]	0.0

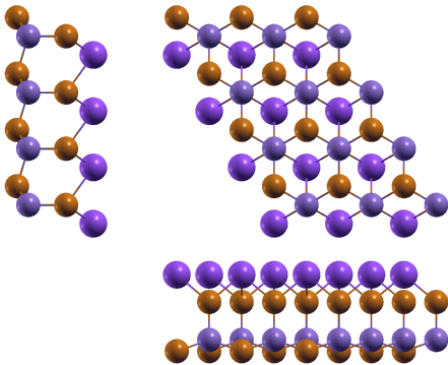


Band structure: Electronic band structure of NaMnTe₂ (P3m1 (156)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NaMnTe₂ (P3m1 (156)) in Cartesian coordinates.

		<i>x</i> [Å]	<i>y</i> [Å]	<i>z</i> [Å]
a₁		4.17772105	−0.00000000	0.00000000
a₂		−2.08886052	3.61801256	0.00000000
a₃		0.00000000	0.00000000	24.99289070
		<i>x</i> [Å]	<i>y</i> [Å]	<i>z</i> [Å]
	Mn	2.08886052	1.20600419	14.32980740
	Te	0.00000000	2.41200837	15.05601905
	Te	2.08886052	1.20600419	11.89095174
	Na	0.00000000	0.00000000	10.13852836



Orthographic projections: views of NaMnTe₂ (P3m1 (156)) as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
InSe	6	0.0077	1	1
AgTl	6	0.1601	1	1
Ag ₂	6	0.458	1	1
PbTe	6	0.0095	1	1
Sb ₂	6	0.0083	1	1
CaCl	6	0.1167	1	1
Cl ₂ Zn	7	1.5657	1	1
I ₂ Mg	7	0.0027	1	1
MoTe ₂	7	1.5322	1	1
PSn ₂	7	1.6396	1	1
Ba ₂ Pt	7	0.4573	1	1
Br ₂ Zn	7	0.2679	1	1
HfS ₂	7	1.5934	1	1
AsSn ₂	7	0.2581	1	1
SiTe ₂	7	0.2739	1	1
Te ₂ V	7	1.546	1	1
I ₂ Pr	7	0.1428	1	1
S ₂ Zr	7	1.6338	1	1
Br ₂ La	7	0.0024	1	1
Ca ₂ Si	7	0.4687	1	1
BrCdI	7	0.0004	1	1
Cl ₂ Zn	7	0.1247	1	1
Te ₂ Ti	7	0.2683	1	1
BaF ₂	7	0.0037	1	1
RhTe ₂	7	0.2621	1	1
GeI ₂	7	0.0045	1	1
Br ₂ Mn	7	1.557	1	1
PtS ₂	7	1.5235	1	1
CoTe ₂	7	1.5958	1	1
CdClO	7	1.5425	1	1
AsKSn	7	0.0023	1	1
Te ₂ W	7	1.5334	1	1
PbTe ₂	7	0.0006	1	1
I ₂ Nd	7	0.1436	1	1
NiTe ₂	7	0.273	1	1
Cl ₂ Cu	7	0.0655	1	1
S ₂ Sn	7	1.6358	1	1
SnTe ₂	7	0.0068	1	1
I ₂ V	7	0.2759	1	1
Se ₂ Zr	7	0.2745	1	1
I ₂ Pb	7	0.4619	1	1
STl ₂	7	0.0047	1	1
PtSe ₂	7	0.259	1	1
OTl ₂	7	1.5438	1	1
GeS ₂	7	0.1117	1	1
TaTe ₂	7	0.2573	1	1
MnSe ₂	7	0.1167	1	1
Br ₂ Ni	7	0.2475	1	1
CeI ₂	7	0.1421	1	1
NbTe ₂	7	1.6322	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

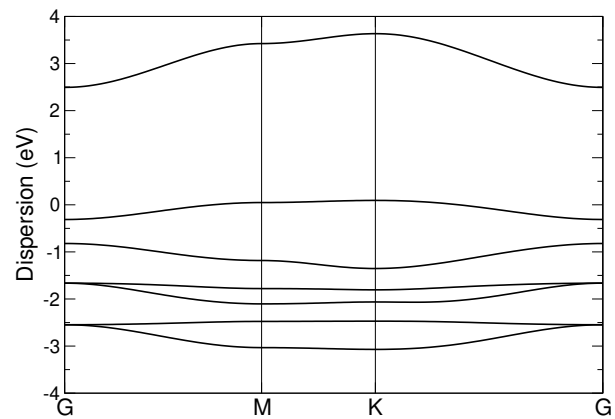
Formula	N° atoms	strain	cell size 1	cell size 2
NbS ₂	139	0.0001	16	25
CCl ₂ Gd ₂	824	0.0001	81	100
Te ₂ V	291	0.0001	36	49
HfS ₂	343	0.0001	43	57
Br ₂ Hf ₂	244	0.0001	25	36
Br ₂ Zn	624	0.0002	81	100
PtSe ₂	499	0.0002	64	81
CuTe ₂	343	0.0002	43	57
BrNZr	208	0.0003	25	36
Ba ₂ F ₂ I ₂	548	0.0003	65	48
I ₂ Pb	643	0.0003	100	81
Cl ₂ H ₂ Zr ₂	214	0.0003	16	25
Hg ₃ N ₂	145	0.0003	25	9
SSb ₂ Te ₂	9	0.0003	1	1
BrCdI	7	0.0004	1	1
Cl ₂ Hf ₂ N ₂	438	0.0004	36	49
OTl ₂	291	0.0004	36	49
CoTe ₂	343	0.0005	43	57
Te ₂ Ti	624	0.0005	81	100
I ₂ N ₂ Zr ₂	838	0.0005	73	91
BN	86	0.0005	9	25
HfSe ₂	624	0.0005	81	100
CBr ₂ Y ₂	824	0.0005	81	100
Sm	164	0.0005	25	64
Ga ₂ Se ₂	656	0.0005	73	91
H ₂ MnO ₂	696	0.0006	49	100
I ₂ Pr ₂ S ₂	886	0.0006	100	81
Br ₂ N ₂ Zr ₂	580	0.0006	49	64
PbTe ₂	7	0.0006	1	1
Sb ₂ Te ₂	656	0.0006	91	73
Ga ₂ S ₂	400	0.0006	43	57
CdClO	291	0.0006	36	49
CBr ₂ Lu ₂	516	0.0006	49	64
CaH ₂ O ₂	457	0.0007	43	57
Cl ₄ Mn	877	0.0007	118	81
Ca ₂ Si	583	0.0007	91	73
Ce ₂ I ₂ S ₂	802	0.0007	91	73
AgTl	386	0.0008	66	61
NbSe ₂	208	0.0008	25	36
S ₂ Ta	139	0.0008	16	25
ClH ₃ O	501	0.0008	64	49
CdClHO	520	0.0008	57	73
Br ₂ OV	44	0.0008	5	6
O ₄ PTl	548	0.0008	65	48
Hf ₂ I ₂ N ₂	666	0.0008	57	73
AsSn ₂	499	0.0008	64	81
Cl ₂ N ₂ Zr ₂	514	0.0009	43	57
Br ₂ Cr ₂ S ₂	400	0.001	40	40
C ₂ F ₂	356	0.001	25	64
Cl ₂ H ₂ Lu ₂	580	0.001	49	64

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

NaO₄ (P3)

Structural and electronic properties

	Formula	NaO ₄
	Spacegroup	P3
	Prototype	NaO4
	Parent 3D	Br ₃ NaO ₅ Zn
	Source DB	ICSD
	DB ID	26038
DF2-C09	Binding energy [meV/ Å²]	93.55
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

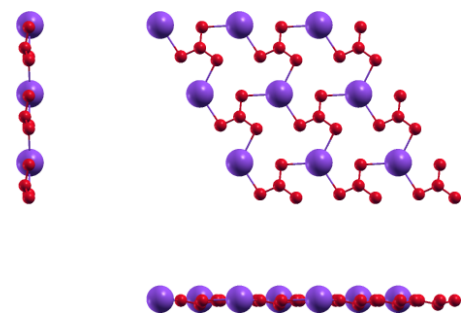


Band structure: Electronic band structure of NaO₄ (P3) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NaO₄ (P3) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		-2.57713361	-4.46372635	0.00000000
a₂		5.15426722	0.00000000	0.00000000
a₃		0.00000000	0.00000000	12.33595371
		x [Å]	y [Å]	z [Å]
●	Na	2.57713361	-1.48790878	-0.11486563
●	O	0.13613202	-1.62647298	-0.03487119
●	O	1.10050068	-3.76838364	-0.03487119
●	O	-1.23663269	-3.53259607	-0.03487119
●	O	0.00000000	-2.97581757	0.21947919



Orthographic projections: views of NaO₄ (P3) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	6	0.1113	1	1
K	6	0.2585	1	1
Ag ₂	7	0.2662	1	1
Ba ₂ Pt	8	0.2658	1	1
CaI ₂	8	0.2462	1	1
Ca ₂ Si	8	0.2724	1	1
HgI ₂	8	0.1186	1	1
CNRb	8	0.1825	1	1
I ₂ Pb	8	0.2685	1	1
DyI ₂	8	0.2499	1	1
Bi ₂ In ₂	9	0.1284	1	1
Cu ₂ Te ₂	9	0.1143	1	1
S ₂ Sn ₂	9	0.1078	1	1
Ge ₂ Te ₂	9	0.1121	1	1
N ₃ Na	9	0.1197	1	1
Ge ₂ S ₂	9	0.1094	1	1
Sb ₂ Te ₂	9	0.2705	1	1
La ₂ S ₂	9	0.1112	1	1
SbSe ₂ Tl	9	0.7979	1	1
Ag ₂ I ₂	9	0.1191	1	1
Br ₂ CsF	9	0.127	1	1
Sn ₂ Te ₂	9	0.1235	1	1
Sm	9	0.0068	1	4
F ₄ Pb	10	0.115	1	1
Cd ₂ I ₃	10	1.5475	1	1
AgNO ₃	10	0.0008	1	1
I ₂ La ₂ Sb	10	0.259	1	1
Cl ₄ Mn	10	0.1324	1	1
I ₂ La ₂ Te	10	0.2552	1	1
Ba ₂ H ₂ I ₂	11	0.1258	1	1
HfS ₂	11	0.2197	1	2
AlH ₄ Na	11	0.1343	1	1
CuTe ₂	11	0.2193	1	2
Cu ₂ Na ₂ Te ₂	11	0.1125	1	1
Cl ₄ Cu ₂	11	0.3148	1	1
Br ₂ Cr ₂ S ₂	11	0.1159	1	1
I ₂ Pr ₂ S ₂	11	0.2672	1	1
C ₂ Br ₂ Gd ₂	11	0.1829	1	1
CoTe ₂	11	0.2201	1	2
Dy ₂ I ₂ S ₂	11	0.249	1	1
Br ₂ Ca ₃ Si	11	0.2551	1	1
Cu ₂ Rb ₂ Te ₂	11	0.1281	1	1
Cl ₂ N ₂ Ti ₂	11	0.1144	1	1
Ag ₂ K ₂ Te ₂	11	0.1387	1	1
Ag ₂ K ₂ Se ₂	11	0.1178	1	1
Br ₂ O ₂ V ₂	11	0.1158	1	1
O ₄ PSn	11	0.1226	1	1
I ₂ S ₂ Tb ₂	11	0.2505	1	1
Ba ₂ F ₂ I ₂	11	0.1211	1	1
Br ₂ Ca ₃ Si	11	0.2532	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

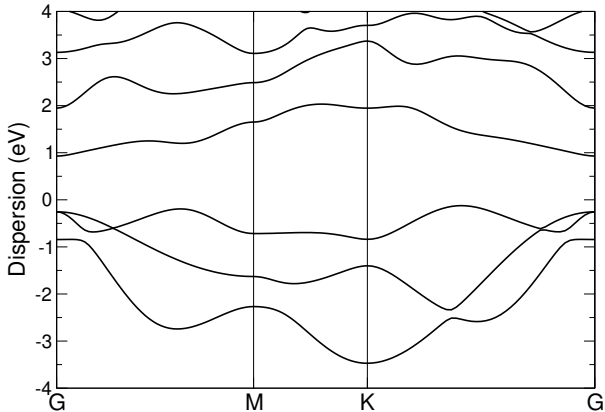
Formula	N° atoms	strain	cell size 1	cell size 2
Cl ₂ N ₂ Zr ₂	669	0.0	39	79
I ₂ Tm	386	0.0	43	57
CCL ₂ Lu ₂	745	0.0	49	100
AsI ₂ La ₂	425	0.0	36	49
Br ₂ Mg	93	0.0001	9	16
Cd ₂ I ₃	425	0.0001	36	49
As ₂	445	0.0001	49	100
PdTe ₂	368	0.0001	37	61
ClNZr	47	0.0001	4	9
Br ₂ Ca ₃ Si	723	0.0002	57	73
Br ₂ Cd	488	0.0002	49	81
Dy ₂ I ₂ S ₂	629	0.0002	49	64
I ₂ La ₂ Te	650	0.0002	57	73
Ga ₂ Gd ₂ I ₂	341	0.0002	25	36
CrI ₂	93	0.0002	9	16
FeI ₂	93	0.0002	9	16
I ₂ La ₂ Sb	725	0.0002	64	81
CrSe ₂	317	0.0002	25	64
Bi ₂	197	0.0002	25	36
CaH ₂ O ₂	590	0.0003	39	79
CeLi ₂ P ₂	205	0.0003	16	25
C	14	0.0003	1	9
Br ₂ Fe	545	0.0003	49	100
Br ₂ Er ₂ Se ₂	440	0.0003	40	40
GeI ₂ La ₂	500	0.0003	43	57
Br ₂ Co	545	0.0003	49	100
Br ₂ PY ₂	650	0.0004	49	81
Br ₂ H ₂ Zr ₂	74	0.0004	4	9
BH ₄ Li	230	0.0004	16	25
Ga ₂ I ₂ Tb ₂	341	0.0005	25	36
CoH ₂ O ₂	170	0.0005	9	25
N ₂ Re	368	0.0005	25	81
DyI ₂	437	0.0005	49	64
Br ₂ Hf ₂ N ₂	669	0.0005	39	79
PSn ₂	272	0.0005	25	49
K	401	0.0006	64	81
C ₂ Br ₂ Gd ₂	613	0.0006	41	68
I ₂ Pb	705	0.0006	81	100
Ca ₂ N	545	0.0006	49	100
Br ₂ HLa	180	0.0007	16	25
C ₂ Br ₂ Tb ₂	613	0.0007	41	68
SnTe ₂	155	0.0007	16	25
CuTe ₂	432	0.0007	39	79
Br ₂ Tb ₂	429	0.0007	37	61
CCL ₂ Sc ₂	65	0.0008	4	9
As ₂ Ir ₂	877	0.0008	81	118
Br ₂ Cd	368	0.0008	37	61
AgNO ₃	10	0.0008	1	1
Bi ₂ SeTe ₂	305	0.0008	25	36
Br ₂ Ca	233	0.0008	25	36

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

NaSnP (P3m1 (156))

Structural and electronic properties

Formula	NaSnP
Spacegroup	P3m1 (156)
Prototype	BiTeI
Parent 3D	Na ₂ Sn ₂ P ₂
Source DB	ICSD
DB ID	409010
DF2-C09 Binding energy [meV/ Å²]	99.35
RVV10 Binding energy [meV/ Å²]	N/A
Band gap (PBE) [eV]	1.05

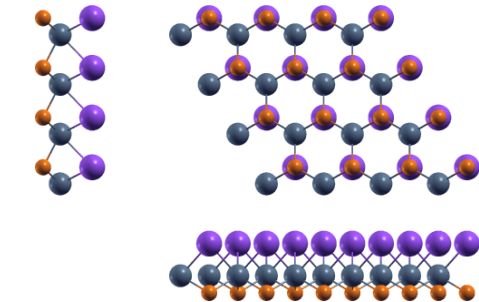


Band structure: Electronic band structure of NaSnP (P3m1 (156)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NaSnP (P3m1 (156)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.96277818	0.00000000	0.00000000
a₂	−1.98138909	3.43186657	0.00000000
a₃	0.00000000	0.00000000	23.87794798
	x [Å]	y [Å]	z [Å]
Na	1.98138909	1.14395552	10.26875877
Sn	0.00000000	0.00000000	12.48472702
P	1.98138909	1.14395552	13.66900712



Orthographic projections: views of NaSnP (P3m1 (156)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	4	2.9325	1	1
Na	4	0.2641	1	1
HgO	5	0.4228	1	1
GeTe	5	0.0082	1	1
As ₂	5	0.2757	1	1
S ₂	5	0.0067	1	1
CaCl	5	0.1318	1	1
IrTe ₂	6	0.0073	1	1
Cl ₂ Zn	6	0.2742	1	1
CdCl ₂	6	0.0092	1	1
MoTe ₂	6	0.2674	1	1
ReSe ₂	6	0.2473	1	1
S ₂ Ta	6	1.5269	1	1
CaI ₂	6	0.4841	1	1
InSe ₂	6	0.0089	1	1
HfTe ₂	6	0.0009	1	1
Te ₂ V	6	0.2702	1	1
I ₂ Mn	6	0.0091	1	1
I ₂ Yb	6	0.4775	1	1
Br ₂ Co	6	0.2751	1	1
AuTe ₂	6	0.0088	1	1
Cl ₂ Zn	6	0.1436	1	1
PdTe ₂	6	0.0063	1	1
S ₂ Ti	6	1.5625	1	1
NbS ₂	6	1.5237	1	1
Te ₂ Zn	6	0.2671	1	1
Bi ₂ Pd	6	0.1109	1	1
Ba ₂ Hg	6	0.2092	1	1
Br ₂ Mn	6	0.2724	1	1
Cl ₂ Ni	6	0.2485	1	1
Cl ₂ Co	6	1.56	1	1
CrTe ₂	6	0.2566	1	1
PtS ₂	6	0.2656	1	1
Br ₂ V	6	0.2462	1	1
ClNZr	6	1.5855	1	1
Cl ₂ Fe	6	1.5548	1	1
CdClO	6	0.2695	1	1
Ba ₂ N	6	0.0024	1	1
Se ₂ Ti	6	0.2619	1	1
Br ₂ Ti	6	0.2559	1	1
Te ₂ Zr	6	0.0014	1	1
Te ₂ W	6	0.2676	1	1
AsSe ₂	6	0.2504	1	1
I ₂ Tm	6	0.481	1	1
I ₂ Pb	6	3.0263	1	1
OTl ₂	6	0.2697	1	1
BiTe	6	0.4579	1	1
BrNZr	6	1.6347	1	1
NbSe ₂	6	0.249	1	1
Br ₂ Fe	6	0.2752	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

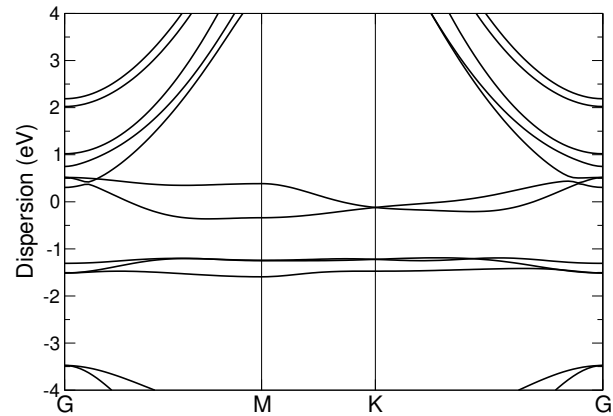
Formula	N° atoms	strain	cell size 1	cell size 2
CCL ₂ Sc ₂	414	0.0	43	57
Te ₂ W	543	0.0	81	100
HNiO ₂	91	0.0	9	16
Se ₂ Ta	339	0.0001	49	64
Na	310	0.0001	73	91
MoTe ₂	543	0.0001	81	100
Pt ₂ Te ₂	7	0.0002	1	1
NbSe ₂	339	0.0002	49	64
H ₂ I ₂ Sr ₂	483	0.0002	65	48
Cl ₂ Cr ₂ O ₂	696	0.0002	70	81
Ga ₂ S ₃	674	0.0002	73	91
Cl ₂ H ₂ Sc ₂	609	0.0003	57	73
Br ₂ Hf ₂ N ₂	462	0.0003	54	50
Br ₂ Ti	390	0.0003	57	73
NS ₂ Zr	583	0.0003	73	91
Te ₂ Zn	543	0.0003	81	100
CaI ₂	390	0.0003	73	57
Ba ₂ Pt	255	0.0004	49	36
Br ₂ H ₂ Zr ₂	471	0.0004	43	57
Cl ₂ Zr ₂	357	0.0004	43	57
Ba ₂ Cu ₂	499	0.0004	81	64
CdH ₂ O ₂	743	0.0004	81	100
Br ₂ H ₂ Zr ₂	609	0.0005	57	73
Se ₂ Ta	390	0.0005	57	73
Br ₂ Cr	390	0.0006	57	73
GeNi ₃ Te ₂	9	0.0006	1	1
HfLiS ₂	643	0.0006	81	100
I ₂ Yb	435	0.0006	81	64
Cl ₂ Ni	339	0.0006	49	64
Cd ₂ I ₃	638	0.0006	91	73
Br ₂ Cr ₂ O ₂	474	0.0006	50	54
Ag ₂	219	0.0006	49	36
Mg ₂	479	0.0006	81	118
AsI ₂ La ₂	638	0.0006	91	73
Er ₂ F ₂ Se ₂	9	0.0007	1	1
Cl ₂ Sc ₂	463	0.0008	57	73
I ₂ N ₂ Ti ₂	801	0.0008	91	88
I ₂ Tm	390	0.0008	73	57
H ₂ MgO ₂	173	0.0008	16	25
AsSe ₂	339	0.0009	49	64
CrTe ₂	390	0.0009	57	73
Br ₂ Ca ₃ Si	429	0.0009	57	43
HfTe ₂	6	0.0009	1	1
Gd ₂ I ₂ S ₂	486	0.0009	64	49
PtS ₂	492	0.0009	73	91
In ₂ Se ₃	8	0.0009	1	1
CuGeO ₃	172	0.0009	24	20
ClNZr	300	0.0009	43	57
Sn ₂ Te ₂	180	0.001	32	21
I ₂ La ₂ Te	386	0.001	57	43

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Ni(OH)₂ (P-3m1 (164))

Structural and electronic properties

	Formula	Ni(OH) ₂
	Spacegroup	P-3m1 (164)
	Prototype	Mn(OH) ₂
	Parent 3D	Ni(OH) ₂
	Source DB	ICSD
	DB ID	28101
DF2-C09	Binding energy [meV/ Å²]	32.27
RVV10	Binding energy [meV/ Å²]	39.65
	Band gap (PBE) [eV]	0.0

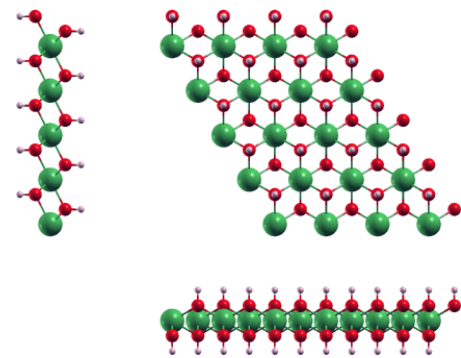


Band structure: Electronic band structure of Ni(OH)₂ (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ni(OH)₂ (P-3m1 (164)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.19602257	0.00000000	0.00000000
a₂		-1.59801128	2.76783673	0.00000000
a₃		0.00000000	0.00000000	23.84520967
		x [Å]	y [Å]	z [Å]
•	H	0.00000000	1.84522449	13.83259764
•	O	0.00000000	1.84522449	12.85662386
•	Ni	0.00000000	0.00000000	11.92260484
•	H	1.59801128	0.92261224	10.01261203
•	O	1.59801128	0.92261224	10.98858581



Orthographic projections: views of Ni(OH)₂ (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Sn	6	0.1381	1	1
Na	6	0.4602	1	1
In	6	0.1419	1	1
In	6	0.0052	1	1
As ₂	7	0.4804	1	1
LiO	7	0.0053	1	1
Mg ₂	7	0.1526	1	1
Cl ₂ Zn	8	0.4777	1	1
S ₂ V	8	0.0021	1	1
MoS ₂	8	0.0014	1	1
MoTe ₂	8	0.4659	1	1
PSn ₂	8	2.9106	1	1
HfS ₂	8	2.8314	1	1
FeO ₂	8	0.2537	1	1
Te ₂ V	8	0.4708	1	1
I ₂ Pr	8	0.3312	1	1
CuTe ₂	8	0.4866	1	1
S ₂ Zr	8	2.9007	1	1
NiO ₂	8	0.2555	1	1
Br ₂ Co	8	0.4793	1	1
Ca ₂ N	8	0.4818	1	1
Te ₂ Zn	8	0.4655	1	1
RhTe ₂	8	2.9975	1	1
S ₂ W	8	0.0013	1	1
Br ₂ Mn	8	0.4747	1	1
PtS ₂	8	0.4628	1	1
CoTe ₂	8	2.8355	1	1
CdClO	8	0.4695	1	1
Se ₂ Ti	8	0.4562	1	1
Te ₂ W	8	0.4663	1	1
I ₂ Nd	8	0.3333	1	1
S ₂ Sn	8	2.9041	1	1
Cl ₂ V	8	0.0027	1	1
PtSe ₂	8	2.9686	1	1
OTl ₂	8	0.47	1	1
Br ₂ Fe	8	0.4795	1	1
Br ₂ Ni	8	0.4928	1	1
CeI ₂	8	0.3296	1	1
FeSe ₂	8	0.133	1	1
NbTe ₂	8	0.5014	1	1
MoS ₂	8	0.0012	1	1
Cl ₂ Mg	8	0.4929	1	1
CrSe ₂	8	0.0015	1	1
CrSe ₂	8	0.004	1	1
O ₂ Pt	8	0.0067	1	1
N ₂ Re	8	0.2639	1	1
F ₂ Zn	8	0.323	1	1
CoO ₂	8	0.2547	1	1
NS ₂ Zr	9	0.4613	1	1
Ir ₂ P ₂	9	0.3328	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

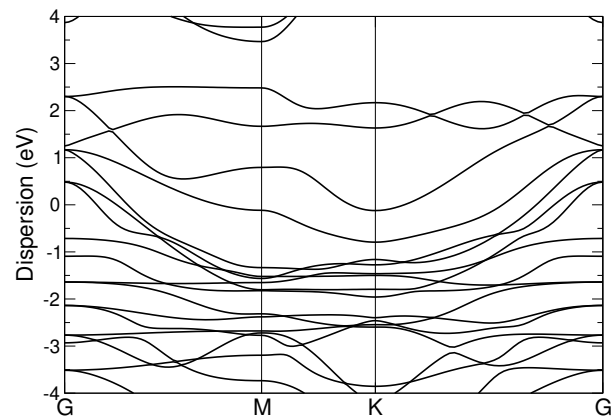
Formula	N° atoms	strain	cell size 1	cell size 2
As ₂ CeLi ₂	125	0.0	16	9
NiO ₂	504	0.0	57	73
Ga ₂ S ₃	905	0.0	100	81
Sb ₂	379	0.0	61	37
GeI ₂ La ₂	370	0.0	49	25
Li ₂ P ₂ Pr	650	0.0	81	49
PbTe	98	0.0	16	9
NS ₂ Zr	824	0.0	100	81
RhTe ₂	353	0.0001	49	36
Ga ₂ Ge ₂ Te ₂	699	0.0001	81	49
Br ₂ Hf ₂ N ₂	707	0.0001	73	57
KS ₂ Ti	661	0.0001	81	64
Br ₂ CsF	866	0.0002	130	54
GeI ₂	107	0.0002	16	9
CdH ₂ O ₂	820	0.0002	91	73
Br ₂ La ₂	453	0.0002	61	37
F ₂ Ho ₂ Se ₂	221	0.0002	25	16
Te ₂ W	674	0.0002	91	73
I ₂ Tm	320	0.0002	49	25
PSn ₂	414	0.0003	57	43
N ₂ Re	638	0.0003	73	91
PTe ₂ Zr ₂	305	0.0003	36	25
Na	581	0.0004	100	81
MoTe ₂	674	0.0004	91	73
I ₂ La ₂ Te	590	0.0004	79	39
Bi ₂ Te ₂	61	0.0005	9	4
LiMnTe ₂	116	0.0005	16	9
Br ₂ Mn	597	0.0005	81	64
CoO ₂	504	0.0005	57	73
Ca ₂ N	536	0.0005	73	57
Te ₂ Zn	674	0.0006	91	73
Br ₂ Ca ₃ Si	629	0.0006	79	39
Li ₂ P ₂ Pr	490	0.0006	61	37
Cl ₂ N ₂ Zr ₂	707	0.0006	73	57
Cl ₂ H ₂ Lu ₂	614	0.0006	64	49
PtS ₂	743	0.0007	100	81
Cl ₂ Zn	597	0.0007	81	64
Ga ₂ Ge ₂ Te ₂	527	0.0007	61	37
CdClHO	389	0.0007	49	36
I ₂ S ₂ Sm ₂	794	0.0007	100	49
Se ₄ TiZr	828	0.0007	114	43
S ₂ Sn	414	0.0008	57	43
Bi ₂ STe ₂	125	0.0008	16	9
HfLiS ₂	747	0.0008	91	73
CaH ₂ O ₂	650	0.0009	73	57
Bi ₂ STe ₂	125	0.0009	16	9
Br ₂ N ₂ Ti ₂	891	0.0009	99	66
Cl ₂ N ₂ Zr ₂	516	0.0009	60	36
I ₂ La ₂ O ₂	315	0.0009	39	20
Br ₂ Ca ₃ Si	629	0.0009	79	39

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Ni₂SbTe₂ (P-6m2 (187))

Structural and electronic properties

Formula	Ni ₂ SbTe ₂
Spacegroup	P-6m2 (187)
Prototype	Ni ₂ SbTe ₂
Parent 3D	Ni ₄ Sb ₂ Te ₄
Source DB	COD
DB ID	1533053
DF2-C09 Binding energy [meV/ Å²]	36.23
RVV10 Binding energy [meV/ Å²]	38.74
Band gap (PBE) [eV]	0.0

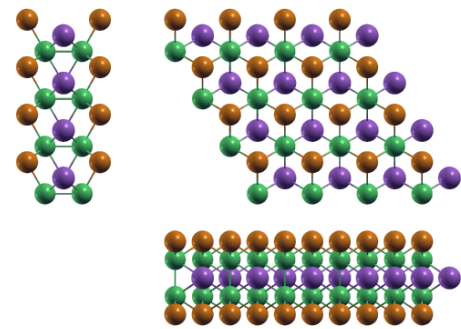


Band structure: Electronic band structure of Ni₂SbTe₂ (P-6m2 (187)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ni₂SbTe₂ (P-6m2 (187)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.90763402	−0.00000000	0.00000000
a₂	−1.95381701	3.38411033	0.00000000
a₃	0.00000000	0.00000000	25.08127536
	x [Å]	y [Å]	z [Å]
● Ni	−0.00000000	0.00000000	13.86287172
● Ni	−0.00000000	0.00000000	11.21840363
● Sb	1.95381701	1.12803678	12.54063768
● Te	−0.00000000	2.25607356	15.13565936
● Te	−0.00000000	2.25607356	9.94561599



Orthographic projections: views of Ni₂SbTe₂ (P-6m2 (187)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	6	3.0204	1	1
Na	6	0.2737	1	1
AsSb	7	0.0077	1	1
Bi ₂	7	0.4492	1	1
GeTe	7	0.0017	1	1
S ₂	7	0.0002	1	1
CaCl	7	0.1369	1	1
IrTe ₂	8	0.0008	1	1
CdCl ₂	8	0.0028	1	1
Cl ₂ Mn	8	1.5594	1	1
ReSe ₂	8	0.2561	1	1
CaI ₂	8	0.5016	1	1
InSe ₂	8	0.0024	1	1
GeTe ₂	8	0.0038	1	1
HfTe ₂	8	0.0076	1	1
I ₂ Mn	8	0.0027	1	1
NSr ₂	8	0.0061	1	1
I ₂ Yb	8	0.4948	1	1
LiO ₂	8	0.0681	1	1
Cl ₂ Zn	8	0.1497	1	1
FeI ₂	8	0.0048	1	1
I ₂ Ni	8	0.0036	1	1
S ₂ Ti	8	0.248	1	1
CrI ₂	8	0.0052	1	1
BiBrTe	8	0.458	1	1
Bi ₂ Pd	8	0.1133	1	1
Cl ₂ Ni	8	0.2573	1	1
Cl ₂ Co	8	0.2475	1	1
CrTe ₂	8	0.2659	1	1
PtS ₂	8	0.2753	1	1
Br ₂ V	8	0.255	1	1
ClN ₂ Zr	8	1.6348	1	1
Cl ₂ Fe	8	0.2466	1	1
S ₂ Ta	8	1.5339	1	1
Ba ₂ N	8	0.0092	1	1
Se ₂ V	8	1.5244	1	1
Se ₂ Ti	8	0.2714	1	1
Br ₂ Ti	8	0.2651	1	1
Te ₂ Zr	8	0.0081	1	1
AsSe ₂	8	0.2593	1	1
I ₂ Tm	8	0.4984	1	1
BiTe	8	0.4745	1	1
CdO ₂	8	0.2474	1	1
BrN ₂ Zr	8	0.2612	1	1
NbSe ₂	8	0.2579	1	1
CoI ₂	8	0.0072	1	1
GeS ₂	8	0.1279	1	1
MnSe ₂	8	0.1369	1	1
Br ₂ Cr	8	0.2655	1	1
Cl ₂ Zr	8	0.2471	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

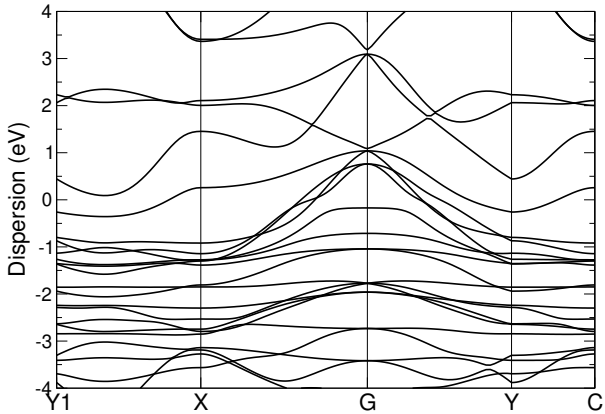
Formula	N° atoms	strain	cell size 1	cell size 2
Cl ₂ H ₂ Sc ₂	911	0.0	73	91
AsSe ₂	563	0.0	64	81
C ₂ F ₂	56	0.0001	4	9
S ₂	7	0.0002	1	1
LiOS ₂ Ti	425	0.0002	36	49
I ₂ Yb	467	0.0002	64	49
Cu ₂ Sr ₂	824	0.0002	100	81
Se ₂ Ta	638	0.0002	73	91
O ₂ Zn	368	0.0003	37	61
NbSe ₂	563	0.0003	64	81
Br ₂ V	504	0.0003	57	73
Cd ₂ I ₃	650	0.0004	73	57
Ba ₂ Cu ₂	516	0.0004	64	49
AsI ₂ La ₂	650	0.0004	73	57
ReSe ₂	504	0.0005	57	73
H ₂ MnO ₂	125	0.0005	9	16
CrO ₂	432	0.0005	39	79
Br ₂ Ti	638	0.0005	73	91
Br ₂ Ca ₃ Si	461	0.0005	49	36
BiTe	597	0.0006	81	64
I ₂ La ₂ Te	425	0.0006	49	36
Ga ₂ Se ₂	9	0.0006	1	1
Bi ₂ Te ₃	725	0.0006	81	64
BrKO ₃	530	0.0007	81	25
I ₂ La ₂ P	905	0.0007	100	81
GdI ₂	674	0.0007	91	73
Cl ₂ H ₂ Zr ₂	474	0.0007	36	49
Br ₂ H ₂ Zr ₂	911	0.0007	73	91
P ₂ Sn ₂	9	0.0008	1	1
Br ₂ Cr	638	0.0008	73	91
IrTe ₂	8	0.0008	1	1
GeI ₂ La ₂	565	0.0009	64	49
Se ₂ Ta	563	0.0009	64	81
F ₂ Se ₂ Yb ₂	11	0.0009	1	1
Br ₂ Hf ₂	644	0.0009	64	81
S ₂ Ti	437	0.001	49	64
NbS ₂	327	0.001	36	49
Dy ₂ I ₂ S ₂	543	0.001	57	43
ClKO ₃	325	0.001	49	16
NbSe ₂	563	0.001	64	81
Cl ₂ Sc ₂	729	0.001	73	91
CrTe ₂	638	0.0011	73	91
I ₂ Se ₂ Tb ₂	455	0.0011	55	30
Cl ₂ Zr ₂	577	0.0011	57	73
Cl ₂ Fe ₂ O ₂	857	0.0011	73	82
I ₂ Tm	467	0.0011	64	49
S ₂ Zn ₂	9	0.0012	1	1
CaI ₂	414	0.0012	57	43
Gd ₂ I ₂ Se ₂	824	0.0012	100	54
Cl ₂ Hf ₂	443	0.0012	43	57

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Ni₃GeTe₂ (P-6m2)

Structural and electronic properties

	Formula	Ni ₃ GeTe ₂
	Spacegroup	P-6m2
	Prototype	GeNi ₃ Te ₂
	Parent 3D	Ge ₂ Ni ₆ Te ₄
	Source DB	MPDS
	DB ID	S1947023
DF2-C09	Binding energy [meV/ Å²]	32.65
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

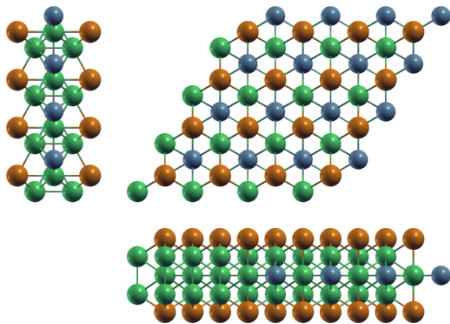


Band structure: Electronic band structure of Ni₃GeTe₂ (P-6m2) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ni₃GeTe₂ (P-6m2) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		1.97888214	-3.42752442	0.00000000
a₂		3.95776429	0.00000000	0.00000000
a₃		0.00000000	0.00000000	22.39729735
		x [Å]	y [Å]	z [Å]
●	Ni	0.00000000	0.00000000	1.34910537
●	Ni	0.00000000	0.00000000	-1.34910537
●	Ni	-1.97888214	-1.14250814	0.00000000
●	Ge	0.00000000	-2.28501628	0.00000000
●	Te	-1.97888214	-1.14250814	2.61256145
●	Te	-1.97888214	-1.14250814	-2.61256145



Orthographic projections: views of Ni₃GeTe₂ (P-6m2) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Na	7	0.265	1	1
HgO	8	0.4242	1	1
GeTe	8	0.0076	1	1
S ₂	8	0.0061	1	1
CaCl	8	0.1323	1	1
IrTe ₂	9	0.0067	1	1
Cl ₂ Zn	9	0.2751	1	1
CdCl ₂	9	0.0086	1	1
MoTe ₂	9	0.2682	1	1
ReSe ₂	9	0.2481	1	1
S ₂ Ta	9	1.5311	1	1
CaI ₂	9	0.4856	1	1
InSe ₂	9	0.0083	1	1
HfTe ₂	9	0.0015	1	1
Te ₂ V	9	0.271	1	1
I ₂ Mn	9	0.0085	1	1
I ₂ Yb	9	0.4791	1	1
AuTe ₂	9	0.0094	1	1
LiO ₂	9	0.0707	1	1
Cl ₂ Zn	9	0.1441	1	1
PdTe ₂	9	0.0069	1	1
NbS ₂	9	1.5279	1	1
Te ₂ Zn	9	0.268	1	1
Bi ₂ Pd	9	0.1111	1	1
Br ₂ Mn	9	0.2733	1	1
Cl ₂ Ni	9	0.2492	1	1
Cl ₂ Co	9	1.5643	1	1
CrTe ₂	9	0.2575	1	1
PtS ₂	9	0.2665	1	1
Br ₂ V	9	0.247	1	1
ClN ₂ Zr	9	1.5899	1	1
Cl ₂ Fe	9	1.5591	1	1
CdClO	9	0.2703	1	1
Ba ₂ N	9	0.003	1	1
Se ₂ Ti	9	0.2627	1	1
Br ₂ Ti	9	0.2567	1	1
Te ₂ Zr	9	0.002	1	1
Te ₂ W	9	0.2685	1	1
I ₂ Tm	9	0.4826	1	1
I ₂ Pb	9	3.0344	1	1
OTl ₂	9	0.2706	1	1
BiTe	9	0.4593	1	1
BrN ₂ Zr	9	1.6392	1	1
NbSe ₂	9	0.2498	1	1
GeS ₂	9	0.124	1	1
MnSe ₂	9	0.1322	1	1
Br ₂ Cr	9	0.257	1	1
DyI ₂	9	0.4931	1	1
Cl ₂ Zr	9	1.5619	1	1
Se ₂ Ta	9	0.2499	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

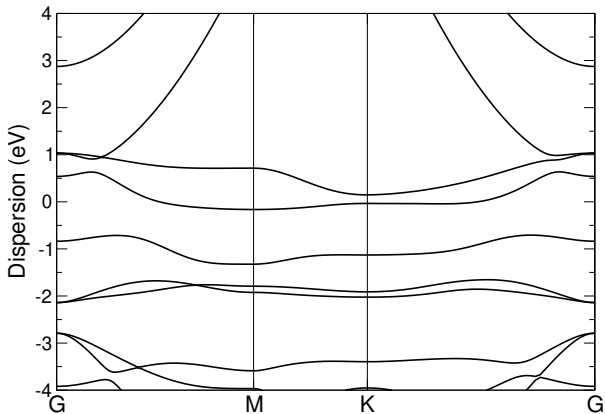
Formula	N° atoms	strain	cell size 1	cell size 2
HfLiS ₂	886	0.0	81	100
Cl ₂ Ni	486	0.0	49	64
Cd ₂ I ₃	911	0.0	91	73
AsI ₂ La ₂	911	0.0	91	73
Se ₂ Ta	561	0.0001	57	73
Br ₂ H ₂ Zr ₂	600	0.0002	43	57
I ₂ Tm	609	0.0002	73	57
Br ₂ Cr ₂ O ₂	624	0.0003	50	54
Te ₂ Zn	786	0.0003	81	100
Br ₂ Ca ₃ Si	600	0.0003	57	43
ClN ₂ Zr	429	0.0003	43	57
Cl ₂ H ₂ Sc ₂	780	0.0003	57	73
I ₂ La ₂ Te	557	0.0004	57	43
NbSe ₂	486	0.0004	49	64
I ₂ S ₂ Tb ₂	678	0.0004	64	49
MoTe ₂	786	0.0005	81	100
NiO ₂	297	0.0005	25	49
Na	529	0.0005	73	91
GeI ₂ La ₂	723	0.0005	73	57
Se ₂ Ta	486	0.0005	49	64
I ₂ N ₂ Zr ₂	618	0.0005	55	48
CCL ₂ Sc ₂	543	0.0006	43	57
NaPSn	9	0.0006	1	1
Te ₂ W	786	0.0006	81	100
HNiO ₂	118	0.0006	9	16
H ₂ I ₂ Sr ₂	678	0.0007	65	48
BiTe	843	0.0007	100	81
Pt ₂ Te ₂	10	0.0008	1	1
PtS ₂	786	0.0008	81	100
Ge ₂ S ₂	890	0.0008	95	80
Cl ₂ Cr ₂ O ₂	906	0.0008	70	81
CuGeO ₃	244	0.0008	24	20
Ga ₂ S ₃	893	0.0008	73	91
HN ₃ OZn	366	0.0008	25	36
In	121	0.0009	16	25
DyI ₂	531	0.0009	64	49
Br ₂ Hf ₂ N ₂	624	0.0009	54	50
Br ₂ Ti	561	0.0009	57	73
NS ₂ Zr	802	0.0009	73	91
ReSe ₂	486	0.0009	49	64
Mg ₂	722	0.0009	81	118
CaI ₂	609	0.0009	73	57
CKN	450	0.001	57	36
I ₂ Nd ₂ S ₂	510	0.001	49	36
Ba ₂ Pt	402	0.001	49	36
Cl ₂ Zr ₂	486	0.001	43	57
CoO ₂	297	0.001	25	49
Cl ₂ Hf ₂	412	0.001	36	49
Ba ₂ Cu ₂	742	0.001	81	64
Bi ₂ Se ₄	270	0.001	32	13

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

NiO₂H (P3m1)

Structural and electronic properties

	Formula	NiO ₂ H
	Spacegroup	P3m1
	Prototype	HNiO2
	Parent 3D	HNiO ₂
	Source DB	ICSD
	DB ID	169980
DF2-C09	Binding energy [meV/ Å²]	105.61
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

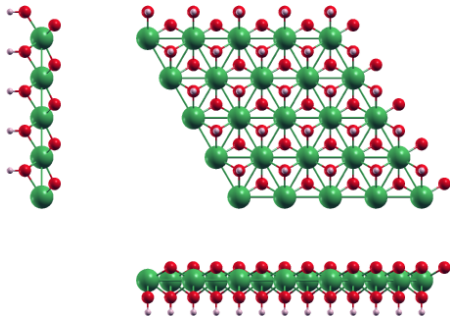


Band structure: Electronic band structure of NiO₂H (P3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NiO₂H (P3m1) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	−1.48610680	−2.57401248	0.00000000
a₂	2.97221360	0.00000000	0.00000000
a₃	0.00000000	0.00000000	17.82827650
	x [Å]	y [Å]	z [Å]
●	Ni	0.00000000	0.00000000
*	H	1.48610680	−0.85800416
●	O	1.48610680	−0.85800416
●	O	0.00000000	−1.71600832



Orthographic projections: views of NiO₂H (P3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Nd	5	0.2758	1	1
Tl	5	0.4678	1	1
Gd	5	0.1144	1	1
P ₂	6	0.4547	1	1
CaCl	6	0.3224	1	1
Cl ₂ Mn	7	0.4825	1	1
MoSe ₂	7	0.4659	1	1
Cl ₂ Ti	7	0.4551	1	1
S ₂ Ti	7	0.5011	1	1
Mg ₃	7	0.2063	1	1
NbS ₂	7	0.4868	1	1
N ₂ W	7	0.0076	1	1
Cl ₂ Co	7	0.5002	1	1
NbS ₂	7	0.4756	1	1
Cl ₂ Fe	7	0.4983	1	1
S ₂ Ta	7	0.4734	1	1
Se ₂ V	7	0.47	1	1
AsSe ₂	7	3.0079	1	1
CdO ₂	7	0.4998	1	1
MnSe ₂	7	0.3222	1	1
Cl ₂ Zr	7	0.4993	1	1
Se ₂ W	7	0.4664	1	1
Cl ₂ OOs	8	0.3412	1	1
Bi ₂ Mn ₂	8	0.3397	1	1
Cl ₂ ORu	8	0.3298	1	1
As ₂ Co ₂	8	0.3328	1	1
C ₂ F ₂	8	0.2504	1	1
Fe ₂ S ₂	8	0.3181	1	1
Co ₂ S ₂	8	0.3237	1	1
O ₂ Sn ₂	8	1.2327	1	1
LiNbS ₂	8	2.8342	1	1
O ₂ Sn ₂	8	1.2304	1	1
Co ₂ Se ₂	8	0.3357	1	1
Ca ₂ Cl ₂	8	0.3313	1	1
NS ₂ Ta	8	0.0053	1	1
CS ₂ Ta ₂	9	0.4553	1	1
Cl ₂ NSc ₂	9	0.4838	1	1
H ₂ MnO ₂	9	0.007	1	1
LiOS ₂ Ti	9	0.4786	1	1
FeH ₂ O ₂	9	0.0088	1	1
CNb ₂ S ₂	9	0.4535	1	1
Cu ₄ Te ₂	10	2.0321	1	1
Cl ₂ H ₂ Zr ₂	10	0.4763	1	1
Hf ₂ Si ₂ Te ₂	10	0.337	1	1
Ge ₂ Se ₂ Zr ₂	10	0.3313	1	1
HN ₃ OZn	10	0.4576	1	1
H ₂ Li ₂ O ₂	10	0.3134	1	1
BrCdI	11	0.219	2	1
BaF ₂	11	0.2233	2	1
CKN	11	0.331	2	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

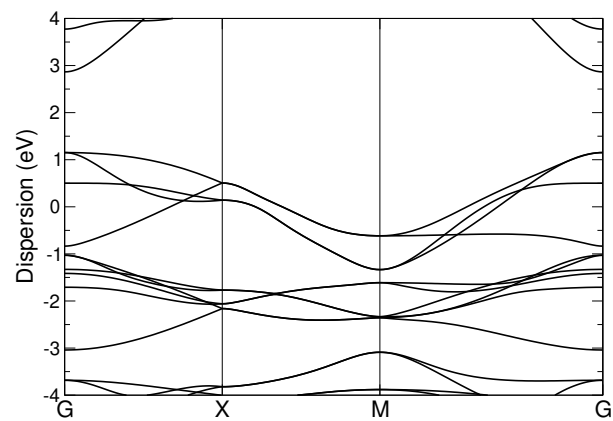
Formula	N° atoms	strain	cell size 1	cell size 2
Te ₂ W	219	0.0	36	25
NaPSn	91	0.0	16	9
Sb ₂ SeTe ₂	511	0.0001	79	39
Br ₂ Y ₂	520	0.0001	81	49
Cu ₂ I ₂	296	0.0001	49	25
Br ₂ Gd ₂ Ge	321	0.0001	49	25
InSe	498	0.0001	100	49
Se ₂ Ta	304	0.0001	49	36
Cl ₂ H ₂ Zr ₂	708	0.0001	81	64
As ₂ Li ₂ Pr	645	0.0001	100	49
In ₂ Te ₃	511	0.0001	79	39
PbS ₂	471	0.0002	81	49
Pt ₂ Te ₂	100	0.0002	16	9
NbS ₂	516	0.0002	81	64
MoTe ₂	219	0.0002	36	25
I ₂ La ₂ Si ₂	694	0.0002	100	49
Br ₂ Cu ₂	236	0.0002	39	20
H ₂ I ₂ Sr ₂	844	0.0002	130	54
AsLi ₃	596	0.0002	100	49
Ga ₂ Se ₂	392	0.0002	61	37
NbSe ₂	304	0.0002	49	36
Cl ₂ NSc ₂	577	0.0002	73	57
Se ₂ W	583	0.0002	91	73
Gd ₂ I ₂	296	0.0002	49	25
Br ₂ Hf ₂ N ₂	342	0.0003	48	25
Cl ₂ Mn	463	0.0003	73	57
Cl ₂ OV	508	0.0003	77	50
Bi ₂ Se ₂ Te	511	0.0003	79	39
Cl ₂ O ₂ Y ₂	466	0.0003	61	37
Te ₂ Zn	219	0.0003	36	25
Tl	437	0.0004	91	73
MoSe ₂	583	0.0004	91	73
Ba ₂ Cu ₂	52	0.0004	9	4
PtSe ₂	148	0.0004	25	16
CdH ₂ O ₂	269	0.0004	36	25
Br ₂ O ₂ Tb ₂	276	0.0004	39	20
Bi ₂ Se ₃	321	0.0005	49	25
Al ₂ Cl ₂ O ₂	628	0.0005	79	52
Br ₂ La	271	0.0005	49	25
Fe ₂ O ₄	766	0.0005	91	67
Br ₂ Y ₂	392	0.0006	61	37
I ₂ Yb	48	0.0006	9	4
Br ₂ F ₂ Yb ₂	276	0.0006	39	20
Cl ₂ ORu	380	0.0006	60	35
GeNi ₃ Te ₂	118	0.0006	16	9
HfLiS ₂	244	0.0006	36	25
Cl ₂ Ni	304	0.0006	49	36
Er ₂ F ₂ Se ₂	118	0.0006	16	9
GeI ₂ Y ₂	511	0.0008	79	39
As ₂ Li ₂ Nd	645	0.0008	100	49

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

NiSe (P4mm (99))

Structural and electronic properties

	Formula	NiSe
	Spacegroup	P4mm (99)
	Prototype	FeSe
	Parent 3D	Ni ₂ TlSe ₂
	Source DB	ICSD
	DB ID	646551
DF2-C09	Binding energy [meV/ Å²]	67.23
RVV10	Binding energy [meV/ Å²]	86.91
	Band gap (PBE) [eV]	0.0

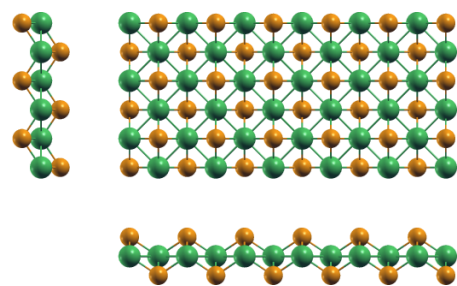


Band structure: Electronic band structure of NiSe (P4mm (99)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NiSe (P4mm (99)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.89782634	0.00000000	0.00000000
a₂		0.00000000	3.89782634	0.00000000
a₃		0.00000000	0.00000000	22.69253003
		x [Å]	y [Å]	z [Å]
●	Se	0.00000000	0.00000000	10.05253306
●	Ni	1.94891317	0.00000000	11.34626866
●	Ni	0.00000000	1.94891317	11.34626866
●	Se	1.94891317	1.94891317	12.63998968



Orthographic projections: views of NiSe (P4mm (99)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.3792	1	1
K	5	0.1853	1	1
InSe	6	0.1465	1	1
Bi ₂	6	0.152	1	1
AgTl	6	0.0233	1	1
Ag ₂	6	0.1924	1	1
LiO	6	0.1095	1	1
PbTe	6	0.1481	1	1
Sb ₂	6	0.1331	1	1
I ₂ Mg	7	0.1376	1	1
S ₂ V	7	0.1111	1	1
MoS ₂	7	0.111	1	1
CdI ₂	7	0.1498	1	1
Ba ₂ Pt	7	0.192	1	1
Br ₂ Ca	7	0.151	1	1
CaI ₂	7	0.1741	1	1
AsSn ₂	7	0.1089	1	1
I ₂ Pr	7	0.001	1	1
Br ₂ La	7	0.1379	1	1
Br ₂ Cu	7	0.106	1	1
Ca ₂ Si	7	0.7532	1	1
I ₂ Yb	7	0.1711	1	1
BiClTe	7	0.1501	1	1
BrCdI	7	0.1402	1	1
HgI ₂	7	1.1225	1	1
I ₂ Zn	7	0.1307	1	1
BaF ₂	7	0.1431	1	1
BiBrTe	7	0.1556	1	1
S ₂ W	7	0.111	1	1
GeI ₂	7	0.1361	1	1
AsKSn	7	0.1418	1	1
PbTe ₂	7	0.1394	1	1
I ₂ Nd	7	0.002	1	1
Cl ₂ Cu	7	0.0987	1	1
I ₂ Tm	7	0.1727	1	1
SnTe ₂	7	0.1343	1	1
Cl ₂ V	7	0.11	1	1
GeI ₂	7	0.1484	1	1
I ₂ Pb	7	0.1944	1	1
STl ₂	7	0.1439	1	1
BiTe	7	0.1624	1	1
GeS ₂	7	0.2195	1	1
DyI ₂	7	0.1774	1	1
CeI ₂	7	0.0002	1	1
Se ₂ Yb	7	0.1363	1	1
MoS ₂	7	0.1109	1	1
BiTe ₂	7	0.1365	1	1
GdI ₂	7	0.1585	1	1
CrSe ₂	7	0.1103	1	1
I ₂ La	7	0.0068	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

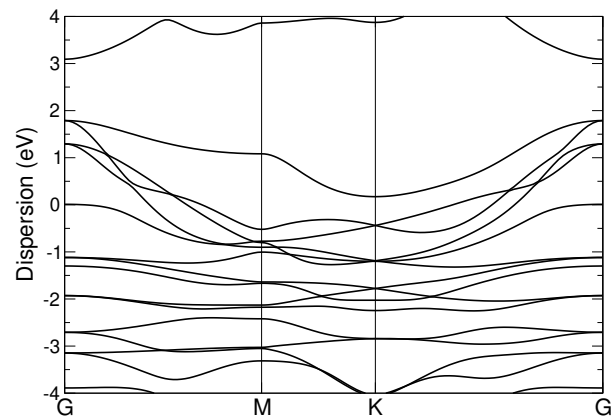
Formula	N° atoms	strain	cell size 1	cell size 2
GeS ₂	624	0.0001	81	100
Cl ₂ S ₂ Tl ₂	814	0.0001	106	65
Se ₂ Sn ₂	724	0.0002	100	81
CeI ₂	7	0.0002	1	1
Cl ₂ Zn	387	0.0003	48	65
Br ₂ Eu ₂ O ₂	10	0.0003	1	1
Pd ₂ S ₄	490	0.0004	70	35
HgO	172	0.0004	25	36
As ₂ Fe ₂	732	0.0004	82	101
O ₄ PSn	412	0.0004	49	36
In	485	0.0005	85	145
Ba ₂ H ₂ I ₂	706	0.0005	85	61
Mg ₂	472	0.0005	65	106
KS ₂ Ti	452	0.0007	48	65
As ₂ Cd ₂ K ₂	412	0.0007	49	36
H ₂ Na ₂ Pd	824	0.0007	81	100
AuI ₄ Li	558	0.0007	81	39
Ag ₂ I ₂	792	0.0007	113	85
Li ₂ Tl ₂	796	0.0007	118	81
Pb ₂ Se ₂	228	0.0007	32	25
Br ₂ Ca ₃ Si	156	0.0008	21	12
Se ₂ Ta	678	0.0008	81	118
AsSe ₂	678	0.0008	81	118
Br ₂ Co	387	0.0008	48	65
NbSe ₂	678	0.0008	81	118
Mg ₃	139	0.0009	16	25
Ag ₂ K ₂ Se ₂	550	0.0009	64	49
Br ₂ Fe	387	0.0009	48	65
K	486	0.0009	101	82
Hf ₂ Se ₂ Si ₂	934	0.0009	82	101
NS ₂ Ta	236	0.0009	20	39
As ₂ Fe ₂	724	0.001	81	100
NbSe ₂	678	0.001	81	118
I ₂ Pr	7	0.001	1	1
Br ₂ Mn	387	0.001	48	65
Se ₂ W	694	0.001	79	126
MoSe ₂	694	0.001	79	126
Au ₂ I ₂	652	0.0011	91	72
CCl ₂ Lu ₂	517	0.0011	48	65
Br ₂ Cr ₂ S ₂	420	0.0011	42	42
C ₂ I ₂ Y ₂	724	0.0011	70	74
Cl ₂ Ni	678	0.0012	81	118
Mg ₄	900	0.0012	89	136
As ₂ Mg ₂ Na ₂	896	0.0012	101	82
Tl	442	0.0012	79	126
Cl ₂ Cu	676	0.0012	88	108
As ₂	322	0.0012	48	65
Bi ₂ Cl ₂ O ₂	10	0.0012	1	1
Cl ₄ Mn	269	0.0013	36	25
H ₂ Na ₂ O ₂	580	0.0013	49	64

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

NiTe (P-3m1 (164))

Structural and electronic properties

	Formula	NiTe
	Spacegroup	P-3m1 (164)
	Prototype	PtTe
	Parent 3D	Ni ₂ Te ₂
	Source DB	ICSD
	DB ID	76730
DF2-C09	Binding energy [meV/ Å²]	40.48
RVV10	Binding energy [meV/ Å²]	41.83
	Band gap (PBE) [eV]	0.0

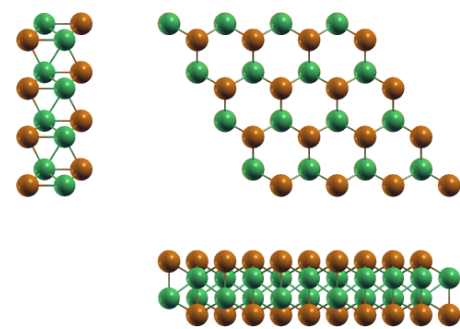


Band structure: Electronic band structure of NiTe (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NiTe (P-3m1 (164)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.88284690	0.00000000	0.00000000
a₂	-1.94142345	3.36264405	0.00000000
a₃	0.00000000	0.00000000	23.74752384
	x [Å]	y [Å]	z [Å]
● Ni	1.94142345	1.12088135	11.17541027
● Te	1.94142345	1.12088135	13.72891757
● Ni	-0.00000000	2.24176270	12.57211358
● Te	-0.00000000	2.24176270	10.01860628



Orthographic projections: views of NiTe (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	5	1.5397	1	1
HgO	6	0.111	1	1
AsSb	6	0.0047	1	1
Bi ₂	6	0.4566	1	1
GeTe	6	0.0013	1	1
S ₂	6	0.0029	1	1
CaCl	6	0.1394	1	1
IrTe ₂	7	0.0022	1	1
CdCl ₂	7	0.0002	1	1
Cl ₂ Mn	7	1.5813	1	1
CdI ₂	7	0.4509	1	1
AgTe ₂	7	0.4242	1	1
MoSe ₂	7	1.5343	1	1
ReSe ₂	7	0.2602	1	1
S ₂ Ta	7	1.5966	1	1
Br ₂ Ca	7	0.4539	1	1
InSe ₂	7	0.0006	1	1
GeTe ₂	7	0.0008	1	1
I ₂ Mn	7	0.0003	1	1
NSr ₂	7	0.0031	1	1
Ca ₂ Si	7	3.1967	1	1
I ₂ Yb	7	2.9052	1	1
PbS ₂	7	0.0073	1	1
BiClTe	7	0.4518	1	1
LiO ₂	7	0.0669	1	1
Cl ₂ Zn	7	0.1526	1	1
FeI ₂	7	0.0019	1	1
I ₂ Ni	7	0.0006	1	1
S ₂ Ti	7	1.6337	1	1
NbS ₂	7	1.5932	1	1
CrI ₂	7	0.0023	1	1
BiBrTe	7	0.4655	1	1
Bi ₂ Pd	7	0.1145	1	1
N ₂ W	7	4.8735	1	1
Cl ₂ Ni	7	0.2615	1	1
Cl ₂ Co	7	1.6311	1	1
CrTe ₂	7	0.2702	1	1
Br ₂ V	7	0.2591	1	1
ClNZr	7	0.2562	1	1
Cl ₂ Fe	7	0.2505	1	1
S ₂ Ta	7	1.5555	1	1
Se ₂ V	7	1.5458	1	1
Se ₂ Ti	7	0.2758	1	1
Br ₂ Ti	7	0.2694	1	1
AsSe ₂	7	0.2636	1	1
I ₂ Tm	7	2.9229	1	1
GeI ₂	7	0.4473	1	1
BiTe	7	0.4823	1	1
BrNZr	7	0.2654	1	1
NbSe ₂	7	0.2621	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

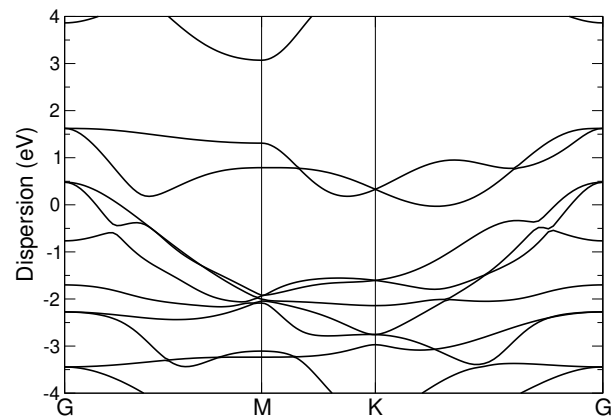
Formula	N° atoms	strain	cell size 1	cell size 2
N ₂ W	439	0.0001	49	81
Sb ₂ Te ₂	244	0.0001	36	25
NbS ₂	343	0.0001	43	57
Sb ₂ Te ₃	805	0.0001	100	81
Br ₂ V	499	0.0001	64	81
N ₃ W ₂	116	0.0001	9	16
Se ₂ V	291	0.0002	36	49
F ₂ Se ₂ Y ₂	196	0.0002	25	16
CdCl ₂	7	0.0002	1	1
Ba ₂ Cd	404	0.0002	65	48
NbSe ₂	565	0.0003	73	91
I ₂ Mn	7	0.0003	1	1
Ge ₂ I ₂ La ₂	550	0.0003	64	49
F ₂ I ₂ Pb ₂	548	0.0003	65	48
Br ₂ Hf ₂	656	0.0004	73	91
BiTe	463	0.0004	73	57
GeI ₂ La ₂	443	0.0004	57	43
Cl ₂ Er ₂ H ₂	10	0.0004	1	1
Bi ₂ Te ₃	577	0.0004	73	57
Cu ₄ Te ₂	886	0.0005	100	81
Br ₂ Cr ₂ O ₂	748	0.0005	73	76
Se ₂ Ta	624	0.0005	81	100
Cu ₂ Sr ₂	656	0.0005	91	73
FeH ₂ O ₂	453	0.0005	37	61
BiBrTe	583	0.0005	91	73
AsSe ₂	565	0.0005	73	91
ClNZr	447	0.0006	57	73
Cl ₂ Cu	436	0.0006	61	64
S ₂ Ta	343	0.0006	43	57
LiO	172	0.0006	25	36
InSe ₂	7	0.0006	1	1
ReS ₂	139	0.0006	16	25
As ₂ O ₃	321	0.0006	49	25
I ₂ Ni	7	0.0006	1	1
LiNbS ₂	400	0.0006	43	57
I ₂ Tm	357	0.0006	57	43
ReSe ₂	499	0.0007	64	81
Cl ₂ H ₂ Sc ₂	924	0.0007	81	100
I ₂ Yb	357	0.0007	57	43
N ₂ W	331	0.0007	37	61
Ho ₂ I ₂ Se ₂	400	0.0008	55	30
BrNZr	565	0.0008	73	91
GeTe ₂	7	0.0008	1	1
Gd ₂ I ₂ S ₂	412	0.0008	49	36
CNNa	488	0.0008	77	60
Ba ₂ Cu ₂	400	0.0009	57	43
H ₂ Si ₂	8	0.0009	1	1
Cl ₂ Zr ₂	580	0.0009	64	81
Cl ₂ Fe	388	0.001	49	64
Tl	193	0.001	36	49

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

NiTe₂ (P-3m1 (164))

Structural and electronic properties

	Formula	NiTe ₂
	Spacegroup	P-3m1 (164)
	Prototype	CdI ₂
	Parent 3D	NiTe ₂
	Source DB	COD
	DB ID	9009113
DF2-C09	Binding energy [meV/ Å²]	48.92
RVV10	Binding energy [meV/ Å²]	48.0
	Band gap (PBE) [eV]	0.0

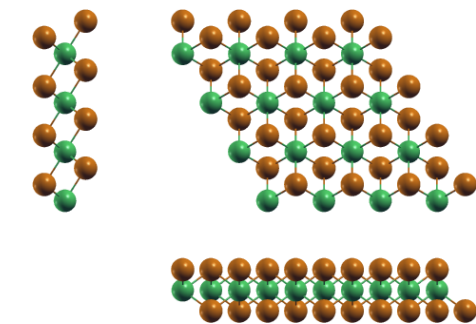


Band structure: Electronic band structure of NiTe₂ (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of NiTe₂ (P-3m1 (164)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.78959609	0.00000000	0.00000000
a₂	−1.89479804	3.28188648	0.00000000
a₃	0.00000000	0.00000000	22.68250423
	x [Å]	y [Å]	z [Å]
● Te	0.00000000	2.18792432	9.95890779
● Ni	0.00000000	0.00000000	11.34125212
● Te	1.89479804	1.09396216	12.72359644



Orthographic projections: views of NiTe₂ (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	4	0.4435	1	1
Tl	4	0.2502	1	1
InSe	5	0.4708	1	1
HgO	5	0.1154	1	1
AsSb	5	0.0068	1	1
Bi ₂	5	0.4857	1	1
P ₂	5	1.5848	1	1
PbTe	5	0.4753	1	1
CaCl	5	0.1497	1	1
Cl ₂ Mn	6	0.258	1	1
CdI ₂	6	0.4798	1	1
AgTe ₂	6	0.1118	1	1
MoSe ₂	6	0.2492	1	1
S ₂ Ta	6	0.2609	1	1
Br ₂ Zn	6	0.0035	1	1
Br ₂ Ca	6	0.4829	1	1
SiTe ₂	6	0.0006	1	1
NSr ₂	6	0.0085	1	1
PbS ₂	6	0.0041	1	1
BiClTe	6	0.4807	1	1
Cl ₂ Ti	6	1.5859	1	1
BrCdI	6	0.453	1	1
S ₂ Ti	6	0.2679	1	1
Mg ₃	6	0.43	1	1
Te ₂ Ti	6	0.0032	1	1
NbS ₂	6	0.2602	1	1
CrI ₂	6	0.0094	1	1
BaF ₂	6	0.4612	1	1
BiBrTe	6	0.4952	1	1
RhTe ₂	6	0.0075	1	1
Bi ₂ Pd	6	0.1201	1	1
Cl ₂ Co	6	0.2674	1	1
NbS ₂	6	0.2543	1	1
Br ₂ V	6	0.2756	1	1
ClNZr	6	0.2725	1	1
Cl ₂ Fe	6	0.2664	1	1
S ₂ Ta	6	1.6404	1	1
Se ₂ V	6	1.6302	1	1
AsKSn	6	0.4576	1	1
PbTe ₂	6	0.4506	1	1
I ₂ V	6	0.0019	1	1
GeI ₂	6	0.4759	1	1
Se ₂ Zr	6	0.001	1	1
STl ₂	6	0.4636	1	1
CdO ₂	6	0.2672	1	1
CoI ₂	6	0.0072	1	1
GeS ₂	6	0.1389	1	1
MnSe ₂	6	0.1496	1	1
Cl ₂ Zr	6	0.2669	1	1
I ₂ Ti	6	0.0076	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

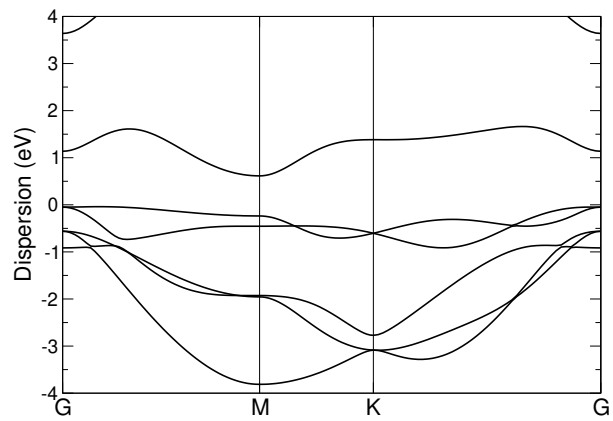
Formula	N° atoms	strain	cell size 1	cell size 2
BaF ₂	543	0.0	100	81
Nd	124	0.0	25	49
MoSe ₂	339	0.0	49	64
GeI ₂	435	0.0	81	64
BiBrTe	339	0.0001	64	49
Br ₂ Ca	390	0.0001	73	57
N ₄	663	0.0001	77	108
HN ₃ OZn	471	0.0001	43	57
Cl ₂ Co	543	0.0001	81	100
Li ₂ Tl ₂	84	0.0002	16	9
Se ₂ W	339	0.0002	49	64
Sb ₂ SeTe ₂	638	0.0002	91	73
ClKO ₃	368	0.0002	81	25
Bi ₂ Se ₂ Te	638	0.0002	91	73
Ga ₂ I ₂ Y ₂	786	0.0002	100	81
As ₂ CeLi ₂	563	0.0002	81	64
In ₂ Te ₃	638	0.0002	91	73
S ₂ Ti	543	0.0002	81	100
Ga ₂ I ₂ Tb ₂	561	0.0003	73	57
PbTe	371	0.0003	81	64
CdO ₂	543	0.0003	81	100
Cd ₂ I ₃	327	0.0003	49	36
LiMnTe ₂	499	0.0003	81	64
AsI ₂ La ₂	327	0.0003	49	36
LiOS ₂ Ti	536	0.0003	57	73
In	111	0.0004	25	36
Br ₂ In ₂ O ₂	963	0.0004	121	100
Br ₂ F ₂ Pb ₂	483	0.0004	65	48
Cl ₂ Zr	543	0.0005	81	100
Cl ₂ NSc ₂	597	0.0005	64	81
CuGeO ₃	375	0.0005	55	42
Ga ₂ Gd ₂ I ₂	561	0.0005	73	57
I ₂ La ₂ Te	233	0.0005	36	25
Cl ₂ H ₂ Zr ₂	609	0.0006	57	73
SiTe ₂	6	0.0006	1	1
CaClHO	7	0.0006	1	1
Bi ₂ STe ₂	563	0.0006	81	64
GeI ₂ Y ₂	638	0.0007	91	73
Br ₂ F ₂ Sr ₂	483	0.0007	65	48
NbS ₂	435	0.0007	64	81
Br ₂ Ca ₃ Si	258	0.0007	36	25
FeH ₂ O ₂	173	0.0007	16	25
GdI ₂	300	0.0007	57	43
Tl	211	0.0007	49	64
Cl ₂ O ₂ Tm ₂	9	0.0007	1	1
Br ₂ Ca ₃ Si	258	0.0008	36	25
CS ₂ Ta ₂	414	0.0008	43	57
Cu ₄ Te ₂	441	0.0008	57	45
Cl ₂ Er ₂ O ₂	9	0.0008	1	1
Cl ₂ Fe	543	0.0008	81	100

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

PbS₂ (P-3m1)

Structural and electronic properties

	Formula	PbS ₂
	Spacegroup	P-3m1
	Prototype	CdI2
	Parent 3D	PbS ₂
	Source DB	MPDS
	DB ID	S1903552
DF2-C09	Binding energy [meV/ Å ²]	38.35
RVV10	Binding energy [meV/ Å ²]	N/A
	Band gap (PBE) [eV]	0.65

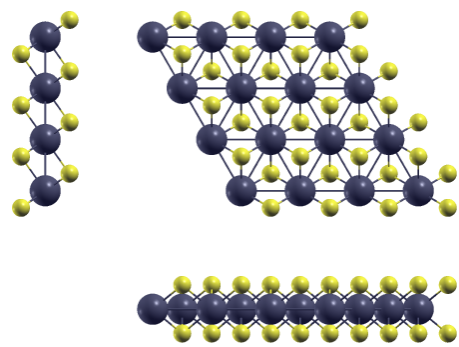


Band structure: Electronic band structure of PbS₂ (P-3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of PbS₂ (P-3m1) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		1.91132413	−3.31051009	0.00000000
a₂		1.91132378	3.31050989	0.00000000
a₃		0.00000000	0.00000000	18.16423751
		x [Å]	y [Å]	z [Å]
●	S	0.95566977	−0.55175620	1.56995427
●	Pb	−0.95566189	−1.65525495	0.00000000
●	S	0.95565436	−2.75875389	−1.56995427



Orthographic projections: views of PbS₂ (P-3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	4	0.4341	1	1
InSe	5	0.4605	1	1
Nd	5	0.2231	1	2
HgO	5	0.1136	1	1
AsSb	5	0.0026	1	1
Bi ₂	5	0.4751	1	1
GeTe	5	0.0088	1	1
PbTe	5	0.4649	1	1
CaCl	5	0.1459	1	1
CdCl ₂	6	0.0077	1	1
CdI ₂	6	0.4693	1	1
ReSe ₂	6	0.2708	1	1
S ₂ Ta	6	0.2552	1	1
Br ₂ Zn	6	0.0075	1	1
Br ₂ Ca	6	0.4724	1	1
InSe ₂	6	0.0081	1	1
GeTe ₂	6	0.0067	1	1
SiTe ₂	6	0.0035	1	1
I ₂ Mn	6	0.0078	1	1
NSr ₂	6	0.0042	1	1
BiClTe	6	0.4702	1	1
FeI ₂	6	0.0055	1	1
I ₂ Ni	6	0.0069	1	1
S ₂ Ti	6	0.2621	1	1
Te ₂ Ti	6	0.0072	1	1
NbS ₂	6	0.2546	1	1
CrI ₂	6	0.0052	1	1
BaF ₂	6	0.4511	1	1
BiBrTe	6	0.4844	1	1
Bi ₂ Pd	6	0.1179	1	1
Cl ₂ Ni	6	0.2721	1	1
Cl ₂ Co	6	0.2616	1	1
NbS ₂	6	0.2488	1	1
Br ₂ V	6	0.2696	1	1
ClNZr	6	0.2665	1	1
Cl ₂ Fe	6	0.2606	1	1
S ₂ Ta	6	0.2477	1	1
AsKSn	6	0.4476	1	1
AsSe ₂	6	0.2742	1	1
NiTe ₂	6	0.0041	1	1
I ₂ V	6	0.0021	1	1
GeI ₂	6	0.4655	1	1
Se ₂ Zr	6	0.0031	1	1
STl ₂	6	0.4534	1	1
CdO ₂	6	0.2614	1	1
NbSe ₂	6	0.2727	1	1
CoI ₂	6	0.003	1	1
GeS ₂	6	0.1356	1	1
MnSe ₂	6	0.1458	1	1
Cl ₂ Zr	6	0.2611	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

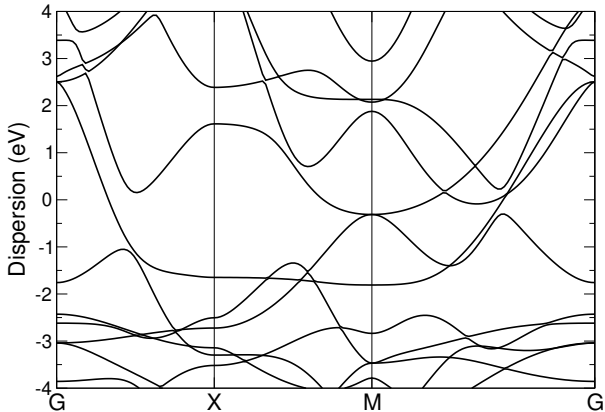
Formula	N° atoms	strain	cell size 1	cell size 2
Cl ₂ H ₂ Zr ₂	531	0.0	49	64
AsLi ₃	624	0.0	100	81
Bi ₂ STe ₂	638	0.0001	91	73
LiNbS ₂	463	0.0001	57	73
Tl	186	0.0001	43	57
HNiO ₂	471	0.0002	49	81
Br ₂ H ₂ Zr ₂	843	0.0002	81	100
MoS ₂	183	0.0002	25	36
S ₂ Ta	390	0.0002	57	73
CCL ₂ Sc ₂	743	0.0002	81	100
Br ₂ Y ₂	7	0.0002	1	1
LiMnTe ₂	565	0.0002	91	73
S ₂ W	183	0.0002	25	36
Bi ₂ SeTe ₂	563	0.0002	81	64
Ba ₂ Cu ₂	291	0.0003	49	36
InSe	462	0.0003	100	81
As ₂ Li ₂ Pr	705	0.0003	100	81
NbS ₂	339	0.0003	49	64
I ₂ La ₂ Si ₂	786	0.0003	100	81
Bi ₂	371	0.0003	81	64
MoS ₂	183	0.0004	25	36
I ₂ Yb	255	0.0004	49	36
Se ₂ W	300	0.0005	43	57
BiBrTe	390	0.0005	73	57
CdI ₂	492	0.0005	91	73
GeI ₂	492	0.0005	91	73
CKN	396	0.0005	83	49
S ₂ V	183	0.0006	25	36
Ga ₂ Se ₂	7	0.0006	1	1
Cl ₂ Zr ₂	643	0.0006	81	100
CNb ₂ S ₂	353	0.0006	36	49
MoSe ₂	300	0.0006	43	57
NbS ₂	390	0.0006	57	73
Br ₂ La ₂ P	638	0.0006	91	73
Bi ₂ STe ₂	705	0.0007	100	81
ClNZr	543	0.0007	81	100
As ₂ CeLi ₂	638	0.0007	91	73
Ga ₂ Gd ₂ I ₂	627	0.0008	81	64
PbTe	419	0.0008	91	73
HNiO ₂	355	0.0008	37	61
I ₂ La ₂ Sb	233	0.0008	36	25
CrS ₂	123	0.0008	16	25
Cl ₂ S ₂ Tl ₂	237	0.0008	39	20
Cu ₄ Te ₂	561	0.0008	73	57
LiOS ₂ Ti	467	0.0008	49	64
Cl ₂ Fe	435	0.0009	64	81
As ₂ Li ₂ Nd	705	0.0009	100	81
Ag ₂ K ₂ Te ₂	411	0.0009	65	36
CdI ₂	492	0.0009	91	73
Se ₂ V	300	0.001	43	57

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

PdBi₂ (P4/mmm (123))

Structural and electronic properties

	Formula	PdBi ₂
	Spacegroup	P4/mmm (123)
	Prototype	Zr2Cu
	Parent 3D	PdBi ₂
	Source DB	COD
	DB ID	9012857
DF2-C09	Binding energy [meV/ Å²]	46.99
RVV10	Binding energy [meV/ Å²]	50.21
	Band gap (PBE) [eV]	0.0

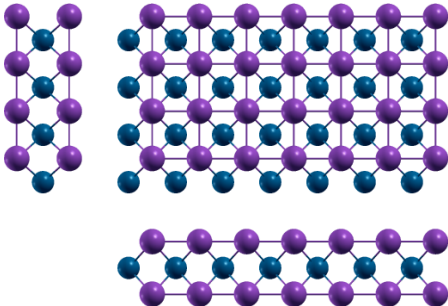


Band structure: Electronic band structure of PdBi₂ (P4/mmm (123)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of PdBi₂ (P4/mmm (123)) in Cartesian coordinates.

	<i>x</i> [Å]	<i>y</i> [Å]	<i>z</i> [Å]
a₁	3.31169211	0.00000000	0.00000000
a₂	0.00000000	3.31169211	0.00000000
a₃	0.00000000	0.00000000	23.51414611
	<i>x</i> [Å]	<i>y</i> [Å]	<i>z</i> [Å]
● Bi	1.65584605	1.65584605	9.91634949
● Bi	1.65584605	1.65584605	13.59779662
● Pd	0.00000000	0.00000000	11.75707306



Orthographic projections: views of PdBi₂ (P4/mmm (123)) as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Sn	4	0.2145	1	1
Na	4	0.1397	1	1
In	4	0.2195	1	1
HgO	5	0.0093	1	1
AsSb	5	0.1786	1	1
GeTe	5	0.1861	1	1
As ₂	5	0.1467	1	1
S ₂	5	0.1881	1	1
IrTe ₂	6	0.1873	1	1
Cl ₂ Zn	6	0.1458	1	1
CdCl ₂	6	0.1848	1	1
MoTe ₂	6	0.1417	1	1
PSn ₂	6	0.1554	1	1
ReSe ₂	6	0.1301	1	1
Br ₂ Zn	6	0.1667	1	1
HfS ₂	6	0.1493	1	1
InSe ₂	6	0.1852	1	1
AsSn ₂	6	0.1592	1	1
GeTe ₂	6	0.1835	1	1
SiTe ₂	6	0.1714	1	1
HfTe ₂	6	0.7538	1	1
Te ₂ V	6	0.1433	1	1
I ₂ Mn	6	0.1849	1	1
CuTe ₂	6	0.149	1	1
S ₂ Zr	6	0.1546	1	1
NSr ₂	6	0.1806	1	1
PbS ₂	6	0.1755	1	1
Br ₂ Co	6	0.1463	1	1
Ca ₂ N	6	0.1472	1	1
AuTe ₂	6	0.7836	1	1
LiO ₂	6	0.1098	1	1
Cl ₂ Zn	6	0.3913	1	1
PdTe ₂	6	0.7741	1	1
FeI ₂	6	0.1822	1	1
I ₂ Ni	6	0.1838	1	1
Te ₂ Ti	6	0.167	1	1
CrI ₂	6	0.1816	1	1
Te ₂ Zn	6	0.1415	1	1
RhTe ₂	6	0.1622	1	1
Br ₂ Mn	6	0.1447	1	1
Cl ₂ Ni	6	0.1307	1	1
CrTe ₂	6	0.1353	1	1
PtS ₂	6	0.1406	1	1
CoTe ₂	6	0.1496	1	1
Br ₂ V	6	0.1295	1	1
CdClO	6	0.1429	1	1
Se ₂ Ti	6	0.1384	1	1
Br ₂ Ti	6	0.1349	1	1
Te ₂ W	6	0.1418	1	1
AsSe ₂	6	0.1318	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

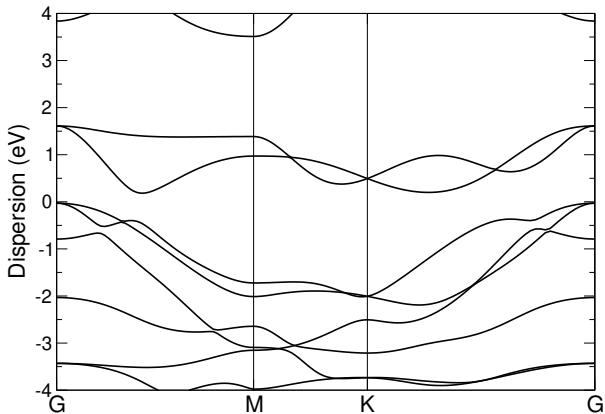
Lattice matching - minimal strain

Formula	N° atoms	strain	cell size 1	cell size 2
I ₂ O ₂ Yb ₂	621	0.0	85	61
Si ₂ Te ₂ Zr ₂	786	0.0001	100	81
F ₂ Ni	543	0.0001	100	81
Fe ₂ Se ₂	631	0.0001	101	82
In	343	0.0001	81	100
Br ₂ Cu ₂	291	0.0001	49	36
Bi ₂ In ₂	247	0.0002	49	25
Ca ₂ Cl ₂ F ₂	495	0.0002	65	50
Cu ₂ I ₂	764	0.0002	136	89
Br ₂ H ₂ Sr ₂	942	0.0002	136	89
Cl ₂ Cu	525	0.0003	93	82
Bi ₂ Se ₂	896	0.0003	164	101
Ir ₂ P ₂	499	0.0004	85	61
Ge ₂ Mn ₂ Sr ₂	258	0.0004	36	25
I ₂ Pr	438	0.0004	85	61
Br ₂ F ₂ Yb ₂	363	0.0004	49	36
Fe ₂ Se ₂	624	0.0004	100	81
I ₂ S ₂ Tl ₂	786	0.0004	100	81
As ₂ Ir ₂	208	0.0005	36	25
Br ₂ Er ₂ O ₂	849	0.0005	113	85
Br ₂ O ₂ Sm ₂	621	0.0005	85	61
Cu ₂ Rb ₂ Te ₂	297	0.0005	49	25
Br ₂ O ₂ Tb ₂	363	0.0005	49	36
Bi ₂ Se ₂	443	0.0006	81	50
I ₂ S ₂ Yb ₂	240	0.0006	40	20
I ₂ Nd	438	0.0006	85	61
I ₂ S ₂ Tm ₂	240	0.0006	40	20
Ga ₂ Gd ₂ I ₂	840	0.0007	118	81
Bi ₂	516	0.0007	118	81
Cu ₂ Se ₂	624	0.0007	100	81
Cu ₂ F ₄	342	0.0007	64	25
Fe ₂ SeTe	887	0.0008	145	113
Ga ₂ I ₂ Tb ₂	840	0.0008	118	81
Cl ₂ S ₂ Tl ₂	51	0.0008	9	4
I ₂ La ₂ Sb	649	0.0008	108	65
Br ₂ Ca ₂ F ₂	363	0.0008	49	36
CrS ₂	339	0.0008	48	65
As ₄	535	0.0008	97	61
Sn	277	0.0008	65	82
K	520	0.0008	145	85
Cu ₂ Te ₂	499	0.0009	81	64
Ca ₂ Cl ₂ F ₂	486	0.0009	64	49
F ₄ Pb	93	0.0009	16	9
Ba ₂ Hg	882	0.0009	181	113
Cl ₄ Mn	817	0.0009	149	74
Cl ₂ Zn	441	0.001	82	65
Br ₂ Ca	597	0.001	118	81
H ₂ I ₂ Sr ₂	639	0.001	97	58
Bi ₂ SeTe ₂	759	0.001	118	81
Br ₂ Eu ₂ O ₂	621	0.0011	85	61

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

PdTe₂ (P-3m1 (164)) Structural and electronic properties

	Formula	PdTe ₂
	Spacegroup	P-3m1 (164)
	Prototype	CdI2
	Parent 3D	PdTe ₂
	Source DB	COD
	DB ID	9009115
DF2-C09	Binding energy [meV/ Å²]	50.82
RVV10	Binding energy [meV/ Å²]	50.86
	Band gap (PBE) [eV]	0.21

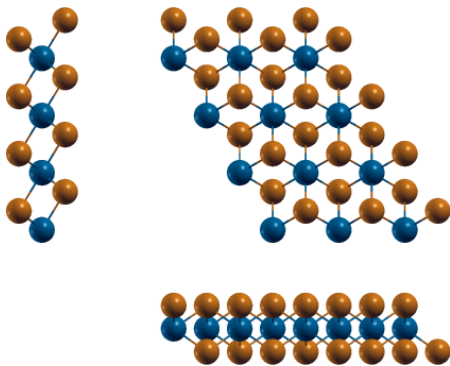


Band structure: Electronic band structure of PdTe₂ (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of PdTe₂ (P-3m1 (164)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.01528942	0.00000000	0.00000000
a₂	−2.00764471	3.47734265	0.00000000
a₃	0.00000000	0.00000000	22.82336998
	x [Å]	y [Å]	z [Å]
● Te	2.00764471	1.15911422	12.81749799
● Te	0.00000000	2.31822843	10.00587199
● Pd	0.00000000	0.00000000	11.41168499



Orthographic projections: views of PdTe₂ (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	4	2.8522	1	1
Na	4	0.2555	1	1
Gd	4	0.2378	1	1
As ₂	5	0.2666	1	1
CaCl	5	0.1274	1	1
Cl ₂ Zn	6	0.2651	1	1
MoTe ₂	6	0.2586	1	1
ReSe ₂	6	1.5614	1	1
HfS ₂	6	0.2706	1	1
CaI ₂	6	0.4681	1	1
HfTe ₂	6	0.0053	1	1
Te ₂ V	6	0.2613	1	1
CuTe ₂	6	0.2701	1	1
Ca ₂ Si	6	2.979	1	1
I ₂ Yb	6	0.4618	1	1
Br ₂ Co	6	0.266	1	1
Ca ₂ N	6	0.2674	1	1
AuTe ₂	6	0.0025	1	1
Cl ₂ Zn	6	0.1383	1	1
I ₂ Zn	6	0.0071	1	1
Te ₂ Zn	6	0.2584	1	1
Bi ₂ Pd	6	0.4305	1	1
Br ₂ Mn	6	0.2634	1	1
CrTe ₂	6	0.2483	1	1
PtS ₂	6	0.2569	1	1
CoTe ₂	6	0.2711	1	1
Br ₂ V	6	1.5556	1	1
ClN ₂ Zr	6	1.5404	1	1
CdClO	6	0.2606	1	1
Ba ₂ N	6	0.0038	1	1
Se ₂ Ti	6	0.2533	1	1
Br ₂ Ti	6	0.2476	1	1
Te ₂ Zr	6	0.0048	1	1
Te ₂ W	6	0.2588	1	1
I ₂ Tm	6	0.4652	1	1
OTl ₂	6	0.2609	1	1
BrN ₂ Zr	6	1.5883	1	1
Br ₂ Fe	6	0.2661	1	1
GeS ₂	6	0.1201	1	1
MnSe ₂	6	0.1274	1	1
Br ₂ Cr	6	0.248	1	1
DyI ₂	6	0.4753	1	1
Br ₂ Ni	6	0.2735	1	1
NbSe ₂	6	1.5806	1	1
Cl ₂ Mg	6	0.2736	1	1
F ₂ Ni	6	0.135	1	1
Se ₂ Ta	6	0.2466	1	1
PtTe ₂	6	0.0021	1	1
Br ₂ Cd	6	0.0009	1	1
NaPSn	6	0.0061	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

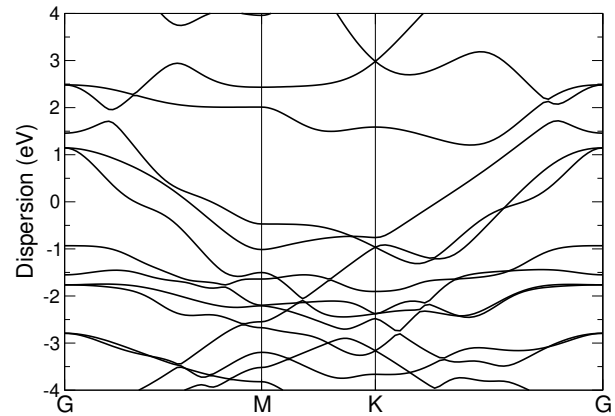
Formula	N° atoms	strain	cell size 1	cell size 2
CCl ₂ Sc ₂	353	0.0	36	49
Na	244	0.0	57	73
CoO ₂	354	0.0	39	79
BN	203	0.0	25	64
AgNO ₃	488	0.0001	81	49
Ba ₂ Cu ₂	624	0.0001	100	81
CdH ₂ O ₂	597	0.0001	64	81
NaO ₄	368	0.0001	61	37
Ca ₂ N	543	0.0001	81	100
I ₂ S ₂ Tb ₂	627	0.0002	81	64
BrKO ₃	227	0.0002	49	16
Cl ₂ H ₂ Zr ₂	291	0.0002	25	36
KS ₂ Ti	583	0.0002	73	91
Cu ₂ Na ₂ Te ₂	483	0.0002	65	48
I ₂ Yb	543	0.0002	100	81
DyI ₂	435	0.0003	81	64
Te ₂ W	435	0.0003	64	81
Cl ₂ V	123	0.0003	16	25
Br ₂ H ₂ Zr ₂	402	0.0003	36	49
Ga ₂ S ₃	536	0.0004	57	73
Ba ₂ Pt	300	0.0004	57	43
Cl ₂ Zr ₂	304	0.0004	36	49
Br ₂ Ca ₃ Si	561	0.0004	73	57
NS ₂ Zr	463	0.0005	57	73
Br ₂ Hf ₂ N ₂	843	0.0005	81	100
C	76	0.0005	9	49
CaI ₂	492	0.0005	91	73
NbS ₂	183	0.0005	25	36
MoTe ₂	435	0.0005	64	81
NiO ₂	354	0.0005	39	79
BrN ₂ Zr	300	0.0005	43	57
Cl ₂ Zn	492	0.0006	73	91
Br ₂ Tb ₂	7	0.0006	1	1
Br ₂ Mn	492	0.0006	73	91
Ag ₂	257	0.0007	57	43
As ₂	443	0.0007	81	100
Te ₂ Zn	435	0.0007	64	81
LiOS ₂ Ti	255	0.0007	25	36
Gd ₂ I ₂ S ₂	561	0.0007	73	57
I ₂ Tm	492	0.0007	91	73
AgNO ₃	368	0.0007	61	37
CrTe ₂	339	0.0007	49	64
Br ₂ O ₂ Sc ₂	570	0.0007	64	63
FHOZn	148	0.0007	16	25
FeO ₂	354	0.0008	39	79
Cl ₂ Sc ₂	403	0.0008	49	64
CCl ₂ Lu ₂	743	0.0008	81	100
Bi ₂ S ₃	8	0.0008	1	1
CrSe ₂	123	0.0009	16	25
ClN ₂ Zr	255	0.0009	36	49

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

PtTe (P3m1 (156))

Structural and electronic properties

	Formula	PtTe
	Spacegroup	P3m1 (156)
	Prototype	PtTe
	Parent 3D	Pt ₄ Te ₆
	Source DB	ICSD
	DB ID	41371
DF2-C09	Binding energy [meV/ Å²]	43.54
RVV10	Binding energy [meV/ Å²]	45.11
	Band gap (PBE) [eV]	0.0

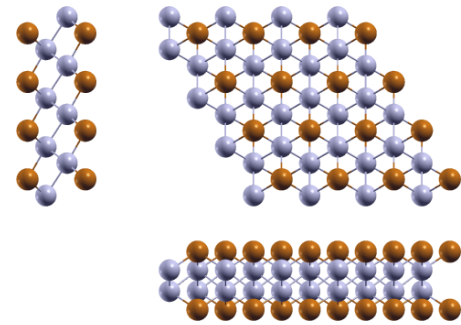


Band structure: Electronic band structure of PtTe (P3m1 (156)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of PtTe (P3m1 (156)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.96424505	0.00000000	0.00000000
a₂		−1.98212253	3.43313692	0.00000000
a₃		0.00000000	0.00000000	24.05625681
		x [Å]	y [Å]	z [Å]
●	Te	1.98212253	1.14437897	9.98304970
●	Pt	0.00000000	2.28875795	11.28144477
●	Pt	0.00000000	0.00000000	12.77481789
●	Te	1.98212253	1.14437897	14.07320127



Orthographic projections: views of PtTe (P3m1 (156)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	2.9303	1	1
Na	5	0.2639	1	1
HgO	6	0.4225	1	1
GeTe	6	0.0084	1	1
As ₂	6	0.2755	1	1
S ₂	6	0.0068	1	1
CaCl	6	0.1317	1	1
IrTe ₂	7	0.0075	1	1
Cl ₂ Zn	7	0.2739	1	1
MoTe ₂	7	0.2671	1	1
ReSe ₂	7	0.247	1	1
S ₂ Ta	7	1.5257	1	1
CaI ₂	7	0.4836	1	1
InSe ₂	7	0.009	1	1
HfTe ₂	7	0.0007	1	1
Te ₂ V	7	0.2699	1	1
I ₂ Yb	7	0.4771	1	1
Br ₂ Co	7	0.2748	1	1
AuTe ₂	7	0.0086	1	1
Cl ₂ Zn	7	0.1434	1	1
PdTe ₂	7	0.0061	1	1
S ₂ Ti	7	1.5613	1	1
NbS ₂	7	1.5224	1	1
Te ₂ Zn	7	0.2669	1	1
Bi ₂ Pd	7	0.1109	1	1
Ba ₂ Hg	7	0.2089	1	1
Br ₂ Mn	7	0.2722	1	1
Cl ₂ Ni	7	0.2482	1	1
Cl ₂ Co	7	1.5587	1	1
CrTe ₂	7	0.2564	1	1
PtS ₂	7	0.2654	1	1
Br ₂ V	7	1.5997	1	1
ClN ₂ Zr	7	1.5842	1	1
Cl ₂ Fe	7	1.5535	1	1
CdClO	7	0.2692	1	1
Ba ₂ N	7	0.0023	1	1
Se ₂ Ti	7	0.2616	1	1
Br ₂ Ti	7	0.2556	1	1
Te ₂ Zr	7	0.0012	1	1
Te ₂ W	7	0.2674	1	1
AsSe ₂	7	0.2501	1	1
I ₂ Tm	7	0.4806	1	1
I ₂ Pb	7	3.0239	1	1
OTl ₂	7	0.2695	1	1
BiTe	7	0.4574	1	1
BrN ₂ Zr	7	1.6334	1	1
NbSe ₂	7	0.2488	1	1
Br ₂ Fe	7	0.2749	1	1
GeS ₂	7	0.1236	1	1
MnSe ₂	7	0.1316	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

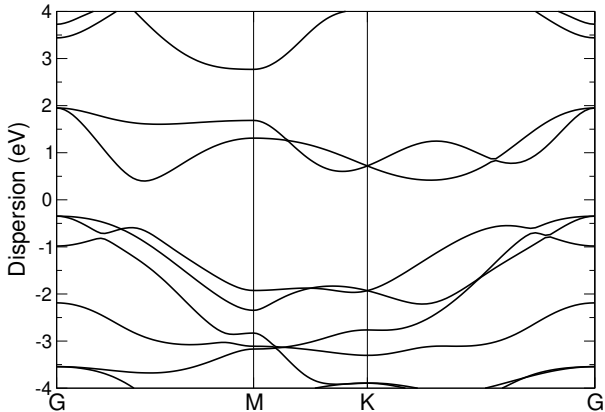
Formula	N° atoms	strain	cell size 1	cell size 2
Cl ₂ Cr ₂ O ₂	766	0.0	70	81
Ga ₂ S ₃	747	0.0001	73	91
Br ₂ Hf ₂ N ₂	516	0.0001	54	50
Br ₂ Ti	447	0.0001	57	73
NS ₂ Zr	656	0.0001	73	91
HNiO ₂	100	0.0002	9	16
Te ₂ W	624	0.0002	81	100
CaI ₂	463	0.0002	73	57
NaPSn	7	0.0002	1	1
CCL ₂ Sc ₂	457	0.0002	43	57
Ba ₂ Pt	304	0.0002	49	36
H ₂ I ₂ Sr ₂	548	0.0002	65	48
Cl ₂ Zr ₂	400	0.0002	43	57
Ba ₂ Cu ₂	580	0.0002	81	64
Se ₂ Ta	388	0.0003	49	64
CdH ₂ O ₂	824	0.0003	81	100
Br ₂ H ₂ Zr ₂	666	0.0003	57	73
Na	383	0.0003	73	91
MoTe ₂	624	0.0003	81	100
NbSe ₂	388	0.0004	49	64
Br ₂ Cr	447	0.0004	57	73
I ₂ Yb	516	0.0004	81	64
Cl ₂ H ₂ Sc ₂	666	0.0004	57	73
Ag ₂	268	0.0004	49	36
Er ₂ F ₂ Se ₂	10	0.0005	1	1
Te ₂ Zn	624	0.0005	81	100
Br ₂ H ₂ Zr ₂	514	0.0005	43	57
Cl ₂ Sc ₂	520	0.0006	57	73
Mg ₂	560	0.0006	81	118
Se ₂ Ta	447	0.0007	57	73
H ₂ MgO ₂	189	0.0007	16	25
AsSe ₂	388	0.0007	49	64
CrTe ₂	447	0.0007	57	73
HfTe ₂	7	0.0007	1	1
Gd ₂ I ₂ S ₂	550	0.0007	64	49
PtS ₂	565	0.0007	73	91
In ₂ Se ₃	9	0.0007	1	1
GeNi ₃ Te ₂	10	0.0008	1	1
HfLiS ₂	724	0.0008	81	100
Cl ₂ Ni	388	0.0008	49	64
Br ₂ Cr ₂ O ₂	524	0.0008	50	54
Cd ₂ I ₃	729	0.0008	91	73
AsI ₂ La ₂	729	0.0008	91	73
Sn ₂ Te ₂	212	0.0008	32	21
I ₂ S ₂ Sm ₂	486	0.0009	57	43
Ge ₂ I ₂ La ₂	802	0.0009	91	73
Cl ₂ Fe	291	0.0009	36	49
ClH ₃ O	269	0.0009	36	25
NbSe ₂	388	0.0009	49	64
Ho ₂ S ₂	548	0.001	72	65

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

PtTe₂ (P-3m1 (164))

Structural and electronic properties

	Formula	PtTe ₂
	Spacegroup	P-3m1 (164)
	Prototype	CdI2
	Parent 3D	PtTe ₂
	Source DB	COD
	DB ID	9009116
DF2-C09	Binding energy [meV/ Å ²]	38.52
RVV10	Binding energy [meV/ Å ²]	40.53
	Band gap (PBE) [eV]	0.75

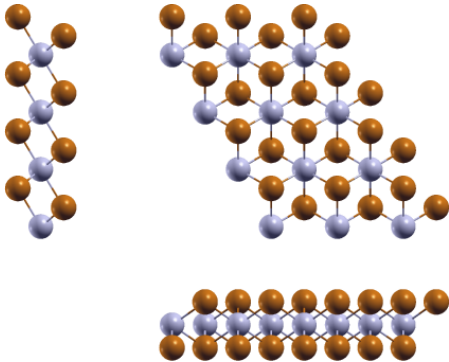


Band structure: Electronic band structure of PtTe₂ (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of PtTe₂ (P-3m1 (164)) in Cartesian coordinates.

	<i>x</i> [Å]	<i>y</i> [Å]	<i>z</i> [Å]
a₁	4.03273334	0.00000000	0.00000000
a₂	−2.01636667	3.49244952	0.00000000
a₃	0.00000000	0.00000000	22.74403087
	<i>x</i> [Å]	<i>y</i> [Å]	<i>z</i> [Å]
● Te	2.01636667	1.16414984	9.97234726
● Te	0.00000000	2.32829968	12.77168360
● Pt	−0.00000000	0.00000000	11.37201543



Orthographic projections: views of PtTe₂ (P-3m1 (164)) as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	4	0.4865	1	1
Na	4	1.6381	1	1
Gd	4	0.2356	1	1
Ag ₂	5	0.501	1	1
As ₂	5	0.2637	1	1
Sb ₂	5	0.0084	1	1
CaCl	5	0.1261	1	1
Cl ₂ Zn	6	0.2622	1	1
MoTe ₂	6	0.2558	1	1
Ba ₂ Pt	6	0.5003	1	1
ReSe ₂	6	1.5466	1	1
HfS ₂	6	0.2676	1	1
CaI ₂	6	0.463	1	1
HfTe ₂	6	0.0072	1	1
Te ₂ V	6	0.2584	1	1
CuTe ₂	6	0.2671	1	1
S ₂ Zr	6	0.2756	1	1
I ₂ Yb	6	0.4567	1	1
Br ₂ Co	6	0.2631	1	1
Ca ₂ N	6	0.2645	1	1
AuTe ₂	6	0.0004	1	1
Cl ₂ Zn	6	0.1366	1	1
PdTe ₂	6	0.002	1	1
I ₂ Zn	6	0.005	1	1
Te ₂ Zn	6	0.2556	1	1
Bi ₂ Pd	6	0.4259	1	1
Br ₂ Mn	6	0.2606	1	1
Cl ₂ Ni	6	1.5532	1	1
CrTe ₂	6	1.5978	1	1
PtS ₂	6	0.2541	1	1
CoTe ₂	6	0.2681	1	1
Br ₂ V	6	1.5408	1	1
ClN ₂ Zr	6	1.5258	1	1
CdClO	6	0.2578	1	1
Ba ₂ N	6	0.0058	1	1
Se ₂ Ti	6	0.2506	1	1
Br ₂ Ti	6	1.5935	1	1
Te ₂ Zr	6	0.0068	1	1
Te ₂ W	6	0.256	1	1
I ₂ Tm	6	0.4601	1	1
S ₂ Sn	6	0.276	1	1
I ₂ Pb	6	2.9168	1	1
OTl ₂	6	0.258	1	1
NbSe ₂	6	1.5562	1	1
Br ₂ Fe	6	0.2632	1	1
GeS ₂	6	0.119	1	1
MnSe ₂	6	0.126	1	1
DyI ₂	6	0.4701	1	1
Br ₂ Ni	6	0.2705	1	1
Se ₂ Ta	6	1.5569	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

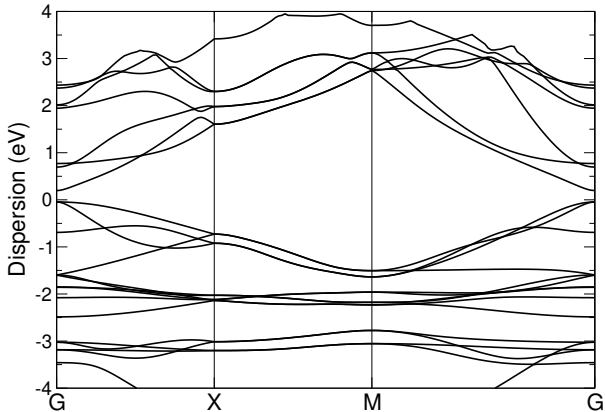
Formula	N° atoms	strain	cell size 1	cell size 2
IO ₃ Tl	120	0.0	25	9
HfS ₂	543	0.0	81	100
ReSe ₂	255	0.0	36	49
Gd ₂ I ₂ S ₂	627	0.0001	81	64
Te ₂ Zn	390	0.0001	57	73
I ₂ Nd ₂ S ₂	486	0.0001	64	49
Ca ₂ N	492	0.0001	73	91
Br ₂ Ti	300	0.0002	43	57
Cl ₂ Mn	183	0.0002	25	36
I ₂ Pb	300	0.0002	57	43
HfLiS ₂	463	0.0002	57	73
NiO ₂	447	0.0002	49	100
MoTe ₂	390	0.0003	57	73
FeSe ₂	519	0.0003	65	108
CoO ₂	447	0.0003	49	100
Br ₂ H ₂ Zr ₂	471	0.0003	43	57
CuTe ₂	543	0.0003	81	100
Br ₂ Ca ₃ Si	627	0.0003	81	64
CoTe ₂	543	0.0003	81	100
Cl ₂ H ₂ Sc ₂	471	0.0004	43	57
AuTe ₂	6	0.0004	1	1
FeH ₂ O ₂	107	0.0004	9	16
Te ₂ W	390	0.0004	57	73
As ₂	401	0.0004	73	91
I ₂ Tm	543	0.0004	100	81
Br ₂ Cr	300	0.0004	43	57
CrSe ₂	123	0.0005	16	25
Ga ₂ S ₂	643	0.0005	81	100
CCl ₂ Lu ₂	674	0.0006	73	91
Dy ₂ I ₂ S ₂	711	0.0006	91	73
Se ₂ Ta	300	0.0006	43	57
Te ₂ V	435	0.0006	64	81
Cl ₂ N ₂ Sc ₂	255	0.0006	25	36
Br ₂ Zr ₂	403	0.0006	49	64
Cl ₂ Sc ₂	357	0.0007	43	57
I ₂ Pr ₂ S ₂	429	0.0007	57	43
Br ₂ Hf ₂ N ₂	666	0.0007	76	73
GeI ₂ La ₂	705	0.0007	100	81
Br ₂ Hf ₂ N ₂	765	0.0007	73	91
CaI ₂	543	0.0007	100	81
CrTe ₂	300	0.0007	43	57
CaH ₂ O ₂	743	0.0008	81	100
Br ₂ Fe	492	0.0008	73	91
N ₂ W	75	0.0008	9	16
LiO	98	0.0008	16	25
Br ₂ V	255	0.0008	36	49
CdH ₂ O ₂	536	0.0008	57	73
Br ₂ Co	492	0.0009	73	91
Cl ₂ Ni	255	0.0009	36	49
C ₄ Ca ₂	558	0.0009	70	58

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Rb₂Cu₂Te₂ (Pmmn)

Structural and electronic properties

Formula	Rb ₂ Cu ₂ Te ₂
Spacegroup	Pmmn
Prototype	PbClF
Parent 3D	Ag ₂ Ce ₂ K ₂ Te ₈
Source DB	None
DB ID	None
DF2-C09 Binding energy [meV/ Å²]	37.64
RVV10 Binding energy [meV/ Å²]	N/A
Band gap (PBE) [eV]	0.24

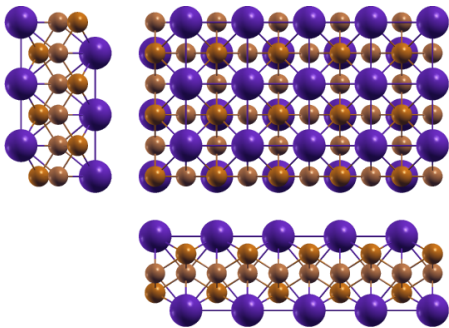


Band structure: Electronic band structure of Rb₂Cu₂Te₂ (Pmmn) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Rb₂Cu₂Te₂ (Pmmn) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		-4.63126704	0.00000000	0.00000000
a₂		0.00000000	-4.63126704	0.00000000
a₃		0.00000000	0.00000000	24.65782961
		x [Å]	y [Å]	z [Å]
●	Rb	-1.15781676	-1.15781676	-2.78398632
●	Cu	1.15781676	-1.15781676	0.00000000
●	Te	1.15781676	1.15781676	-1.45995160
●	Rb	1.15781676	1.15781676	2.78398632
●	Cu	-1.15781676	1.15781676	0.00000000
●	Te	-1.15781676	-1.15781676	1.45995160



Orthographic projections: views of Rb₂Cu₂Te₂ (Pmmn) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
AsSb	8	0.1094	1	1
AgTl	8	0.622	1	1
Sm	8	0.1436	1	2
SiTe ₂	9	0.1107	1	1
Br ₂ Cu	9	0.1013	1	1
NSr ₂	9	0.1091	1	1
FeI ₂	9	0.1088	1	1
CrI ₂	9	0.1089	1	1
Ba ₂ Hg	9	0.2213	1	1
CNRb	9	0.0407	1	1
CKN	9	0.0492	1	1
NiTe ₂	9	0.1109	1	1
I ₂ V	9	0.1104	1	1
Se ₂ Zr	9	0.1106	1	1
BiITe	9	0.1086	1	1
CoI ₂	9	0.1093	1	1
Br ₂ Mg	9	0.1089	1	1
I ₂ La	9	0.5606	1	1
Se ₂ Sn	9	0.1091	1	1
Li ₂ Tl ₂	10	0.1471	1	1
Bi ₂ In ₂	10	0.0003	1	1
Cu ₂ I ₂	10	0.2096	1	1
Ag ₂ Br ₂	10	0.5621	1	1
S ₂ Sn ₂	10	0.2124	1	1
K	10	2.3086	1	4
N ₃ Na	10	0.0258	1	1
As ₂ Ir ₂	10	0.5689	1	1
O ₂ Pb ₂	10	0.5988	1	1
Ga ₂ Se ₂	10	0.1101	1	1
P ₄	10	0.1676	1	1
CaClHO	10	0.111	1	1
Bi ₂ O ₂	10	0.2075	1	1
PbS ₂ Sn	10	0.2219	1	1
As ₂ Rh ₂	10	0.5613	1	1
Br ₂ CsF	10	0.0017	1	1
Sn ₂ Te ₂	10	0.0074	1	1
As ₂ O ₃	11	0.1844	1	1
F ₄ Sn	11	0.2204	1	1
Bi ₂ Te ₃	11	0.1086	1	1
PTe ₂ Zr ₂	11	0.1096	1	1
FKO ₂ Se	11	0.5026	1	1
F ₄ Nb	11	0.2138	1	1
NaO ₄	11	0.1564	1	1
AgNO ₃	11	0.1573	1	1
Cl ₄ Mn	11	0.006	1	1
Ba ₂ H ₂ I ₂	12	0.0036	1	1
Br ₂ Ho ₂ S ₂	12	0.0634	1	1
Br ₂ F ₂ Sr ₂	12	0.2118	1	1
Au ₂ K ₂ S ₂	12	2.518	1	1
Cu ₄ Te ₂	12	0.3449	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

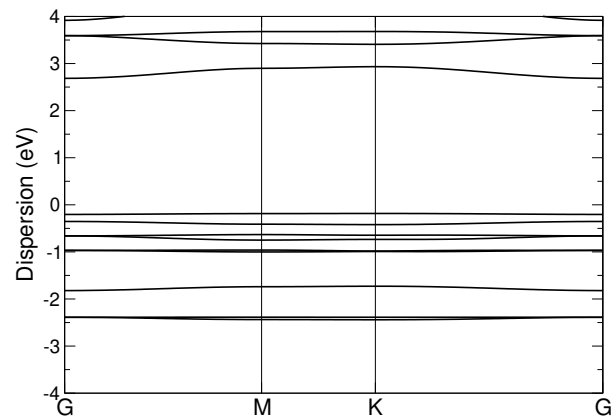
Formula	N° atoms	strain	cell size 1	cell size 2
I ₂ O ₂ Pr ₂	678	0.0	49	64
F ₂ I ₂ Sm ₂	690	0.0	50	65
Br ₂ O ₂ Tb ₂	366	0.0	25	36
I ₂ O ₂ Tm ₂	876	0.0001	61	85
Ge ₂ Mn ₂ Sr ₂	510	0.0001	36	49
F ₄ Nb	800	0.0002	65	82
Hf ₃ Te ₂	221	0.0002	16	25
O ₂ Pb ₂	560	0.0002	50	65
CdI ₂	483	0.0002	48	65
Te ₂ Zn	237	0.0002	20	39
FHOZn	844	0.0002	54	130
Gd ₂ GeI ₂	613	0.0002	48	65
TaTe ₂	411	0.0002	36	65
CrSe ₂	714	0.0002	54	130
MoTe ₂	237	0.0003	20	39
CaCl	456	0.0003	49	81
HfLiS ₂	276	0.0003	20	39
Bi ₂ In ₂	10	0.0003	1	1
F ₄ Sn	997	0.0003	82	101
K ₂ PdSe ₂	390	0.0003	45	24
MnSe ₂	537	0.0004	49	81
Br ₂ La ₂ P	613	0.0004	48	65
Br ₂ Cu ₂	294	0.0004	25	36
Co ₂ S ₂	618	0.0004	49	81
Ca ₂ Cl ₂ H ₂	246	0.0004	16	25
BiClTe	483	0.0004	48	65
Te ₂ W	237	0.0004	20	39
Fe ₂ S ₂	736	0.0004	58	97
I ₂ Pr	483	0.0005	48	65
CdI ₂	483	0.0005	48	65
Bi ₂ Pd	297	0.0005	25	49
HgO	494	0.0006	49	100
K ₂ PdS ₂	316	0.0006	36	20
Br ₂ Eu ₂ F ₂	876	0.0006	61	85
Er ₂ I ₂ O ₂	876	0.0007	61	85
Er ₂ I ₂ S ₂	852	0.0008	72	70
Se ₄ TiZr	966	0.0008	84	77
Ca ₂ Cl ₂	814	0.0008	65	106
CdH ₂ O ₂	315	0.0008	20	39
Br ₂ F ₂ Sr ₂	870	0.0008	64	81
Bi ₂ STe ₂	613	0.0009	48	65
F ₄ Sn	986	0.0009	81	100
Br ₂ N ₂ Zr ₂	876	0.0009	60	86
Cl ₂ Zn	171	0.0009	16	25
O ₂ Sn ₂	294	0.0009	25	36
F ₄ Nb	789	0.0009	64	81
Br ₂ HLa	958	0.0009	81	118
Br ₂ O ₂ Pr ₂	510	0.0009	36	49
Br ₂ F ₂ Yb ₂	366	0.0009	25	36
Eu ₂ F ₂ I ₂	690	0.0009	50	65

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

RbGeI₃ (P3m1)

Structural and electronic properties

	Formula	RbGeI ₃
	Spacegroup	P3m1
	Prototype	KNO3
	Parent 3D	GeI ₃ Rb
	Source DB	COD
	DB ID	1535399
DF2-C09	Binding energy [meV/ Å²]	40.34
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	2.87

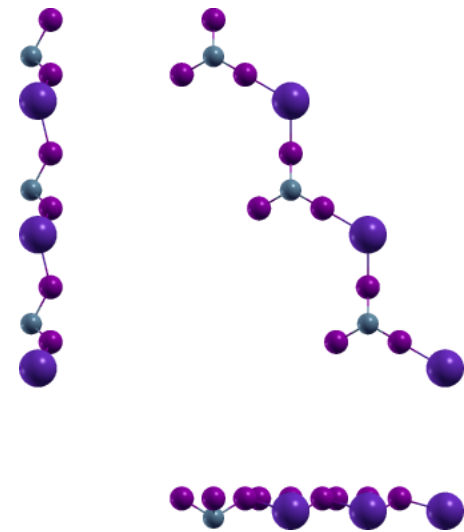


Band structure: Electronic band structure of RbGeI₃ (P3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of RbGeI₃ (P3m1) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		-5.03043862	-8.71297528	0.00000000
a₂		10.06087725	0.00000000	0.00000000
a₃		0.00000000	0.00000000	18.57119167
		x [Å]	y [Å]	z [Å]
●	Ge	5.03043862	-2.90432509	0.84687271
●	I	-0.00000000	-9.23354861	-0.41720985
●	I	2.96604904	-4.09620097	-0.41720985
●	I	-2.96604904	-4.09620097	-0.41720985
●	Rb	-0.00000000	-5.80865019	0.40475684



Orthographic projections: views of RbGeI₃ (P3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	9	0.044	1	4
Br ₂ Hg ₃	10	0.0034	1	1
Bi ₂ Se ₄	11	0.1459	1	1
Tl	14	0.0046	1	9
IKO ₃	15	0.2215	1	2
K ₂ O ₄	17	0.1198	1	2
HgI ₂	17	0.1252	1	4
K	20	0.0402	2	10
Li ₂ Tl ₂	21	0.0019	1	4
Au ₂ I ₂	21	0.0425	1	4
La ₂ S ₂	21	0.0489	1	4
Se ₂ Sn ₂	21	0.0459	1	4
AuI ₄ Li	23	0.2042	1	3
F ₄ Pb	25	0.039	1	4
Au ₂ K ₂ Se ₂	28	0.0491	2	3
K	29	0.0196	3	14
Cu ₂ Na ₂ Te ₂	29	0.042	1	4
Au ₂ Br ₂	29	0.1217	1	6
N ₃ Na	29	0.3229	1	6
Ag ₂ K ₂ Se ₂	29	0.1242	1	4
Ge ₂ Se ₂	29	0.089	1	6
As ₂ Mg ₂ Na ₂	29	0.0442	1	4
AgTl	30	0.0298	2	10
Cl ₂ Mn	32	0.0011	1	9
MoSe ₂	32	0.0053	1	9
S ₂ Ta	32	0.0032	1	9
S ₂ Ti	32	0.0083	1	9
NbS ₂	32	0.0028	1	9
Cl ₂ Co	32	0.008	1	9
NbS ₂	32	0.0016	1	9
Cl ₂ Fe	32	0.0072	1	9
S ₂ Ta	32	0.0024	1	9
Se ₂ V	32	0.0037	1	9
CdO ₂	32	0.0078	1	9
Cl ₂ Zr	32	0.0076	1	9
Se ₂ W	32	0.0051	1	9
GeTe	33	0.6075	1	14
N ₃ Na	34	0.155	2	6
Br ₂ Cu	35	0.2955	1	10
Hg ₃ S ₂	35	0.1127	3	4
Ge ₂ S ₂	37	0.2411	1	8
BN	37	0.0011	1	16
C ₂	37	0.0091	1	16
K	38	0.0182	4	18
Hg ₄ O ₂	39	0.0396	3	4
Cl ₂ Hf ₂	41	0.0045	1	9
Bi ₂ Mn ₂	41	0.1088	1	9
Br ₂ Hf ₂ N ₂	41	0.0569	1	6
LiNbS ₂	41	0.0033	1	9
H ₂ I ₂ Sr ₂	41	0.1298	1	6

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

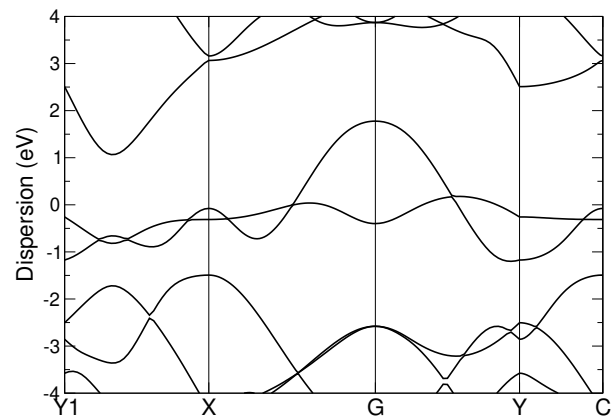
Formula	N° atoms	strain	cell size 1	cell size 2
Br ₂ Ho ₂	120	0.0	4	25
Sb ₂ Te ₃	290	0.0001	9	49
N ₂ W	345	0.0002	9	100
Bi ₂ S ₃	145	0.0002	4	25
Br ₂ Pr ₂	301	0.0002	9	64
GeI ₂ La ₂	485	0.0003	16	81
LiOS ₂ Ti	50	0.0004	1	9
Br ₂ Tb ₂	120	0.0005	4	25
Cl ₂ O ₂ Yb ₂	429	0.0005	9	64
F ₂ Na	237	0.0005	9	64
I ₂ Tm	323	0.0005	16	81
Cu ₄ Te ₂	339	0.0007	9	49
I ₂ Yb	323	0.0008	16	81
PtTe ₂	95	0.001	4	25
Ba ₂ Cu ₂	404	0.001	16	81
IO ₃ Tl	65	0.001	4	9
Bi ₂ SeTe ₂	290	0.001	9	49
PdTe ₂	95	0.0011	4	25
HfSe ₂	237	0.0011	9	64
BN	37	0.0011	1	16
Te ₂ Ti	237	0.0011	9	64
Cl ₂ Mn	32	0.0011	1	9
BrKO ₃	745	0.0013	49	100
Cl ₂ H ₂ Zr ₂	59	0.0013	1	9
Cl ₂ O ₂ Tm ₂	429	0.0014	9	64
AuTe ₂	95	0.0014	4	25
FeH ₂ O ₂	545	0.0014	9	100
Ag ₂ Te ₂	348	0.0014	12	72
Br ₂ Zn	237	0.0014	9	64
CaClHO	301	0.0015	9	64
CCL ₂ Gd ₂	365	0.0015	9	64
NbS ₂	32	0.0016	1	9
Bi ₂	143	0.0016	9	49
Cl ₂ NSc ₂	50	0.0016	1	9
H ₂ Li ₂ Pt	445	0.0017	9	80
CaI ₂	323	0.0017	16	81
K ₂ O ₂ Tl ₂	411	0.0018	15	56
Hg ₄ O ₂	843	0.0019	63	88
Br ₂ Er ₂	120	0.0019	4	25
Li ₂ Tl ₂	21	0.0019	1	4
Br ₂ Cd	95	0.002	4	25
Ga ₂ Gd ₂ I ₂	339	0.002	9	49
NS ₂ Ta	445	0.002	9	100
BiBrTe	192	0.002	9	49
NiTe ₂	237	0.0021	9	64
CBr ₂ Y ₂	365	0.0021	9	64
Cu ₂ Na ₂ Te ₂	949	0.0021	29	134
Br ₂ PY ₂	145	0.0022	4	25
Cl ₂ Fe ₂ O ₂	747	0.0022	15	112
Ga ₂ I ₂ Tb ₂	339	0.0023	9	49

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

ReN₂ (P3m1)

Structural and electronic properties

	Formula	ReN ₂
	Spacegroup	P3m1
	Prototype	MoS2
	Parent 3D	N ₄ Re ₂
	Source DB	MPDS
	DB ID	S1937030
DF2-C09	Binding energy [meV/ Å²]	40.09
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

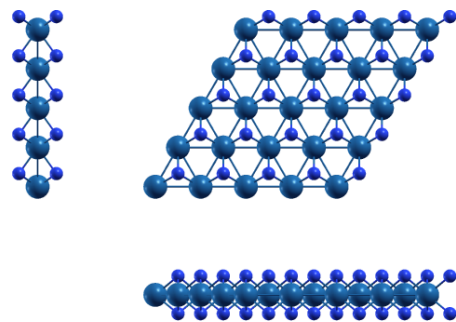


Band structure: Electronic band structure of ReN₂ (P3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of ReN₂ (P3m1) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		1.43027249	−2.47730463	0.00000000
a₂		2.86054499	0.00000000	0.00000000
a₃		0.00000000	0.00000000	16.73205078
		x [Å]	y [Å]	z [Å]
●	Re	−1.43027249	−0.82576821	0.00000000
●	N	0.00000000	−1.65153642	1.18570349
●	N	0.00000000	−1.65153642	−1.18570349



Orthographic projections: views of ReN₂ (P3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	4	2.9661	1	1
In	4	0.4545	1	1
LiO	5	0.4811	1	1
BN	5	1.6273	1	1
P ₂	5	0.5012	1	1
C ₂	5	1.5664	1	1
S ₂ V	6	0.4624	1	1
MoS ₂	6	0.4643	1	1
Cl ₂ Mn	6	3.0431	1	1
PSn ₂	6	13.6012	1	1
FeO ₂	6	0.0072	1	1
NiO ₂	6	0.006	1	1
Cl ₂ Ti	6	0.5016	1	1
S ₂ W	6	0.4644	1	1
S ₂ Ta	6	2.9953	1	1
Se ₂ V	6	2.9774	1	1
Cl ₂ Cu	6	0.631	1	1
Cl ₂ V	6	0.4746	1	1
GeS ₂	6	0.3349	1	1
MoS ₂	6	0.4648	1	1
CrSe ₂	6	0.4716	1	1
CrSe ₂	6	0.4779	1	1
O ₂ Pt	6	0.4507	1	1
CoO ₂	6	0.0065	1	1
C ₂ F ₂	7	0.2759	1	1
As ₂ Fe ₂	7	0.3367	1	1
FHOZn	7	0.4719	1	1
CS ₂ Ta ₂	8	2.9003	1	1
H ₂ Na ₂ Pd	8	0.3332	1	1
Tl	8	0.9175	2	2
N ₃ W ₂	8	0.0087	1	1
H ₂ NiO ₂	8	0.4677	1	1
H ₂ MgO ₂	8	0.4602	1	1
In	8	0.1997	2	2
CNb ₂ S ₂	8	0.4999	1	1
Cu ₄ Te ₂	9	2.2064	1	1
Br ₂ Cu	9	5.154	1	2
AuTe ₂	9	0.2208	2	1
CNRb	9	0.2858	2	1
PtTe ₂	9	0.2203	2	1
Br ₂ Er ₂	10	0.2215	2	1
Cl ₂ La ₂	10	0.2237	2	1
As ₄	10	0.2642	2	1
Br ₂ Gd ₂	10	0.2223	2	1
C ₂ Li ₂	10	0.1839	2	1
P ₄	10	0.1971	2	1
BN	10	0.4692	2	2
Br ₂ Ho ₂	10	0.2191	2	1
O ₂ Sn ₂	10	0.4426	2	1
In ₂ Se ₂	10	0.2253	2	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

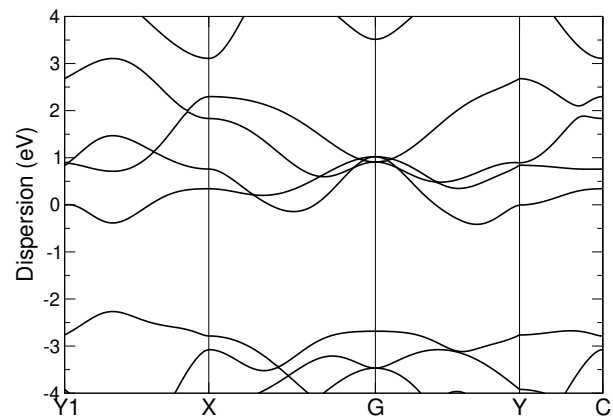
Formula	N° atoms	strain	cell size 1	cell size 2
Ga ₂ I ₂ Tb ₂	51	0.0	9	4
Cl ₂ O ₂ Y ₂	102	0.0	16	9
PSn ₂	390	0.0001	81	49
S ₂ Sn	294	0.0001	61	37
CdClO	123	0.0001	25	16
K	217	0.0001	64	25
S ₂ Ta	255	0.0001	49	36
Cl ₄ Cu ₂	267	0.0001	65	12
ClH ₃ O	120	0.0001	25	9
Br ₂ PY ₂	272	0.0001	49	25
HN ₃ OZn	429	0.0002	57	43
S ₂ Zr	294	0.0002	61	37
F ₂ Lu ₂ Se ₂	594	0.0002	100	49
OTl ₂	123	0.0003	25	16
I ₂ La ₂ Sb	317	0.0003	64	25
Cl ₂ Hf ₂ N ₂	171	0.0003	25	16
Ga ₂ Gd ₂ I ₂	51	0.0003	9	4
Br ₂ Cd	222	0.0003	49	25
H ₂ NiO ₂	638	0.0003	91	73
ClNZr	183	0.0003	36	25
Br ₂ Ca	39	0.0003	9	4
H ₂ MgO ₂	705	0.0004	100	81
NbTe ₂	294	0.0004	61	37
Br ₂ Cu	351	0.0004	77	40
I ₂ S ₂ Sm ₂	342	0.0004	64	25
Ga ₂ Se ₂	84	0.0005	16	9
NaO ₄	368	0.0005	81	25
I ₂ Zn	354	0.0005	79	39
S ₂ V	543	0.0005	100	81
Cl ₂ V	435	0.0005	81	64
Te ₂ V	123	0.0006	25	16
PSn ₂	294	0.0006	61	37
In ₂ Se ₂	393	0.0006	79	39
Cl ₂ Rh ₂ Te ₂	342	0.0006	72	21
F ₄ Nb	660	0.0007	130	54
Cl ₂ Zn	177	0.0007	39	20
CrSe ₂	435	0.0007	81	64
Bi ₂	35	0.0007	9	4
Cl ₂ Ho ₂ O ₂	102	0.0007	16	9
NbS ₂	255	0.0007	49	36
C	52	0.0008	9	25
CdH ₂ O ₂	155	0.0008	25	16
LiO	333	0.0008	73	57
MoS ₂	492	0.0008	91	73
Br ₂ Y ₂	84	0.0008	16	9
Br ₂ H ₂ Zr ₂	258	0.0009	36	25
Br ₂ O ₂ Ti ₂	534	0.0009	88	45
Ho ₂ S ₂	604	0.0009	124	58
F ₂ Ho ₂ Se ₂	297	0.0009	49	25
Br ₂ Hf ₂ N ₂	147	0.0009	25	12

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

ReS₂ (P3m1)

Structural and electronic properties

	Formula	ReS ₂
	Spacegroup	P3m1
	Prototype	MoS2
	Parent 3D	Re ₂ S ₄
	Source DB	MPDS
	DB ID	S309035
DF2-C09	Binding energy [meV/ Å ²]	31.81
RVV10	Binding energy [meV/ Å ²]	N/A
	Band gap (PBE) [eV]	0.0

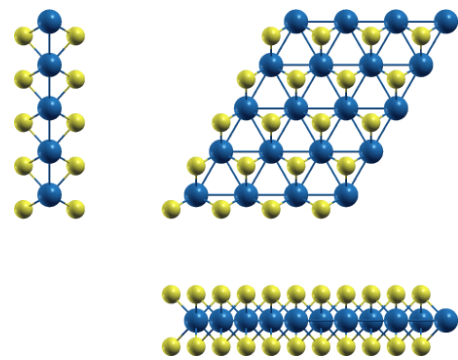


Band structure: Electronic band structure of ReS₂ (P3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of ReS₂ (P3m1) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		1.55121674	−2.68678621	0.00000000
a₂		3.10243349	0.00000000	0.00000000
a₃		0.00000000	0.00000000	18.42285117
		x [Å]	y [Å]	z [Å]
●	Re	0.00000000	−1.79119081	0.00000000
●	S	−1.55121674	−0.89559540	−1.62085814
●	S	−1.55121674	−0.89559540	1.62085814



Orthographic projections: views of ReS₂ (P3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Nd	4	0.2475	1	1
Sn	4	0.1507	1	1
Na	4	0.4964	1	1
In	4	0.0089	1	1
As ₂	5	2.9779	1	1
CrS ₂	6	0.0059	1	1
Cl ₂ Zn	6	2.964	1	1
MoTe ₂	6	2.9031	1	1
ReSe ₂	6	0.4643	1	1
HfS ₂	6	3.0145	1	1
FeO ₂	6	0.2736	1	1
Te ₂ V	6	2.9282	1	1
NiO ₂	6	0.2755	1	1
Br ₂ Co	6	2.9722	1	1
CrO ₂	6	0.2571	1	1
Ca ₂ N	6	2.9849	1	1
Cl ₂ Zn	6	0.3106	1	1
MnO ₂	6	0.2602	1	1
S ₂ Ti	6	0.4493	1	1
RhTe ₂	6	3.1908	1	1
Cl ₂ Ni	6	0.4666	1	1
Cl ₂ Co	6	0.4485	1	1
CrTe ₂	6	0.4822	1	1
PtS ₂	6	0.4991	1	1
CoTe ₂	6	3.0188	1	1
Br ₂ V	6	0.4623	1	1
ClN ₂ Zr	6	0.4571	1	1
CdClO	6	2.9218	1	1
Se ₂ Ti	6	2.8533	1	1
Br ₂ Ti	6	0.4807	1	1
Te ₂ W	6	2.9052	1	1
AsSe ₂	6	0.4703	1	1
OTl ₂	6	2.9242	1	1
CdO ₂	6	0.4481	1	1
BrN ₂ Zr	6	0.4737	1	1
NbSe ₂	6	0.4677	1	1
Br ₂ Fe	6	2.9731	1	1
O ₂ Zn	6	0.0091	1	1
Br ₂ Cr	6	0.4814	1	1
Br ₂ Ni	6	3.0412	1	1
Cl ₂ Zr	6	0.4477	1	1
FeSe ₂	6	0.1446	1	1
Se ₂ Ta	6	0.4679	1	1
NbSe ₂	6	0.471	1	1
Cl ₂ Mg	6	3.0419	1	1
Se ₂ Ta	6	0.4787	1	1
O ₂ Pt	6	0.0073	1	1
CoO ₂	6	0.2747	1	1
Fe ₂ Te ₂	7	0.334	1	1
Ca ₂ Cl ₂	7	0.3349	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

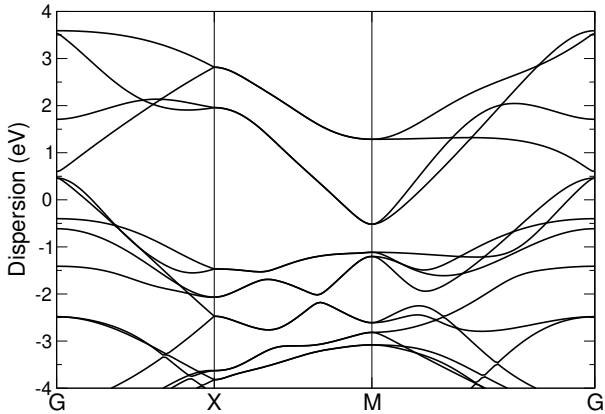
Formula	N° atoms	strain	cell size 1	cell size 2
As ₂ O ₃	227	0.0	49	16
I ₂ Ni	123	0.0	25	16
CdClHO	208	0.0	36	25
Ba ₂ N	294	0.0	61	37
GeI ₂	75	0.0001	16	9
Cl ₂ Ni	492	0.0001	91	73
Ba ₂ Ni ₃	93	0.0001	16	9
Ga ₂ Te ₂	84	0.0001	16	9
GeTe ₂	123	0.0002	25	16
I ₂ Pr ₂ Si ₂	102	0.0002	16	9
Ge ₂ I ₂ La ₂	594	0.0003	100	49
Cl ₂ N ₂ Zr ₂	363	0.0003	49	36
Br ₂ Hf ₂ N ₂	363	0.0003	49	36
CdH ₂ O ₂	386	0.0003	57	43
Cu ₃ Se ₃	405	0.0003	61	37
HgI ₂	552	0.0003	130	54
NbSe ₂	492	0.0003	91	73
AsI ₂ La ₂	432	0.0003	79	39
Se ₂ Yb	75	0.0003	16	9
Cl ₂ Zr ₂	624	0.0003	100	81
Cd ₂ I ₃	432	0.0003	79	39
Na	241	0.0004	64	49
CrTe ₂	390	0.0004	73	57
I ₂ Nd ₂ O ₂	237	0.0004	39	20
Se ₂ Ta	492	0.0004	91	73
AsCuLi ₂	84	0.0004	16	9
Cu ₂ Sr ₂	247	0.0004	49	25
Br ₂ V	543	0.0005	100	81
Cl ₂ Sc ₂	447	0.0005	73	57
Sb ₂ Te ₂	43	0.0005	9	4
I ₂ La ₂ P	272	0.0005	49	25
CaH ₂ O ₂	327	0.0005	49	36
Cl ₂ O ₂ Ti ₂	429	0.0005	63	40
Cl ₂ F ₂ Pb ₂	237	0.0006	39	20
CdClO	300	0.0006	57	43
BiTe ₂	75	0.0006	16	9
Au ₂ I ₂	568	0.0006	120	52
Ni ₂ Te ₂	139	0.0006	25	16
Bi ₂ I ₂ O ₂	237	0.0006	39	20
Cu ₂ Na ₂ Se ₂	237	0.0006	39	20
MnO ₂	435	0.0007	64	81
Br ₂ Cr	390	0.0007	73	57
AgNO ₃	120	0.0007	25	9
Te ₂ W	300	0.0007	57	43
Ga ₂ S ₃	437	0.0007	64	49
CCl ₂ Sc ₂	705	0.0007	100	81
F ₂ I ₂ Tm ₂	237	0.0007	39	20
OTl ₂	300	0.0008	57	43
Cl ₂ Hf ₂ N ₂	429	0.0008	57	43
NS ₂ Zr	388	0.0008	64	49

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Rh₂As₂ (P4/nmm)

Structural and electronic properties

	Formula	Rh ₂ As ₂
	Spacegroup	P4/nmm
	Prototype	FeSe
	Parent 3D	As ₂ KRh ₂
	Source DB	MPDS
	DB ID	S1714016
DF2-C09	Binding energy [meV/ Å²]	77.07
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

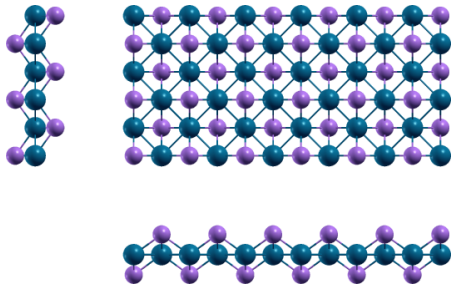


Band structure: Electronic band structure of Rh₂As₂ (P4/nmm) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Rh₂As₂ (P4/nmm) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.95584717	0.00000009	0.00000000
a₂	0.00000009	3.95584717	0.00000000
a₃	0.00000000	0.00000000	17.58335920
	x [Å]	y [Å]	z [Å]
As	2.96688324	-0.98896384	-1.42663753
As	0.98896384	-2.96688324	1.42663753
Rh	2.96688740	-2.96688740	0.00000000
Rh	0.98895968	-0.98895968	0.00000000



Orthographic projections: views of Rh₂As₂ (P4/nmm) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.1767	1	1
InSe	6	0.1403	1	1
Bi ₂	6	0.1454	1	1
AgTl	6	0.0175	1	1
Ag ₂	6	0.1834	1	1
LiO	6	0.111	1	1
P ₂	6	0.1094	1	1
PbTe	6	0.1419	1	1
I ₂ Mg	7	0.1321	1	1
CdI ₂	7	0.1434	1	1
Nd	7	0.1911	1	3
Ba ₂ Pt	7	0.1831	1	1
Br ₂ Zn	7	0.1089	1	1
Br ₂ Ca	7	0.1444	1	1
CaI ₂	7	0.1661	1	1
I ₂ Pr	7	0.0059	1	1
Br ₂ La	7	0.1324	1	1
Br ₂ Cu	7	0.103	1	1
Ca ₂ Si	7	0.1888	1	1
I ₂ Yb	7	0.1633	1	1
BiClTe	7	0.1437	1	1
Cl ₂ Ti	7	0.1093	1	1
BrCdI	7	0.1345	1	1
HgI ₂	7	0.4014	1	1
Te ₂ Ti	7	0.109	1	1
BaF ₂	7	0.1372	1	1
BiBrTe	7	0.1487	1	1
GeI ₂	7	0.1308	1	1
AsKSn	7	0.136	1	1
PbTe ₂	7	0.1338	1	1
I ₂ Nd	7	0.005	1	1
Cl ₂ Cu	7	0.0975	1	1
I ₂ Tm	7	0.1648	1	1
GeI ₂	7	0.1421	1	1
I ₂ Pb	7	0.1854	1	1
STl ₂	7	0.1379	1	1
BiTe	7	0.1551	1	1
GeS ₂	7	0.2116	1	1
DyI ₂	7	0.1693	1	1
CeI ₂	7	0.0066	1	1
Se ₂ Yb	7	0.131	1	1
BiTe ₂	7	0.1312	1	1
GdI ₂	7	0.1515	1	1
I ₂ La	7	0.0003	1	1
CrSe ₂	7	0.1113	1	1
CdI ₂	7	0.143	1	1
I ₂ Pr	7	0.1438	1	1
HfSe ₂	7	0.109	1	1
Bi ₂ Te ₂	8	0.7751	1	1
Bi ₂ In ₂	8	1.1736	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

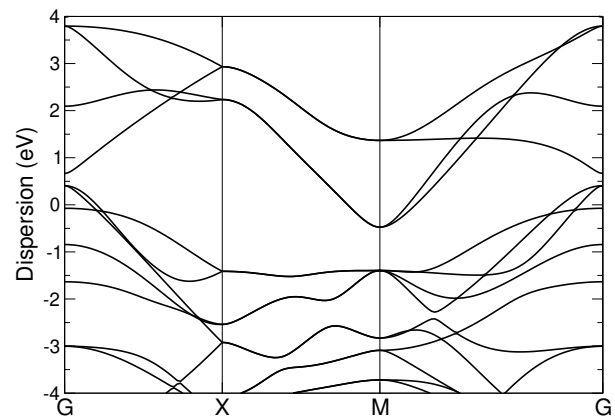
Formula	N° atoms	strain	cell size 1	cell size 2
Br ₂ CsF	340	0.0	49	36
Ba ₂ F ₂ I ₂	550	0.0001	64	49
As ₂ Fe ₂	580	0.0001	64	81
Tl	89	0.0002	16	25
Ag ₂ Br ₂	8	0.0003	1	1
Mg ₃	995	0.0003	113	181
I ₂ La	7	0.0003	1	1
H ₂ Li ₂ O ₂	934	0.0003	82	101
Hf ₂ Se ₂ Si ₂	742	0.0004	64	81
HgI ₂	919	0.0004	145	113
O ₂ Zn	197	0.0004	20	39
Mg ₂	426	0.0005	58	97
O ₄ PTl	550	0.0005	64	49
Mg ₄	164	0.0005	16	25
Br ₂ Lu ₂ S ₂	34	0.0006	4	3
Cu ₂ K ₂ Te ₂	962	0.0006	113	85
Br ₂ Lu ₂ S ₂	34	0.0006	4	3
Cl ₂ H ₂ Lu ₂	582	0.0007	48	65
Br ₂ O ₂ Pr ₂	10	0.0007	1	1
H ₄ Ti	601	0.0008	49	81
H ₂ Li ₂ O ₂	924	0.0009	81	100
O ₂ Sn ₂	920	0.0009	102	128
P ₄	284	0.0009	35	36
H ₂ I ₂ Yb ₂	10	0.0009	1	1
Se ₂ Ta ₄	438	0.0009	36	49
Br ₂ N ₂ Zr ₂	582	0.0009	48	65
CBr ₂ Lu ₂	517	0.001	48	65
Bi ₂ Se ₄	914	0.001	134	63
Cl ₂ Mg	387	0.001	48	65
GeS ₂	499	0.001	64	81
Cl ₂ NSc ₂	946	0.001	79	126
Br ₂ Ni	387	0.001	48	65
O ₂ Sn ₂	920	0.001	102	128
Cl ₄ KTl	154	0.0011	25	9
Bi ₂ Se ₄	218	0.0011	32	15
PTe ₂ Ti ₂	517	0.0012	48	65
Cl ₂ Mn	694	0.0012	79	126
O ₄ PSn	962	0.0012	113	85
F ₄ Pb	805	0.0012	100	81
Ho ₂ S ₂	860	0.0013	106	109
H ₂ Li ₂ Pd	601	0.0013	49	81
Ag ₂ K ₂ Se ₂	708	0.0013	81	64
Br ₂ OV	640	0.0014	71	89
C ₄ Ca ₂	838	0.0014	88	81
I ₂ S ₂ Sm ₂	946	0.0014	103	89
Se ₂ Si ₂ Zr ₂	924	0.0014	81	100
K	501	0.0015	103	89
NbS ₂	694	0.0015	79	126
Ga ₂ S ₂	452	0.0015	48	65
Te ₄ W ₂	526	0.0015	64	45

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

RhP (P4mm (99))

Structural and electronic properties

	Formula	RhP
	Spacegroup	P4mm (99)
	Prototype	FeSe
	Parent 3D	KRh ₂ P ₂
	Source DB	ICSD
	DB ID	641292
DF2-C09	Binding energy [meV/ Å²]	89.86
RVV10	Binding energy [meV/ Å²]	87.76
	Band gap (PBE) [eV]	0.0

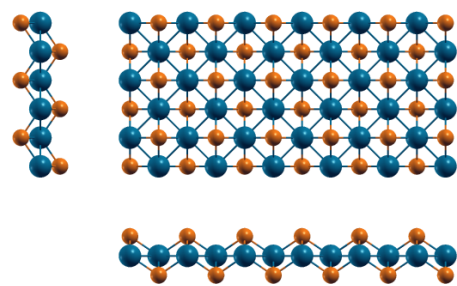


Band structure: Electronic band structure of RhP (P4mm (99)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of RhP (P4mm (99)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.84209064	0.00000000	0.00000000
a₂	0.00000000	3.84209064	0.00000000
a₃	0.00000000	0.00000000	22.59475484
	x [Å]	y [Å]	z [Å]
● P	0.00000000	0.00000000	9.99265600
● Rh	3.84209064	1.92104532	11.29736765
● Rh	1.92104532	0.00000000	11.29736765
● P	1.92104532	1.92104532	12.60211837



Orthographic projections: views of RhP (P4mm (99)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.3939	1	1
K	5	0.1941	1	1
In	5	0.1103	1	1
InSe	6	0.153	1	1
Bi ₂	6	0.1589	1	1
PbTe	6	0.1547	1	1
Sb ₂	6	0.1385	1	1
I ₂ Mg	7	0.1434	1	1
S ₂ V	7	0.1096	1	1
MoS ₂	7	0.1095	1	1
CdI ₂	7	0.1565	1	1
Nd	7	0.786	1	3
Br ₂ Ca	7	0.1578	1	1
CaI ₂	7	0.1823	1	1
I ₂ Pr	7	0.0079	1	1
Br ₂ La	7	0.1437	1	1
Br ₂ Cu	7	0.1093	1	1
Ca ₂ Si	7	0.7792	1	1
I ₂ Yb	7	0.1792	1	1
BiClTe	7	0.1569	1	1
AuTe ₂	7	0.1323	1	1
BrCdI	7	0.1462	1	1
PdTe ₂	7	0.1305	1	1
HgI ₂	7	1.1596	1	1
I ₂ Zn	7	0.1359	1	1
BaF ₂	7	0.1493	1	1
BiBrTe	7	0.1627	1	1
S ₂ W	7	0.1095	1	1
GeI ₂	7	0.1417	1	1
AsKSn	7	0.1479	1	1
PbTe ₂	7	0.1453	1	1
I ₂ Nd	7	0.0089	1	1
Cl ₂ Cu	7	0.1005	1	1
I ₂ Tm	7	0.1808	1	1
SnTe ₂	7	0.1398	1	1
GeI ₂	7	0.155	1	1
I ₂ Pb	7	0.7688	1	1
STl ₂	7	0.1502	1	1
BiTe	7	0.17	1	1
DyI ₂	7	0.1858	1	1
Br ₂ Ni	7	0.1087	1	1
CeI ₂	7	0.0071	1	1
Se ₂ Yb	7	0.1419	1	1
MoS ₂	7	0.1094	1	1
Cl ₂ Mg	7	0.1087	1	1
BiTe ₂	7	0.1422	1	1
GdI ₂	7	0.1658	1	1
CrSe ₂	7	0.1089	1	1
PtTe ₂	7	0.132	1	1
Br ₂ Cd	7	0.1299	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

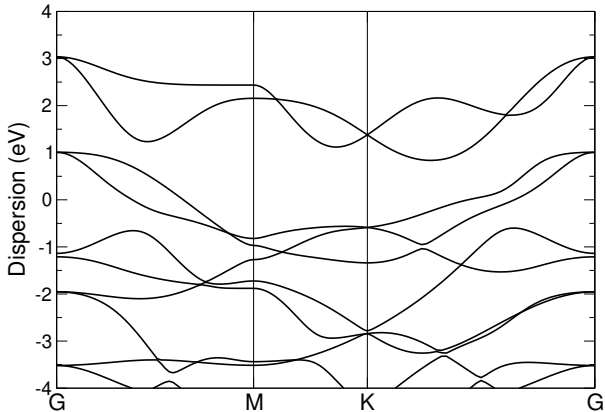
Formula	N° atoms	strain	cell size 1	cell size 2
As ₂ Mg ₂ Na ₂	718	0.0001	82	65
Mg ₆	316	0.0001	25	36
F ₂ Tl ₂	8	0.0001	1	1
Na	257	0.0002	48	65
K	393	0.0003	82	65
H ₄ Ti	189	0.0003	16	25
Br ₂ CsF	244	0.0004	36	25
Ga ₂ S ₃	517	0.0005	48	65
Ag ₂ I ₂	340	0.0005	49	36
K	388	0.0005	81	64
NS ₂ Zr	452	0.0005	48	65
HgI ₂	304	0.0005	49	36
Br ₂ Dy ₂ O ₂	10	0.0005	1	1
I ₃ Sn	52	0.0006	9	4
Br ₂ O ₂ Y ₂	10	0.0006	1	1
As ₂ Cd ₂ K ₂	706	0.0006	85	61
Cu ₂ S ₂	8	0.0007	1	1
Ho ₂ S ₂	860	0.0007	109	106
Cl ₂ S ₂ Tl ₂	736	0.0007	97	58
La ₂ S ₂	640	0.0007	89	71
Pb ₂ Se ₂	628	0.0008	89	68
Bi ₂ Se ₂	716	0.0008	98	81
As ₂ Mg ₂ Na ₂	708	0.0008	81	64
H ₂ Li ₂ Pd	189	0.0008	16	25
Cu ₂ O ₂	396	0.0009	50	49
C ₂ I ₂ La ₂	114	0.001	12	11
C ₄ Ca ₂	636	0.001	69	60
In	277	0.0011	49	81
C ₂ Li ₂	196	0.0011	25	24
PtS ₂	387	0.0011	48	65
Ho ₂ S ₂	396	0.0012	50	49
Br ₂ Ho ₂ O ₂	10	0.0012	1	1
O ₂ Sn ₂	8	0.0012	1	1
Se ₂ Sn ₂	572	0.0012	80	63
P ₄	284	0.0013	36	35
S ₂ Ti	678	0.0013	81	118
Au ₂ Br ₂	724	0.0013	100	81
HgO	414	0.0013	61	85
Ca ₂ Mn ₂ Si ₂	10	0.0014	1	1
Ba ₂ F ₂ I ₂	706	0.0014	85	61
Mo ₂ Te ₄	360	0.0014	45	30
AuI ₄ Li	612	0.0014	90	42
H ₂ Na ₂ O ₂	742	0.0014	64	81
C ₂	422	0.0014	44	123
Ba ₂ H ₂ I ₂	294	0.0015	36	25
In	365	0.0015	64	109
BrNZr	427	0.0015	52	73
CNRb	891	0.0015	150	97
Se ₂ Ti	387	0.0015	48	65
O ₄ PSn	706	0.0016	85	61

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

RhTe₂ (P-3m1 (164))

Structural and electronic properties

	Formula	RhTe ₂
	Spacegroup	P-3m1 (164)
	Prototype	CdI2
	Parent 3D	RhTe ₂
	Source DB	COD
	DB ID	9009118
DF2-C09	Binding energy [meV/ Å²]	54.93
RVV10	Binding energy [meV/ Å²]	54.44
	Band gap (PBE) [eV]	0.0

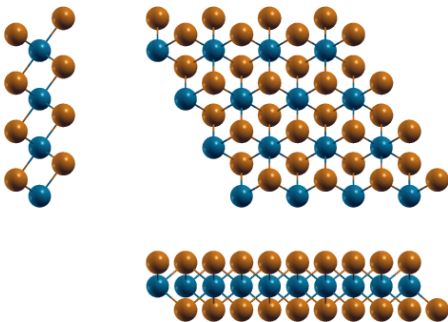


Band structure: Electronic band structure of RhTe₂ (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of RhTe₂ (P-3m1 (164)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.72914031	0.00000000	0.00000000
a₂	−1.86457015	3.22953024	0.00000000
a₃	0.00000000	0.00000000	22.78362116
	x [Å]	y [Å]	z [Å]
● Te	1.86457015	1.07651008	12.97009407
● Te	0.00000000	2.15302016	9.81352709
● Rh	0.00000000	0.00000000	11.39181058



Orthographic projections: views of RhTe₂ (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	4	0.1135	1	1
Tl	4	0.2605	1	1
InSe	5	2.8455	1	1
HgO	5	0.1191	1	1
Bi ₂	5	2.92	1	1
P ₂	5	0.2533	1	1
PbTe	5	0.4951	1	1
Mg ₂	5	0.4236	1	1
Sb ₂	5	0.45	1	1
I ₂ Mg	6	0.464	1	1
S ₂ V	6	1.5315	1	1
MoS ₂	6	1.5367	1	1
Cl ₂ Mn	6	0.2687	1	1
CdI ₂	6	0.4997	1	1
AgTe ₂	6	0.1147	1	1
PSn ₂	6	0.0065	1	1
MoSe ₂	6	0.2595	1	1
S ₂ Ta	6	0.2717	1	1
Br ₂ Zn	6	0.0041	1	1
Br ₂ Ca	6	2.906	1	1
AsSn ₂	6	0.0028	1	1
SiTe ₂	6	0.0083	1	1
S ₂ Zr	6	0.0072	1	1
Br ₂ La	6	0.4649	1	1
Br ₂ Cu	6	0.971	1	1
BiClTe	6	0.5007	1	1
ReS ₂	6	1.4487	1	1
Cl ₂ Ti	6	0.2535	1	1
BrCdI	6	0.4719	1	1
HgI ₂	6	0.3139	1	1
Mg ₃	6	0.1113	1	1
Te ₂ Ti	6	0.0044	1	1
NbS ₂	6	0.2711	1	1
BaF ₂	6	0.4805	1	1
S ₂ W	6	1.5371	1	1
Bi ₂ Pd	6	0.1245	1	1
GeI ₂	6	0.4594	1	1
NbS ₂	6	0.2649	1	1
S ₂ Ta	6	0.2636	1	1
Se ₂ V	6	0.2617	1	1
AsKSn	6	0.4768	1	1
PbTe ₂	6	0.4695	1	1
NiTe ₂	6	0.0077	1	1
S ₂ Sn	6	0.007	1	1
SnTe ₂	6	0.4538	1	1
Cl ₂ V	6	1.5662	1	1
GeI ₂	6	0.4958	1	1
Se ₂ Zr	6	0.0087	1	1
STl ₂	6	0.4829	1	1
PtSe ₂	6	0.0022	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

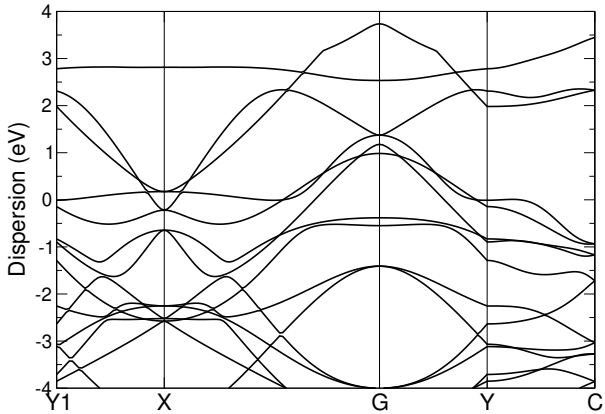
Formula	N° atoms	strain	cell size 1	cell size 2
Ga ₂ Gd ₂ I ₂	429	0.0	57	43
H ₂ NiO ₂	353	0.0001	36	49
As ₂ CeLi ₂	437	0.0001	64	49
GeI ₂ La ₂	233	0.0001	36	25
PbTe	290	0.0001	64	49
STl ₂	390	0.0001	73	57
Sb ₂ Se ₂ Te	705	0.0001	100	81
GeI ₂	339	0.0001	64	49
MoSe ₂	435	0.0001	64	81
I ₂ Tm	183	0.0002	36	25
Br ₂ Gd ₂ Ge	638	0.0002	91	73
Cu ₂ I ₂	565	0.0002	91	73
BiTe ₂	543	0.0002	100	81
I ₂ La ₂	499	0.0002	81	64
AgClO ₄	237	0.0003	39	20
I ₂ La ₂ P	327	0.0003	49	36
Ga ₂ I ₂ Tb ₂	429	0.0003	57	43
Sb ₂ Te ₂	139	0.0003	25	16
AsKSn	435	0.0003	81	64
Se ₂ W	435	0.0003	64	81
NbS ₂	492	0.0004	73	91
HN ₃ OZn	609	0.0004	57	73
Bi ₂ Te ₂	439	0.0004	81	49
Bi ₂	257	0.0004	57	43
LiMnTe ₂	388	0.0004	64	49
K ₂ PtTe ₂	393	0.0005	91	24
I ₂ Nd ₂ O ₂	483	0.0005	65	48
Se ₂ Yb	543	0.0005	100	81
S ₂ Ta	492	0.0005	73	91
Gd ₂ I ₂	565	0.0005	91	73
Br ₂ Cr ₂ O ₂	666	0.0005	76	73
Sb ₂ Se ₂ Te	705	0.0006	100	81
IO ₃ Tl	368	0.0006	81	25
Sm	247	0.0006	49	100
Cl ₂ H ₂ Zr ₂	765	0.0006	73	91
GdI ₂	255	0.0006	49	36
Br ₂ Ca	300	0.0006	57	43
GeI ₂	543	0.0007	100	81
Cr ₂ O ₄	459	0.0007	47	53
Bi ₂ Se ₃	638	0.0007	91	73
Br ₂ Ca ₃ Si	840	0.0007	118	81
CdClHO	7	0.0008	1	1
LiOS ₂ Ti	743	0.0008	81	100
Cl ₂ Mn	543	0.0008	81	100
Bi ₂ STe ₂	437	0.0008	64	49
ReS ₂	183	0.0008	25	36
Br ₂ La	492	0.0008	91	73
Ho ₂ I ₂ Se ₂	621	0.0008	103	52
Bi ₂ Mn ₂	378	0.0009	54	54
C ₂ F ₂	547	0.0009	49	100

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Ru₂As₂ (P4/nmm)

Structural and electronic properties

	Formula	Ru ₂ As ₂
	Spacegroup	P4/nmm
	Prototype	FeSe
	Parent 3D	As ₂ KRu ₂
	Source DB	MPDS
	DB ID	S2110346
DF2-C09	Binding energy [meV/ Å²]	94.76
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

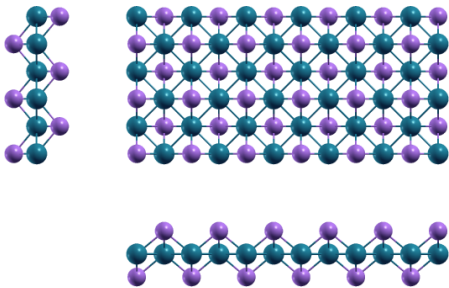


Band structure: Electronic band structure of Ru₂As₂ (P4/nmm) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ru₂As₂ (P4/nmm) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.80713336	−0.00014793	0.00000000
a₂		−0.00014793	3.80713336	0.00000000
a₃		0.00000000	0.00000000	17.43906930
		x [Å]	y [Å]	z [Å]
●	As	−0.95187075	−0.95187075	−1.59393718
●	As	0.95201868	−2.85526262	1.59393718
●	Ru	−0.95163010	−2.85535533	0.00000000
●	Ru	0.95177803	−0.95177803	0.00000000



Orthographic projections: views of Ru₂As₂ (P4/nmm) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.4035	1	1
In	5	0.1094	1	1
InSe	6	0.1573	1	1
HgO	6	0.5591	1	1
Bi ₂	6	0.1634	1	1
Ag ₂	6	0.7794	1	1
As ₂	6	0.1085	1	1
PbTe	6	0.1592	1	1
Sb ₂	6	0.1421	1	1
I ₂ Mg	7	0.1472	1	1
S ₂ V	7	0.1087	1	1
CdI ₂	7	0.161	1	1
Ba ₂ Pt	7	0.7784	1	1
Br ₂ Ca	7	0.1623	1	1
CaI ₂	7	0.1877	1	1
HfTe ₂	7	0.1298	1	1
Br ₂ La	7	0.1476	1	1
Br ₂ Cu	7	0.1118	1	1
I ₂ Yb	7	0.1845	1	1
Br ₂ Co	7	0.1084	1	1
BiClTe	7	0.1614	1	1
ReS ₂	7	0.1113	1	1
Ca ₂ N	7	0.1087	1	1
AuTe ₂	7	0.1356	1	1
BrCdI	7	0.1502	1	1
PdTe ₂	7	0.1337	1	1
I ₂ Zn	7	0.1393	1	1
BaF ₂	7	0.1534	1	1
BiBrTe	7	0.1674	1	1
Bi ₂ Pd	7	0.5865	1	1
GeI ₂	7	0.1455	1	1
Ba ₂ N	7	0.1309	1	1
AsKSn	7	0.152	1	1
Te ₂ Zr	7	0.1301	1	1
PbTe ₂	7	0.1493	1	1
Cl ₂ Cu	7	0.1018	1	1
I ₂ Tm	7	0.1862	1	1
SnTe ₂	7	0.1435	1	1
GeI ₂	7	0.1594	1	1
I ₂ Pb	7	0.7855	1	1
STl ₂	7	0.1544	1	1
BiTe	7	0.175	1	1
Br ₂ Fe	7	0.1085	1	1
DyI ₂	7	0.1914	1	1
Se ₂ Yb	7	0.1458	1	1
BiTe ₂	7	0.146	1	1
GdI ₂	7	0.1707	1	1
PtTe ₂	7	0.1353	1	1
Br ₂ Cd	7	0.133	1	1
O ₂ Pt	7	0.1097	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

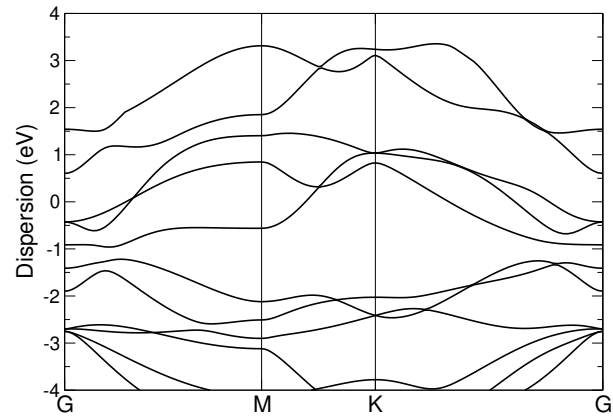
Formula	N° atoms	strain	cell size 1	cell size 2
Se ₂ Ta ₄	742	0.0	64	81
In	366	0.0	65	106
Cu ₂ Na ₂ Te ₂	550	0.0001	64	49
Cu ₂ K ₂ Te ₂	294	0.0001	36	25
Ca ₂ Cl ₂	8	0.0002	1	1
Br ₂ O ₂ Tm ₂	10	0.0002	1	1
FeSe ₂	775	0.0003	85	145
H ₂ MnO ₂	275	0.0003	20	39
I ₂ S ₂ Tb ₂	550	0.0004	70	45
Bi ₂ Se ₂	472	0.0005	65	53
O ₂ Zn	339	0.0005	36	65
K	693	0.0006	145	113
Ho ₂ S ₂	696	0.0006	89	85
Fe ₂ Te ₂	8	0.0006	1	1
Ag ₂ I ₂	584	0.0007	85	61
C ₂ I ₂ Y ₂	676	0.0008	67	68
Hg ₃ S ₂	617	0.0008	113	33
H ₂ I ₂ Sr ₂	708	0.001	81	64
CrTe ₂	387	0.001	48	65
Br ₂ O ₂ Yb ₂	10	0.0011	1	1
Hg ₃ S ₂	562	0.0011	103	30
Cl ₂ Sc ₂	452	0.0011	48	65
Hg ₃ S ₂	486	0.0011	89	26
Ag ₂ K ₂ Te ₂	196	0.0012	25	16
Sn	277	0.0012	49	81
Dy ₂ I ₂ S ₂	584	0.0012	74	48
Br ₂ Cr	387	0.0013	48	65
Ho ₂ I ₂ S ₂	584	0.0013	74	48
Tl	136	0.0014	25	36
Bi ₂ Pd	679	0.0014	85	113
Br ₂ H ₂ Zr ₂	582	0.0014	48	65
Ca ₂ O ₂	452	0.0015	49	64
Au ₂ I ₂	428	0.0015	61	46
LiO	568	0.0015	79	126
Pb ₂ Se ₂	680	0.0015	97	73
Dy ₂ I ₂ S ₂	550	0.0015	70	45
Br ₂ V	427	0.0015	52	73
Mg ₂	114	0.0016	16	25
F ₂ Se ₂ Y ₂	604	0.0016	73	52
Br ₂ Ti	387	0.0016	48	65
S ₂ Zr	479	0.0016	62	77
NbTe ₂	479	0.0016	62	77
ReSe ₂	427	0.0016	52	73
H ₂ Na ₂ O ₂	838	0.0016	73	91
AgTe ₂	208	0.0016	25	36
Cl ₂ Hg ₂ N ₂	564	0.0016	81	40
S ₂ Sn	479	0.0016	62	77
NaPSn	763	0.0016	106	113
Cl ₄ Mn	989	0.0016	136	89
Pt ₂ Te ₂	876	0.0017	106	113

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Sb₂Te₂ (P-3m1)

Structural and electronic properties

	Formula	Sb ₂ Te ₂
	Spacegroup	P-3m1
	Prototype	PtTe
	Parent 3D	GeSb ₂ Te ₄
	Source DB	MPDS
	DB ID	S1407163
DF2-C09	Binding energy [meV/ Å²]	76.62
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

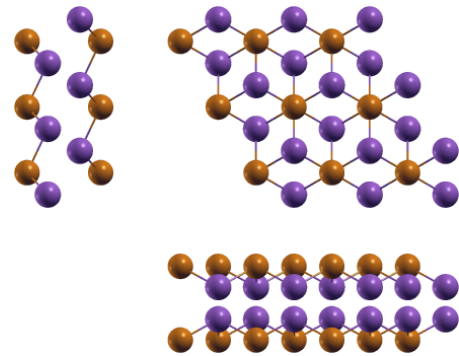


Band structure: Electronic band structure of Sb₂Te₂ (P-3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Sb₂Te₂ (P-3m1) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		2.32927117	-4.03441602	0.00000000
a₂		2.32927117	4.03441602	0.00000000
a₃		0.00000000	0.00000000	22.98972743
		x [Å]	y [Å]	z [Å]
●	Sb	3.49390676	0.67240267	-0.98691537
●	Sb	1.16463559	-0.67240267	0.98691537
●	Te	1.16463559	2.01720801	-2.26353695
●	Te	1.16463559	2.01720801	2.26353695



Orthographic projections: views of Sb₂Te₂ (P-3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.1393	1	1
K	5	0.0083	1	1
AgTl	6	0.1194	1	1
Ag ₂	6	0.0029	1	1
Sb ₂	6	0.2535	1	1
I ₂ Mg	7	0.2613	1	1
Ba ₂ Pt	7	0.0032	1	1
GeTe ₂	7	1.4493	1	1
I ₂ Pr	7	0.1115	1	1
Br ₂ La	7	0.2618	1	1
Ca ₂ Si	7	0.0013	1	1
BrCdI	7	0.2657	1	1
I ₂ Zn	7	0.2492	1	1
BaF ₂	7	0.2705	1	1
GeI ₂	7	0.2587	1	1
Ba ₂ Hg	7	0.1279	1	1
AsKSn	7	0.2684	1	1
PbTe ₂	7	0.2643	1	1
I ₂ Nd	7	0.1118	1	1
Cl ₂ Cu	7	0.3069	1	1
SnTe ₂	7	0.2556	1	1
I ₂ Pb	7	0.0014	1	1
STl ₂	7	0.2719	1	1
CeI ₂	7	0.1112	1	1
Se ₂ Yb	7	0.259	1	1
BiTe ₂	7	0.2594	1	1
I ₂ La	7	0.1136	1	1
Ba ₂ Cd	7	0.1297	1	1
Cu ₂ I ₂	8	0.1214	1	1
Cu ₂ Te ₂	8	0.111	1	1
Ir ₂ P ₂	8	0.1117	1	1
Ag ₂ Br ₂	8	0.1138	1	1
Br ₂ Er ₂	8	1.5878	1	1
O ₂ Sn ₂	8	0.1111	1	1
Cu ₂ S ₂	8	0.432	1	1
Au ₂ Br ₂	8	0.1268	1	1
As ₂ Ir ₂	8	0.1148	1	1
O ₂ Pb ₂	8	0.1196	1	1
AgBrO ₂	8	0.2864	1	1
Br ₂ Gd ₂	8	1.5918	1	1
MnNaTe ₂	8	0.2652	1	1
O ₂ Sn ₂	8	0.4332	1	1
AsCuLi ₂	8	0.2581	1	1
Cu ₂ I ₂	8	0.2626	1	1
P ₂ Rh ₂	8	0.4305	1	1
F ₂ Tl ₂	8	0.4307	1	1
I ₂ La ₂	8	0.2677	1	1
P ₂	8	0.2204	1	2
O ₂ Sn ₂	8	0.1298	1	1
Ge ₂ Se ₂	8	0.4811	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

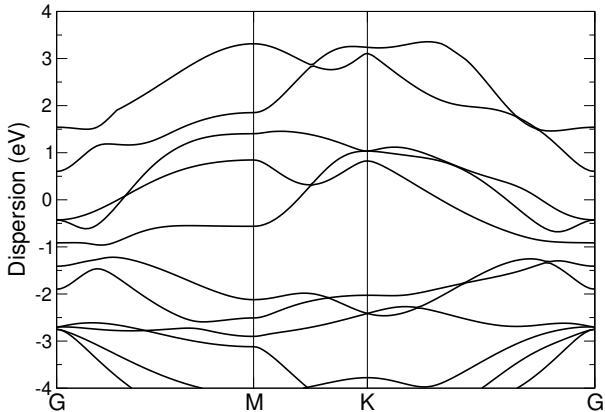
Formula	N° atoms	strain	cell size 1	cell size 2
PbTe ₂	565	0.0	73	91
CaH ₂ O ₂	601	0.0	49	81
As ₂ Sn ₂	400	0.0	43	57
Se ₂ V	247	0.0001	25	49
I ₂ La ₂	724	0.0001	81	100
I ₂ Zn	388	0.0001	49	64
BiTe ₂	499	0.0001	64	81
Br ₂ Gd ₂	400	0.0001	43	57
Ni ₂ Te ₂	244	0.0001	25	36
SnTe ₂	447	0.0001	57	73
CuTe ₂	331	0.0002	37	61
Se ₂ Yb	499	0.0002	64	81
HfS ₂	331	0.0002	37	61
Cl ₂ N ₂ Zr ₂	682	0.0002	49	81
N ₃ W ₂	420	0.0002	25	64
RhTe ₂	139	0.0003	16	25
CdCl ₂	208	0.0003	25	36
BH ₄ Li	666	0.0004	57	73
I ₂ Mn	208	0.0004	25	36
Sb ₂ Se ₂ Te	661	0.0004	64	81
GeI ₂	499	0.0004	64	81
F ₂ Ho ₂ Se ₂	438	0.0005	36	49
CdClHO	164	0.0005	16	25
ReS ₂	43	0.0005	4	9
As ₂ O ₃	376	0.0005	49	36
I ₂ Ni	208	0.0005	25	36
CoTe ₂	331	0.0005	37	61
Cl ₂ Er ₂ H ₂	316	0.0005	25	36
Se ₂ Ta	84	0.0006	9	16
O ₂ Sn ₂	100	0.0006	11	14
AsKSn	624	0.0006	81	100
MnNaTe ₂	656	0.0006	73	91
Br ₂ Er ₂	400	0.0006	43	57
CaH ₂ O ₂	453	0.0006	37	61
Ba ₂ Ni ₃	661	0.0006	64	81
Ga ₂ Te ₂	580	0.0006	64	81
Gd ₂ I ₂ Se ₂	784	0.0007	91	70
Ga ₂ S ₂	392	0.0007	37	61
InSe ₂	208	0.0007	25	36
In ₂ Se ₂	752	0.0007	103	85
GeTe ₂	208	0.0007	25	36
I ₂ Pr ₂ Si ₂	742	0.0007	64	81
Cl ₂ O ₂ Ti ₂	88	0.0007	7	10
Br ₂ Hf ₂ N ₂	682	0.0008	49	81
Ga ₂ Ge ₂ Te ₂	666	0.0008	57	73
Cl ₂ H ₂ Sc ₂	132	0.0008	9	16
Cl ₂ N ₂ Zr ₂	514	0.0009	37	61
Li ₂ P ₂ Pr	593	0.0009	57	73
Sb ₂ Se ₂ Te	661	0.0009	64	81
Te ₄ W ₂	300	0.0009	33	28

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Sb₂Te₂ (P-3m1)

Structural and electronic properties





	Formula	Sb ₂ Te ₂
	Spacegroup	P-3m1
	Prototype	PtTe
	Parent 3D	GeSb ₂ Te ₄
	Source DB	MPDS
	DB ID	S1407163
DF2-C09	Binding energy [meV/ Å²]	76.62
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

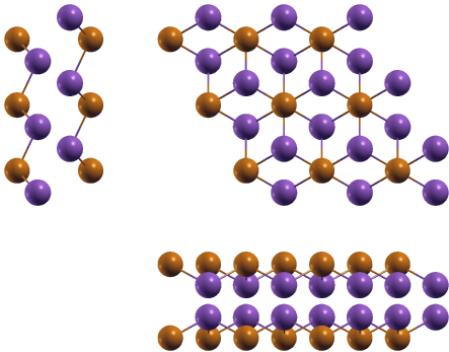


Band structure: Electronic band structure of Sb₂Te₂ (P-3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Sb₂Te₂ (P-3m1) in Cartesian coordinates.

		<i>x</i> [Å]	<i>y</i> [Å]	<i>z</i> [Å]
a₁		2.32927117	−4.03441602	0.00000000
a₂		2.32927117	4.03441602	0.00000000
a₃		0.00000000	0.00000000	22.98972743
		<i>x</i> [Å]	<i>y</i> [Å]	<i>z</i> [Å]
	Sb	3.49390676	0.67240267	−0.98691537
	Sb	1.16463559	−0.67240267	0.98691537
	Te	1.16463559	2.01720801	−2.26353695
	Te	1.16463559	2.01720801	2.26353695



Orthographic projections: views of Sb₂Te₂ (P-3m1) as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.1393	1	1
K	5	0.0083	1	1
AgTl	6	0.1194	1	1
Ag ₂	6	0.0029	1	1
Sb ₂	6	0.2535	1	1
I ₂ Mg	7	0.2613	1	1
Ba ₂ Pt	7	0.0032	1	1
GeTe ₂	7	1.4493	1	1
I ₂ Pr	7	0.1115	1	1
Br ₂ La	7	0.2618	1	1
Ca ₂ Si	7	0.0013	1	1
BrCdI	7	0.2657	1	1
I ₂ Zn	7	0.2492	1	1
BaF ₂	7	0.2705	1	1
GeI ₂	7	0.2587	1	1
Ba ₂ Hg	7	0.1279	1	1
AsKSn	7	0.2684	1	1
PbTe ₂	7	0.2643	1	1
I ₂ Nd	7	0.1118	1	1
Cl ₂ Cu	7	0.3069	1	1
SnTe ₂	7	0.2556	1	1
I ₂ Pb	7	0.0014	1	1
STl ₂	7	0.2719	1	1
CeI ₂	7	0.1112	1	1
Se ₂ Yb	7	0.259	1	1
BiTe ₂	7	0.2594	1	1
I ₂ La	7	0.1136	1	1
Ba ₂ Cd	7	0.1297	1	1
Cu ₂ I ₂	8	0.1214	1	1
Cu ₂ Te ₂	8	0.111	1	1
Ir ₂ P ₂	8	0.1117	1	1
Ag ₂ Br ₂	8	0.1138	1	1
Br ₂ Er ₂	8	1.5878	1	1
O ₂ Sn ₂	8	0.1111	1	1
Cu ₂ S ₂	8	0.432	1	1
Au ₂ Br ₂	8	0.1268	1	1
As ₂ Ir ₂	8	0.1148	1	1
O ₂ Pb ₂	8	0.1196	1	1
AgBrO ₂	8	0.2864	1	1
Br ₂ Gd ₂	8	1.5918	1	1
MnNaTe ₂	8	0.2652	1	1
O ₂ Sn ₂	8	0.4332	1	1
AsCuLi ₂	8	0.2581	1	1
Cu ₂ I ₂	8	0.2626	1	1
P ₂ Rh ₂	8	0.4305	1	1
F ₂ Tl ₂	8	0.4307	1	1
I ₂ La ₂	8	0.2677	1	1
P ₂	8	0.2204	1	2
O ₂ Sn ₂	8	0.1298	1	1
Ge ₂ Se ₂	8	0.4811	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

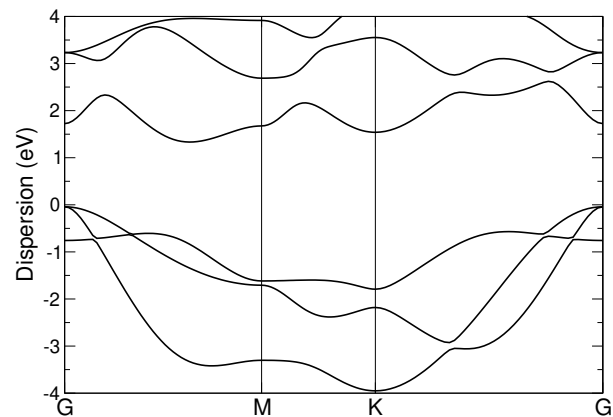
Formula	N° atoms	strain	cell size 1	cell size 2
PbTe ₂	565	0.0	73	91
CaH ₂ O ₂	601	0.0	49	81
As ₂ Sn ₂	400	0.0	43	57
Se ₂ V	247	0.0001	25	49
I ₂ La ₂	724	0.0001	81	100
I ₂ Zn	388	0.0001	49	64
BiTe ₂	499	0.0001	64	81
Br ₂ Gd ₂	400	0.0001	43	57
Ni ₂ Te ₂	244	0.0001	25	36
SnTe ₂	447	0.0001	57	73
CuTe ₂	331	0.0002	37	61
Se ₂ Yb	499	0.0002	64	81
HfS ₂	331	0.0002	37	61
Cl ₂ N ₂ Zr ₂	682	0.0002	49	81
N ₃ W ₂	420	0.0002	25	64
RhTe ₂	139	0.0003	16	25
CdCl ₂	208	0.0003	25	36
BH ₄ Li	666	0.0004	57	73
I ₂ Mn	208	0.0004	25	36
Sb ₂ Se ₂ Te	661	0.0004	64	81
GeI ₂	499	0.0004	64	81
F ₂ Ho ₂ Se ₂	438	0.0005	36	49
CdClHO	164	0.0005	16	25
ReS ₂	43	0.0005	4	9
As ₂ O ₃	376	0.0005	49	36
I ₂ Ni	208	0.0005	25	36
CoTe ₂	331	0.0005	37	61
Cl ₂ Er ₂ H ₂	316	0.0005	25	36
Se ₂ Ta	84	0.0006	9	16
O ₂ Sn ₂	100	0.0006	11	14
AsKSn	624	0.0006	81	100
MnNaTe ₂	656	0.0006	73	91
Br ₂ Er ₂	400	0.0006	43	57
CaH ₂ O ₂	453	0.0006	37	61
Ba ₂ Ni ₃	661	0.0006	64	81
Ga ₂ Te ₂	580	0.0006	64	81
Gd ₂ I ₂ Se ₂	784	0.0007	91	70
Ga ₂ S ₂	392	0.0007	37	61
InSe ₂	208	0.0007	25	36
In ₂ Se ₂	752	0.0007	103	85
GeTe ₂	208	0.0007	25	36
I ₂ Pr ₂ Si ₂	742	0.0007	64	81
Cl ₂ O ₂ Ti ₂	88	0.0007	7	10
Br ₂ Hf ₂ N ₂	682	0.0008	49	81
Ga ₂ Ge ₂ Te ₂	666	0.0008	57	73
Cl ₂ H ₂ Sc ₂	132	0.0008	9	16
Cl ₂ N ₂ Zr ₂	514	0.0009	37	61
Li ₂ P ₂ Pr	593	0.0009	57	73
Sb ₂ Se ₂ Te	661	0.0009	64	81
Te ₄ W ₂	300	0.0009	33	28

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

SbAs (P3m1)

Structural and electronic properties

	Formula	SbAs
	Spacegroup	P3m1
	Prototype	GeTe
	Parent 3D	AsSb
	Source DB	MPDS
	DB ID	S1636232
DF2-C09	Binding energy [meV/ Å²]	41.59
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	1.37

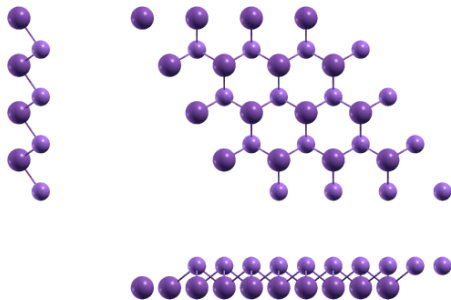


Band structure: Electronic band structure of SbAs (P3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of SbAs (P3m1) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	-1.92182724	-3.32870242	0.00000000
a₂	3.84365448	-0.00000000	0.00000000
a₃	0.00000000	0.00000000	14.82870073
	x [Å]	y [Å]	z [Å]
● Sb	1.92182724	-1.10956747	0.76738881
● As	1.92182724	-3.32870242	-0.76738881



Orthographic projections: views of SbAs (P3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	3	0.4282	1	1
InSe	4	0.4541	1	1
Nd	4	0.2198	1	2
HgO	4	0.1126	1	1
Bi ₂	4	0.4686	1	1
GeTe	4	0.0061	1	1
S ₂	4	0.0077	1	1
PbTe	4	0.4585	1	1
CaCl	4	0.1435	1	1
IrTe ₂	5	0.0071	1	1
CdCl ₂	5	0.005	1	1
Cl ₂ Mn	5	0.249	1	1
CdI ₂	5	0.4628	1	1
AgTe ₂	5	0.435	1	1
ReSe ₂	5	0.267	1	1
Br ₂ Ca	5	0.4658	1	1
InSe ₂	5	0.0054	1	1
GeTe ₂	5	0.004	1	1
SiTe ₂	5	0.006	1	1
I ₂ Mn	5	0.0052	1	1
NSr ₂	5	0.0016	1	1
PbS ₂	5	0.0026	1	1
BiClTe	5	0.4637	1	1
FeI ₂	5	0.0029	1	1
I ₂ Ni	5	0.0042	1	1
S ₂ Ti	5	0.2585	1	1
CrI ₂	5	0.0025	1	1
BiBrTe	5	0.4777	1	1
Bi ₂ Pd	5	0.1167	1	1
Cl ₂ Ni	5	0.2683	1	1
Cl ₂ Co	5	0.258	1	1
NbS ₂	5	1.5968	1	1
Br ₂ V	5	0.2659	1	1
ClNZr	5	0.2629	1	1
Cl ₂ Fe	5	0.257	1	1
AsSe ₂	5	0.2704	1	1
NiTe ₂	5	0.0066	1	1
Cl ₂ Cu	5	2.7535	1	1
I ₂ V	5	0.0047	1	1
Sn	5	0.159	2	1
GeI ₂	5	0.4591	1	1
Se ₂ Zr	5	0.0056	1	1
BiTe	5	0.4948	1	1
CdO ₂	5	0.2578	1	1
BrNZr	5	0.2724	1	1
NbSe ₂	5	0.2689	1	1
CoI ₂	5	0.0004	1	1
GeS ₂	5	0.1336	1	1
MnSe ₂	5	0.1435	1	1
Cl ₂ Zr	5	0.2575	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

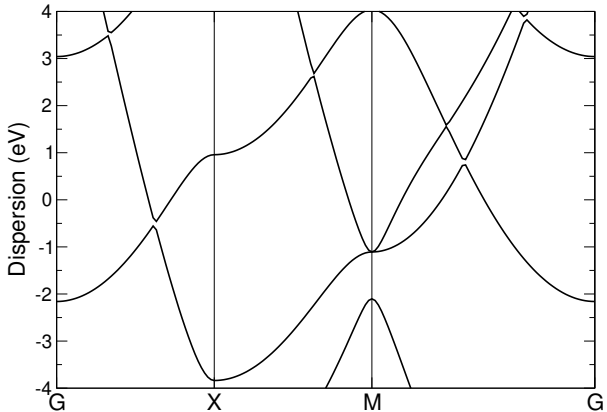
Formula	N° atoms	strain	cell size 1	cell size 2
Ga ₂ I ₂ Tb ₂	620	0.0001	91	73
CCl ₂ Sc ₂	601	0.0001	73	91
I ₂ La ₂ P	431	0.0002	73	57
Bi ₂ STe ₂	605	0.0002	100	81
CdI ₂	443	0.0002	100	81
Cl ₂ Mn	290	0.0002	49	64
BiTe	275	0.0002	64	49
Ga ₂ Gd ₂ I ₂	620	0.0002	91	73
I ₂ La ₂ O ₂	418	0.0002	65	48
I ₂ S ₂ Tb ₂	476	0.0003	88	50
Cl ₂ NSc ₂	418	0.0003	49	64
S ₂ Ta	257	0.0003	43	57
Bi ₂ Te ₃	373	0.0003	64	49
Cl ₂ Zr ₂	510	0.0003	73	91
HN ₃ OZn	366	0.0003	36	49
Br ₂ La ₂ P	605	0.0003	100	81
IO ₃ Tl	178	0.0004	49	16
CaI ₂	206	0.0004	49	36
Cl ₂ Fe ₂ O ₂	940	0.0004	110	120
ReSe ₂	462	0.0004	81	100
Br ₂ Ca	401	0.0004	91	73
CoI ₂	5	0.0004	1	1
I ₂ Nd ₂ S ₂	222	0.0005	36	25
Br ₂ H ₂ Zr ₂	692	0.0005	73	91
CrSe ₂	158	0.0005	25	36
CrO ₂	197	0.0005	25	49
Cl ₂ Ni	462	0.0005	81	100
LiMnTe ₂	524	0.0005	100	81
Bi ₂ Te ₂	114	0.0006	25	16
Cl ₂ Cu	366	0.0006	72	74
Cl ₂ Hg ₂ N ₂	602	0.0006	130	57
NbS ₂	257	0.0006	43	57
S ₂ Ti	371	0.0006	64	81
FHOZn	194	0.0006	25	36
Br ₂ Cr ₂ O ₂	390	0.0006	48	49
Cu ₄ Te ₂	546	0.0006	81	64
K	317	0.0006	118	81
CdI ₂	443	0.0006	100	81
Br ₂ Er ₂ S ₂	412	0.0006	74	44
Bi ₂	328	0.0007	91	73
BiBrTe	354	0.0007	81	64
As ₂ Mg ₂ Na ₂	722	0.0007	118	81
PTe ₂ Zr ₂	7	0.0007	1	1
Cd ₂ I ₃	329	0.0007	57	43
GdI ₂	317	0.0007	73	57
AsI ₂ La ₂	329	0.0007	57	43
Gd ₂ GeI ₂	605	0.0008	100	81
I ₂ Ti	5	0.0008	1	1
I ₂ Tm	206	0.0008	49	36
GeI ₂	443	0.0008	100	81

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Sn (P4/mmm (123))

Structural and electronic properties

	Formula	Sn
	Spacegroup	P4/mmm (123)
	Prototype	Sn
	Parent 3D	Sn
	Source DB	ICSD
	DB ID	652713
DF2-C09	Binding energy [meV/ Å ²]	87.52
RVV10	Binding energy [meV/ Å ²]	79.55
	Band gap (PBE) [eV]	0.0

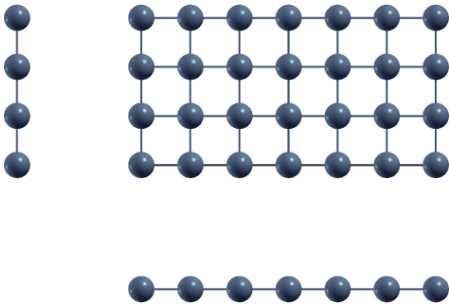


Band structure: Electronic band structure of Sn (P4/mmm (123)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Sn (P4/mmm (123)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	2.95366241	0.00000000	0.00000000
a₂	0.00000000	2.95366241	0.00000000
a₃	0.00000000	0.00000000	20.00000000
	x [Å]	y [Å]	z [Å]
● Sn	1.47683121	1.47683121	10.00000000



Orthographic projections: views of Sn (P4/mmm (123)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	2	0.1615	1	1
In	2	0.0044	1	1
In	2	0.1392	1	1
As ₂	3	0.7882	1	1
LiO	3	0.1485	1	1
P ₂	3	0.156	1	1
C ₂	3	0.1088	1	1
Cl ₂ Zn	4	0.7841	1	1
S ₂ V	4	0.1419	1	1
MoS ₂	4	0.1425	1	1
Cl ₂ Mn	4	0.1678	1	1
MoSe ₂	4	0.1607	1	1
ReSe ₂	4	0.1834	1	1
S ₂ Ta	4	0.1702	1	1
Te ₂ V	4	0.7735	1	1
Br ₂ Co	4	0.7865	1	1
ReS ₂	4	0.1323	1	1
Cl ₂ Ti	4	0.1562	1	1
S ₂ Ti	4	0.176	1	1
NbS ₂	4	0.1696	1	1
S ₂ W	4	0.1426	1	1
Bi ₂ Pd	4	0.3916	1	1
Br ₂ Mn	4	0.7795	1	1
Cl ₂ Ni	4	0.1845	1	1
Cl ₂ Co	4	0.1755	1	1
CrTe ₂	4	0.1924	1	1
NbS ₂	4	0.1648	1	1
Br ₂ V	4	0.1824	1	1
ClN ₂ Zr	4	0.1798	1	1
Cl ₂ Fe	4	0.1747	1	1
CdClO	4	0.7716	1	1
S ₂ Ta	4	0.1639	1	1
Se ₂ V	4	0.1624	1	1
Se ₂ Ti	4	0.1974	1	1
Br ₂ Ti	4	0.1916	1	1
Te ₂ W	4	0.7667	1	1
AsSe ₂	4	0.1863	1	1
Cl ₂ V	4	0.1462	1	1
OTl ₂	4	0.7723	1	1
CdO ₂	4	0.1754	1	1
BrN ₂ Zr	4	0.188	1	1
NbSe ₂	4	0.185	1	1
Br ₂ Fe	4	0.7868	1	1
Br ₂ Cr	4	0.192	1	1
Cl ₂ Zr	4	0.1751	1	1
FeSe ₂	4	0.0064	1	1
Se ₂ Ta	4	0.1852	1	1
NbSe ₂	4	0.1867	1	1
MoS ₂	4	0.1427	1	1
CrSe ₂	4	0.1451	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

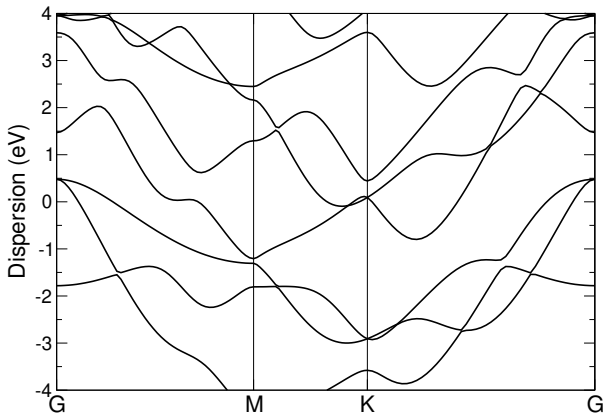
Formula	N° atoms	strain	cell size 1	cell size 2
AgClO ₄	530	0.0001	164	61
Br ₂ O ₂ Yb ₂	375	0.0001	81	49
Br ₂ O ₂ Tb ₂	655	0.0002	145	85
I ₂ O ₂ Y ₂	70	0.0002	16	9
Ca ₂ O ₂	337	0.0003	81	64
Hf ₂ Si ₂ Te ₂	670	0.0003	136	89
Ge ₂ Hf ₂ Te ₂	859	0.0003	181	113
As ₂ Co ₂ Li ₂	859	0.0003	181	113
Co ₂ Se ₂	492	0.0003	136	89
Br ₂ Er ₂ O ₂	445	0.0003	97	58
F ₂ Lu ₂ Se ₂	498	0.0004	108	65
Br ₂ Nd ₂ O ₂	70	0.0004	16	9
As ₄	120	0.0005	40	20
PbS ₂ Sn	296	0.0005	100	49
Gd	153	0.0005	63	90
Dy ₂ I ₂ S ₂	300	0.0005	90	35
Fe ₂ Te ₂	277	0.0006	81	49
Br ₂ Cu ₂	485	0.0006	145	85
Br ₂ Ca ₃ Si	314	0.0006	80	39
Se ₂ Si ₂ Zr ₂	186	0.0007	36	25
Br ₂ Ca ₃ Si	593	0.0007	149	74
Ca ₂ Cl ₂ F ₂	496	0.0007	106	65
O ₂ Sn ₂	485	0.0007	145	85
Bi ₂ Br ₂ O ₂	70	0.0007	16	9
Cu ₂ Te ₂	633	0.0007	181	113
C ₄ Ca ₂	143	0.0007	35	18
I ₂ La ₂ Te	275	0.0007	80	39
Ag ₂ K ₂ Te ₂	293	0.0008	89	34
Ge ₂ Te ₂ Zr ₂	496	0.0008	106	65
Br ₂ Cu	233	0.0008	80	51
Bi ₂ Pd	277	0.0008	82	65
Cu ₂ Sr ₂	411	0.0008	131	70
Cu ₂ F ₄	231	0.0009	81	25
Gd ₂ I ₂ S ₂	314	0.0009	80	39
Br ₂ Ca ₃ Si	314	0.0009	80	39
Cu ₂ Se ₂	89	0.0009	25	16
Ba ₂ Hg	371	0.0009	149	74
I ₂ S ₂ Tb ₂	300	0.0009	90	35
I ₂ S ₂ Yb ₂	213	0.001	63	25
Ca ₂ Cl ₂	277	0.001	81	49
AlH ₄ Na	214	0.001	64	25
Br ₂ Lu ₂ O ₂	496	0.001	106	65
I ₂ La ₂ P	481	0.0011	131	70
P ₂ Te ₂ Zr ₂	523	0.0011	118	81
Er ₂ I ₂ O ₂	70	0.0011	16	9
GdI ₂	205	0.0011	79	42
Br ₂ F ₂ Yb ₂	655	0.0011	145	85
Br ₂ Eu ₂ F ₂	70	0.0011	16	9
I ₂ S ₂ Tl ₂	121	0.0011	25	16
Cl ₂ N ₂ Zr ₂	192	0.0011	42	25

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Sn₂As (P-3m1 (164))

Structural and electronic properties

Formula	Sn ₂ As
Spacegroup	P-3m1 (164)
Prototype	CdI ₂
Parent 3D	Sn ₄ As ₃
Source DB	COD
DB ID	1010003
DF2-C09 Binding energy [meV/ Å ²]	96.44
RVV10 Binding energy [meV/ Å ²]	88.51
Band gap (PBE) [eV]	0.0

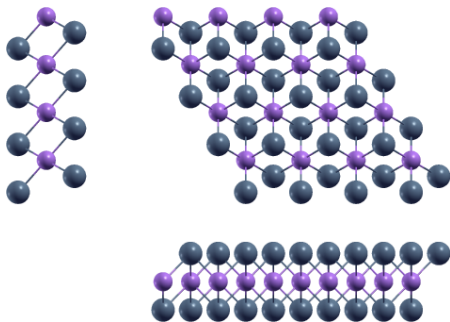


Band structure: Electronic band structure of Sn₂As (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Sn₂As (P-3m1 (164)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.70696883	0.00000000	0.00000000
a₂	−1.85348442	3.21032918	0.00000000
a₃	0.00000000	0.00000000	23.23789655
	x [Å]	y [Å]	z [Å]
● Sn	1.85348442	1.07010973	9.72403310
● Sn	0.00000000	0.00000000	13.51386346
● As	−0.00000000	2.14021945	11.61894828



Orthographic projections: views of Sn₂As (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	4	0.1146	1	1
Tl	4	0.2645	1	1
In	4	1.5287	1	1
InSe	5	0.4979	1	1
HgO	5	0.1206	1	1
LiO	5	0.247	1	1
P ₂	5	0.2572	1	1
PbTe	5	2.9043	1	1
Mg ₂	5	0.43	1	1
Sb ₂	5	0.4569	1	1
Sm	5	0.2205	1	2
I ₂ Mg	6	0.4711	1	1
S ₂ V	6	1.5516	1	1
MoS ₂	6	1.5569	1	1
Cl ₂ Mn	6	0.2728	1	1
CdI ₂	6	2.9267	1	1
AgTe ₂	6	0.1159	1	1
PSn ₂	6	0.0037	1	1
MoSe ₂	6	0.2634	1	1
S ₂ Ta	6	0.2759	1	1
Br ₂ Zn	6	0.007	1	1
I ₂ Pr	6	0.208	1	1
S ₂ Zr	6	0.0045	1	1
Br ₂ La	6	0.472	1	1
Br ₂ Cu	6	0.9843	1	1
BiClTe	6	2.9315	1	1
Cl ₂ Ti	6	0.2574	1	1
BrCdI	6	0.4792	1	1
HgI ₂	6	0.3196	1	1
Mg ₃	6	0.1123	1	1
Te ₂ Ti	6	0.0073	1	1
NbS ₂	6	0.2752	1	1
I ₂ Zn	6	0.4489	1	1
RhTe ₂	6	0.0028	1	1
S ₂ W	6	1.5574	1	1
Bi ₂ Pd	6	0.1263	1	1
GeI ₂	6	0.4664	1	1
NbS ₂	6	0.2689	1	1
S ₂ Ta	6	0.2676	1	1
Se ₂ V	6	0.2657	1	1
AsKSn	6	0.484	1	1
PbTe ₂	6	0.4766	1	1
I ₂ Nd	6	0.2094	1	1
S ₂ Sn	6	0.0042	1	1
SnTe ₂	6	0.4608	1	1
Cl ₂ V	6	1.5867	1	1
GeI ₂	6	2.9074	1	1
STl ₂	6	2.8446	1	1
PtSe ₂	6	0.0006	1	1
GeS ₂	6	0.1481	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

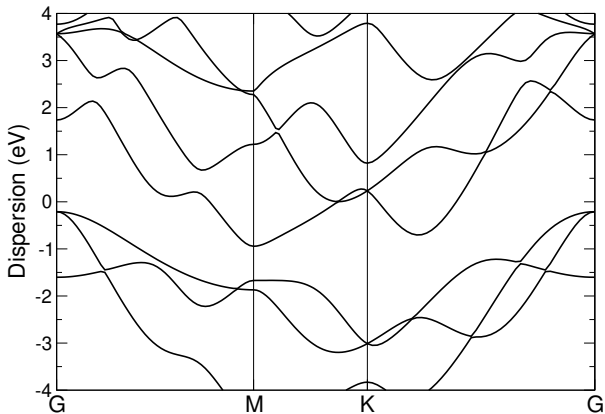
Formula	N° atoms	strain	cell size 1	cell size 2
ClH ₃ O	488	0.0	81	49
S ₂ Ta	543	0.0	81	100
GeI ₂ Y ₂	437	0.0001	64	49
Se ₂ Yb	492	0.0001	91	73
Bi ₂ STe ₂	386	0.0001	57	43
BH ₄ Li	786	0.0001	100	81
Tl	310	0.0001	73	91
SnTe ₂	543	0.0002	100	81
C ₂ F ₂	433	0.0002	39	79
GeI ₂	492	0.0002	91	73
Ba ₂ Ge ₂ Mn ₂	483	0.0002	65	48
I ₂ La ₂	447	0.0002	73	57
H ₂ MgO ₂	353	0.0002	36	49
LiMnTe ₂	343	0.0002	57	43
PbTe ₂	435	0.0002	81	64
I ₂ Pr ₂ S ₂	171	0.0003	25	16
As ₂ Li ₂ Nd	437	0.0003	64	49
F ₂ I ₂ Yb ₂	483	0.0003	65	48
BiTe ₂	492	0.0003	91	73
AsKSn	390	0.0003	73	57
Ba ₂ Ni ₃	638	0.0004	91	73
HN ₃ OZn	678	0.0004	64	81
Ga ₂ Te ₂	565	0.0004	91	73
Bi ₂ Se ₂ Te	437	0.0004	64	49
Ag ₂	107	0.0004	25	16
CKN	336	0.0005	72	40
Se ₂ W	492	0.0005	73	91
I ₂ Pr ₂ Si ₂	711	0.0005	91	73
CrSe ₂	300	0.0005	43	57
CdI ₂	300	0.0005	57	43
GeI ₂	300	0.0005	57	43
TaTe ₂	6	0.0006	1	1
BiBrTe	255	0.0006	49	36
MoSe ₂	492	0.0006	73	91
Br ₂ La ₂ P	386	0.0006	57	43
Eu ₂ H ₂ I ₂	483	0.0006	65	48
PtSe ₂	6	0.0006	1	1
Al ₂ Cl ₂ O ₂	438	0.0006	48	49
S ₂ V	255	0.0007	36	49
AsCuLi ₂	565	0.0007	91	73
Sb ₂ Se ₂ Te	638	0.0007	91	73
ClH ₃ O	368	0.0007	61	37
Cu ₄ Te ₂	363	0.0007	49	36
Ba ₂ Pt	123	0.0007	25	16
I ₂ La ₂ O ₂	840	0.0007	118	81
CNb ₂ S ₂	536	0.0007	57	73
As ₂ CeLi ₂	386	0.0007	57	43
Cl ₂ V	300	0.0008	43	57
Sb ₂ SeTe ₂	437	0.0008	64	49
PbTe	257	0.0008	57	43

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Sn₂P (P-3m1 (164))

Structural and electronic properties

	Formula	Sn ₂ P
	Spacegroup	P-3m1 (164)
	Prototype	CdI ₂
	Parent 3D	Sn ₄ P ₃
	Source DB	ICSD
	DB ID	15014
DF2-C09	Binding energy [meV/ Å²]	106.71
RVV10	Binding energy [meV/ Å²]	95.98
	Band gap (PBE) [eV]	0.0

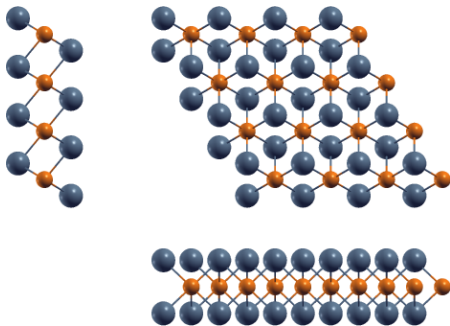


Band structure: Electronic band structure of Sn₂P (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Sn₂P (P-3m1 (164)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.67742646	0.00000000	0.00000000
a₂		−1.83871323	3.18474473	0.00000000
a₃		0.00000000	0.00000000	23.16539814
		x [Å]	y [Å]	z [Å]
●	Sn	0.00000000	2.12316315	13.33031314
●	Sn	0.00000000	0.00000000	9.83508500
●	P	1.83871323	1.06158158	11.58269907



Orthographic projections: views of Sn₂P (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	4	0.1163	1	1
Tl	4	0.2699	1	1
In	4	1.5558	1	1
InSe	5	2.9305	1	1
HgO	5	0.1227	1	1
Bi ₂	5	3.0072	1	1
As ₂	5	0.0087	1	1
P ₂	5	0.2624	1	1
Sb ₂	5	0.4663	1	1
Sm	5	0.2254	1	2
I ₂ Mg	6	0.4808	1	1
MoS ₂	6	1.5844	1	1
CdI ₂	6	2.9765	1	1
AgTe ₂	6	0.1178	1	1
MoSe ₂	6	0.2689	1	1
Br ₂ Ca	6	2.9928	1	1
HfS ₂	6	0.0061	1	1
AsSn ₂	6	0.0038	1	1
CuTe ₂	6	0.0064	1	1
S ₂ Zr	6	0.0008	1	1
Br ₂ La	6	0.4817	1	1
Br ₂ Co	6	0.0091	1	1
BiClTe	6	2.9813	1	1
Ca ₂ N	6	0.0082	1	1
Cl ₂ Ti	6	0.2626	1	1
HgI ₂	6	0.3275	1	1
Mg ₃	6	0.1137	1	1
I ₂ Zn	6	0.4582	1	1
BaF ₂	6	0.4978	1	1
RhTe ₂	6	0.0067	1	1
S ₂ W	6	1.5849	1	1
Bi ₂ Pd	6	0.1289	1	1
GeI ₂	6	0.476	1	1
NbS ₂	6	0.2744	1	1
CoTe ₂	6	0.0058	1	1
S ₂ Ta	6	0.2732	1	1
Se ₂ V	6	0.2712	1	1
AsKSn	6	0.494	1	1
PbTe ₂	6	0.4864	1	1
S ₂ Sn	6	0.0005	1	1
SnTe ₂	6	0.4703	1	1
Cl ₂ V	6	0.2486	1	1
STl ₂	6	0.5003	1	1
PtSe ₂	6	0.0045	1	1
Br ₂ Fe	6	0.0091	1	1
GeS ₂	6	0.1517	1	1
TaTe ₂	6	0.0032	1	1
Br ₂ Ni	6	0.0041	1	1
NbTe ₂	6	0.001	1	1
Se ₂ Yb	6	0.4766	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

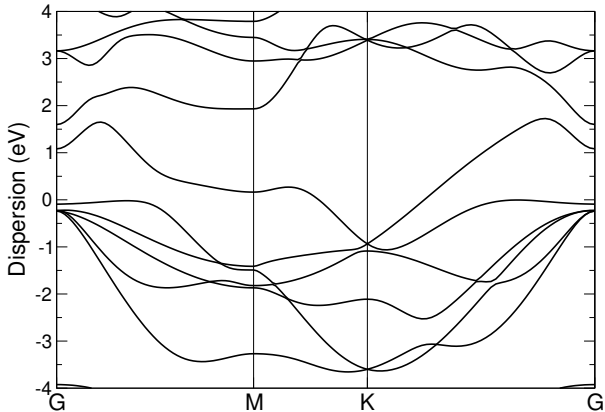
Formula	N° atoms	strain	cell size 1	cell size 2
GeI ₂	435	0.0	81	64
Cu ₂ I ₂	447	0.0	73	57
Br ₂ Gd ₂ Ge	504	0.0	73	57
N ₂ Re	390	0.0001	49	81
Ga ₂ I ₂ Tb ₂	363	0.0001	49	36
Bi ₂ Se ₂ Te	386	0.0001	57	43
Ba ₂ Ni ₃	563	0.0002	81	64
CrS ₂	183	0.0002	25	36
HN ₃ OZn	765	0.0002	73	91
Ga ₂ Te ₂	499	0.0002	81	64
Sb ₂	419	0.0002	91	73
Se ₂ Yb	435	0.0003	81	64
F ₂ Lu ₂ Se ₂	786	0.0003	100	81
Gd ₂ I ₂	447	0.0003	73	57
I ₂ Pr ₂ Si ₂	627	0.0003	81	64
H ₂ NiO ₂	414	0.0003	43	57
Br ₂ Ca	255	0.0003	49	36
O ₂ Pt	255	0.0003	36	49
Au ₂ K ₂ Se ₂	153	0.0003	35	8
Cu ₂ F ₄	714	0.0003	130	54
GeI ₂ Y ₂	386	0.0003	57	43
Li ₂ P ₂ Pr	638	0.0003	91	73
Ga ₂ Gd ₂ I ₂	363	0.0004	49	36
Se ₄ TiZr	12	0.0004	2	1
Ga ₂ Ge ₂ Te ₂	711	0.0005	91	73
Br ₂ La ₂	565	0.0005	91	73
AsCuLi ₂	499	0.0005	81	64
Cl ₂ V	339	0.0005	49	64
Sb ₂ SeTe ₂	386	0.0005	57	43
S ₂ Sn	6	0.0005	1	1
BiTe ₂	435	0.0005	81	64
Ca ₂ H ₂ I ₂	483	0.0005	65	48
Bi ₂ Se ₃	504	0.0005	73	57
I ₂ S ₂ Yb ₂	279	0.0005	45	24
NaO ₄	272	0.0005	49	25
AsKSn	339	0.0005	64	49
In ₂ Te ₃	386	0.0005	57	43
As ₂ Ir ₂	387	0.0006	65	48
As ₂ Li ₂ Nd	386	0.0006	57	43
N ₂ Re	294	0.0006	37	61
Br ₂ La	390	0.0006	73	57
AsI ₂ La ₂	233	0.0006	36	25
MnO ₂	75	0.0006	9	16
Cd ₂ I ₃	233	0.0006	36	25
Ga ₂ I ₂ Y ₂	486	0.0007	64	49
Gd	123	0.0007	25	48
Ho ₂ I ₂ S ₂	492	0.0007	80	42
S ₂ Zr	6	0.0008	1	1
CrSe ₂	339	0.0008	49	64
Bi ₂	219	0.0008	49	36

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

SnAs (P-3m1 (164))

Structural and electronic properties

	Formula	SnAs
	Spacegroup	P-3m1 (164)
	Prototype	PtTe
	Parent 3D	Sn ₄ As ₃
	Source DB	COD
	DB ID	1010003
DF2-C09	Binding energy [meV/ Å ²]	96.44
RVV10	Binding energy [meV/ Å ²]	88.51
	Band gap (PBE) [eV]	0.0

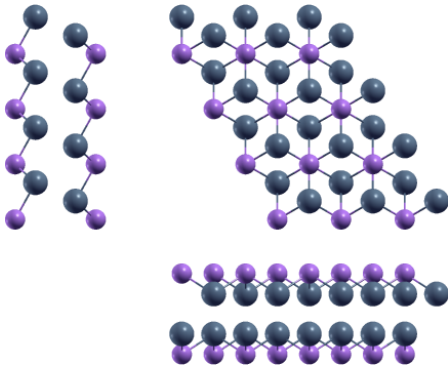


Band structure: Electronic band structure of SnAs (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of SnAs (P-3m1 (164)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.04633238	0.00000000	0.00000000
a₂	−2.02316619	3.50422663	0.00000000
a₃	0.00000000	0.00000000	25.10500954
	x [Å]	y [Å]	z [Å]
● Sn	2.02316619	1.16807554	11.28238524
● As	0.00000000	0.00000000	9.98667669
● As	0.00000000	0.00000000	15.11833285
● Sn	−0.00000000	2.33615109	13.82262430



Orthographic projections: views of SnAs (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.4824	1	1
Na	5	0.2506	1	1
Ag ₂	6	0.4968	1	1
As ₂	6	0.2615	1	1
Sb ₂	6	0.0068	1	1
CaCl	6	0.1251	1	1
Cl ₂ Zn	7	0.26	1	1
MoTe ₂	7	0.2537	1	1
PSn ₂	7	0.2743	1	1
Ba ₂ Pt	7	0.4961	1	1
ReSe ₂	7	1.5353	1	1
HfS ₂	7	0.2653	1	1
CaI ₂	7	0.459	1	1
HfTe ₂	7	0.0088	1	1
Te ₂ V	7	0.2563	1	1
CuTe ₂	7	0.2648	1	1
S ₂ Zr	7	0.2732	1	1
Ca ₂ Si	7	2.9311	1	1
I ₂ Yb	7	0.4528	1	1
Br ₂ Co	7	0.2609	1	1
Ca ₂ N	7	0.2622	1	1
AuTe ₂	7	0.0012	1	1
Cl ₂ Zn	7	0.1353	1	1
PdTe ₂	7	0.0036	1	1
I ₂ Zn	7	0.0034	1	1
Te ₂ Zn	7	0.2534	1	1
Bi ₂ Pd	7	0.4223	1	1
Br ₂ Mn	7	0.2584	1	1
Cl ₂ Ni	7	1.5417	1	1
CrTe ₂	7	1.5861	1	1
PtS ₂	7	1.6339	1	1
CoTe ₂	7	0.2658	1	1
Br ₂ V	7	1.5295	1	1
CdClO	7	0.2556	1	1
Ba ₂ N	7	0.0073	1	1
Se ₂ Ti	7	0.2485	1	1
Br ₂ Ti	7	1.5818	1	1
Te ₂ Zr	7	0.0083	1	1
Te ₂ W	7	0.2539	1	1
I ₂ Tm	7	0.4561	1	1
S ₂ Sn	7	0.2736	1	1
SnTe ₂	7	0.0084	1	1
I ₂ Pb	7	0.501	1	1
OTl ₂	7	0.2558	1	1
BrNZr	7	1.5618	1	1
NbSe ₂	7	1.5448	1	1
Br ₂ Fe	7	0.261	1	1
GeS ₂	7	0.1182	1	1
MnSe ₂	7	0.125	1	1
DyI ₂	7	0.4661	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

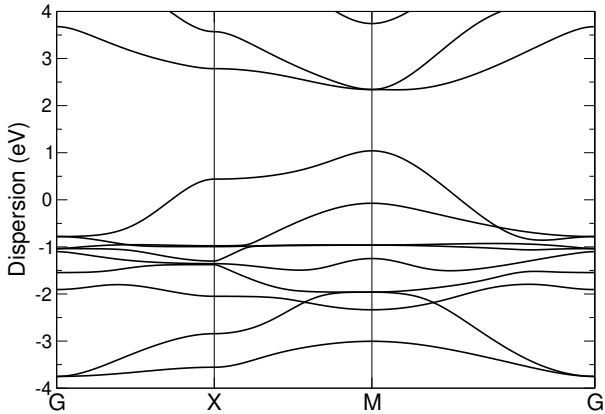
Formula	N° atoms	strain	cell size 1	cell size 2
Sb ₂ Te ₂	400	0.0	57	43
I ₂ La ₂ Sb	577	0.0	73	57
Ga ₂ S ₂	724	0.0	81	100
I ₂ La ₂ Te	644	0.0001	81	64
CaH ₂ O ₂	747	0.0001	73	91
Br ₂ Gd ₂	8	0.0001	1	1
CdClO	447	0.0001	57	73
I ₂ S ₂ Tb ₂	802	0.0001	91	73
NbS ₂	208	0.0002	25	36
O ₂ Pt	331	0.0002	37	61
Se ₂ Ta	291	0.0002	36	49
Ba ₂ Pt	403	0.0002	64	49
Br ₂ Ca ₃ Si	708	0.0003	81	64
PTe ₂ Ti ₂	824	0.0003	81	100
OTl ₂	447	0.0003	57	73
KS ₂ Ti	580	0.0003	64	81
Cl ₂ Hf ₂ N ₂	666	0.0003	57	73
NbSe ₂	291	0.0003	36	49
DyI ₂	583	0.0003	91	73
K	349	0.0003	73	57
Cl ₂ N ₂ Zr ₂	838	0.0003	73	91
CuTe ₂	565	0.0004	73	91
F ₂ Se ₂ Y ₂	294	0.0004	36	25
Br ₂ Ni	624	0.0004	81	100
Cl ₂ Mg	624	0.0005	81	100
Ag ₂	354	0.0005	64	49
Cl ₂ Zn	499	0.0005	64	81
Br ₂ Ca ₃ Si	324	0.0005	45	24
Se ₂ Ti	388	0.0006	49	64
Te ₂ V	447	0.0006	57	73
SbSe ₂ Tl	492	0.0006	75	48
Li ₂ Tl ₂	164	0.0006	25	16
Br ₂ Er ₂	8	0.0006	1	1
S ₂ Ta	208	0.0006	25	36
I ₂ Se ₂ Tm ₂	684	0.0007	90	54
Br ₂ Mn	499	0.0007	64	81
I ₂ S ₂ Sm ₂	634	0.0007	73	57
LiNbS ₂	244	0.0007	25	36
Cl ₂ Ni	291	0.0007	36	49
HfS ₂	565	0.0007	73	91
AsSe ₂	291	0.0007	36	49
As ₂ Cd ₂ K ₂	958	0.0007	118	81
CdH ₂ O ₂	593	0.0007	57	73
Cl ₂ H ₂ Lu ₂	924	0.0008	81	100
LiO	114	0.0008	16	25
Br ₂ N ₂ Ti ₂	468	0.0008	45	48
Cl ₂ N ₂ Ti ₂	974	0.0008	92	101
Br ₂ Hg ₃	120	0.0008	25	4
O ₄ PSn	958	0.0008	118	81
CrTe ₂	343	0.0009	43	57

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

SnI₃ (P4mm)

Structural and electronic properties

	Formula	SnI ₃
	Spacegroup	P4mm
	Prototype	I3Sn
	Parent 3D	Cl ₃ NSn
	Source DB	ICSD
	DB ID	250733
DF2-C09	Binding energy [meV/ Å ²]	65.05
RVV10	Binding energy [meV/ Å ²]	N/A
	Band gap (PBE) [eV]	0.0

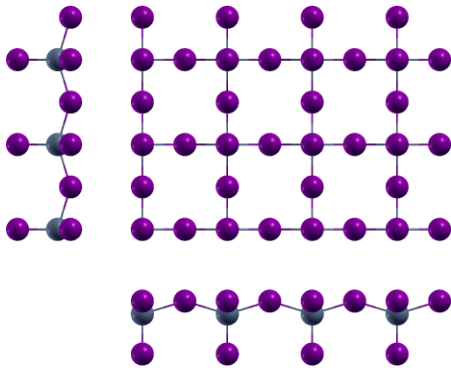


Band structure: Electronic band structure of SnI₃ (P4mm) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of SnI₃ (P4mm) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		-5.76993809	0.00000000	0.00000000
a₂		0.00000000	-5.76993809	0.00000000
a₃		0.00000000	0.00000000	19.90224402
		x [Å]	y [Å]	z [Å]
●	Sn	0.00000000	0.00000000	-0.24356509
●	I	0.00000000	-2.88496904	-1.11897398
●	I	-2.88496904	0.00000000	-1.11897398
●	I	0.00000000	0.00000000	2.48151304



Orthographic projections: views of SnI₃ (P4mm) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	6	0.1465	1	2
Cl ₂ Rb ₂	8	0.3892	1	1
Br ₃ Cs	8	0.1854	1	1
Au ₂ I ₂	8	0.4486	1	1
In	8	0.1491	1	4
IO ₃ Tl	9	0.1807	1	1
ClKO ₃	9	0.1898	1	1
ClH ₃ O	9	0.1099	1	1
BrKO ₃	9	0.7815	1	1
KNO ₃	9	0.1682	1	1
Cl ₂ Mn	10	0.1486	1	2
MoSe ₂	10	0.1462	1	2
Hg ₄ O ₂	10	1.8519	1	1
S ₂ Ti	10	0.1515	1	2
NbS ₂	10	0.1492	1	2
Cl ₂ Co	10	0.1514	1	2
NbS ₂	10	0.1476	1	2
Cl ₂ Fe	10	0.1511	1	2
S ₂ Ta	10	0.1473	1	2
Se ₂ V	10	0.1468	1	2
Cl ₂ Ga ₂ Te ₂	10	0.1733	1	1
Au ₄ Li	10	0.3889	1	1
Cl ₂ Zr	10	0.1512	1	2
Br ₂ O ₂ Ti ₂	10	0.3358	1	1
Cl ₄ KTl	10	1.1032	1	1
Br ₂ Ca ₃ Si	10	0.1921	1	1
Se ₂ W	10	0.1463	1	2
In ₂ Se ₂	12	0.4279	1	2
Bi ₂ Mn ₂	12	0.171	1	2
Br ₂ Zn	13	0.1636	1	3
GeTe ₂	13	0.1801	1	3
K ₂ PtTe ₂	13	0.1036	2	1
CuTe ₂	13	0.1464	1	3
PbS ₂	13	0.1722	1	3
Te ₂ Ti	13	0.164	1	3
IO ₃ Tl	13	0.1485	2	1
Te ₂ Zn	13	0.1391	1	3
ClKO ₃	13	0.1515	2	1
TaTe ₂	13	0.1558	1	3
I ₂ Ti	13	0.1762	1	3
HfSe ₂	13	0.164	1	3
Cl ₂ NSc ₂	14	0.1488	1	2
GeI ₂	14	0.3508	2	2
Tl	14	0.0734	2	6
CNRb	14	0.1885	2	2
LiOS ₂ Ti	14	0.148	1	2
Se ₂ Yb	14	0.3512	2	2
BiTe ₂	14	0.3517	2	2
C ₂ I ₂ Y ₂	14	0.1591	2	1
Bi ₂ Te ₂	16	0.6476	1	3

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

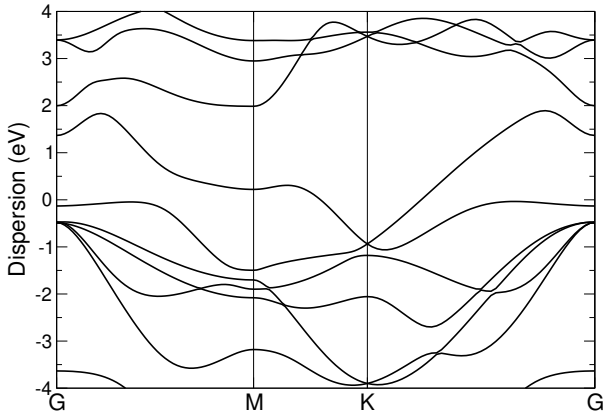
Formula	N° atoms	strain	cell size 1	cell size 2
Br ₂ O ₂ Y ₂	70	0.0	4	9
Br ₂ Dy ₂ O ₂	70	0.0	4	9
H ₂ Li ₂ O ₂	670	0.0001	34	89
Ag ₂ I ₂	520	0.0001	49	81
Cu ₂ S ₂	52	0.0001	4	9
Cl ₄ KTl	560	0.0001	65	50
Br ₂ CsF	164	0.0001	16	25
Ag ₂ K ₂ Se ₂	814	0.0001	58	97
Co ₂ S ₂	356	0.0002	25	64
F ₂ I ₂ Tm ₂	866	0.0003	53	109
Sn ₂ Te ₂	884	0.0003	85	136
O ₂ Pb ₂	892	0.0003	74	149
F ₄ Nb	345	0.0004	25	49
Cu ₂ Na ₂ Se ₂	866	0.0004	53	109
Bi ₂ I ₂ O ₂	866	0.0004	53	109
Ba ₂ F ₂ I ₂	896	0.0004	65	106
F ₂ Tl ₂	52	0.0004	4	9
Cl ₂ F ₂ Pb ₂	866	0.0004	53	109
Mg ₆	586	0.0004	25	81
I ₂ Nd ₂ O ₂	796	0.0005	49	100
P ₂ Rh ₂	52	0.0006	4	9
O ₄ PTl	896	0.0006	65	106
Ge ₂ I ₂ La ₂	314	0.0006	20	39
O ₂ Sn ₂	52	0.0007	4	9
I ₂ Nd ₂ S ₂	534	0.0007	36	65
HgO	424	0.0008	41	130
CaCl	228	0.0008	25	64
P ₄	204	0.0009	16	35
MnSe ₂	292	0.0009	25	64
Bi ₂ O ₂	892	0.001	74	149
Ba ₂ Ge ₂ Mn ₂	866	0.001	53	109
Br ₂ Cd	537	0.001	48	115
K	52	0.0011	9	16
HgI ₂	439	0.0011	49	81
Cl ₄ KTl	550	0.0012	64	49
F ₂ I ₂ Yb ₂	866	0.0013	53	109
Ba ₂ Pt	339	0.0013	36	65
AsSn ₂	545	0.0013	44	123
CNRb	368	0.0014	44	64
Br ₂ OV	220	0.0014	15	40
Mo ₂ Te ₄	838	0.0014	64	97
C ₂ I ₂ La ₂	262	0.0014	16	33
Br ₂ F ₂ Sr ₂	394	0.0014	25	49
As ₂ Mg ₂ Na ₂	132	0.0014	9	16
Cl ₂ F ₂ Pb ₂	796	0.0014	49	100
PtSe ₂	545	0.0014	44	123
K ₂ PdSe ₂	147	0.0014	18	15
Bi ₂ I ₂ O ₂	796	0.0014	49	100
Cu ₂ Na ₂ Se ₂	796	0.0014	49	100
PdTe ₂	537	0.0015	48	115

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

SnP (P-3m1 (164))

Structural and electronic properties

	Formula	SnP
	Spacegroup	P-3m1 (164)
	Prototype	PtTe
	Parent 3D	Sn ₄ P ₃
	Source DB	ICSD
	DB ID	15014
DF2-C09	Binding energy [meV/ Å ²]	106.71
RVV10	Binding energy [meV/ Å ²]	95.98
	Band gap (PBE) [eV]	0.0

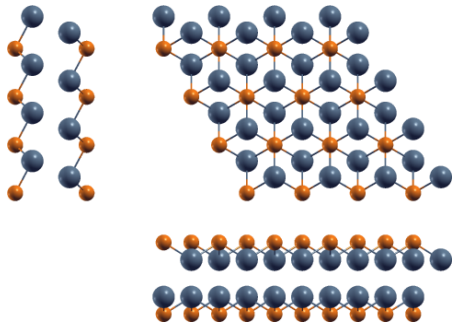


Band structure: Electronic band structure of SnP (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of SnP (P-3m1 (164)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.91417873	0.00000000	0.00000000
a₂		−1.95708937	3.38977822	0.00000000
a₃		0.00000000	0.00000000	25.15735730
		x [Å]	y [Å]	z [Å]
●	Sn	−0.00000000	2.25985215	13.88976292
●	P	0.00000000	0.00000000	10.05716490
●	P	0.00000000	0.00000000	15.10019240
●	Sn	1.95708937	1.12992607	11.26759438



Orthographic projections: views of SnP (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	3.0098	1	1
Na	5	0.2726	1	1
AsSb	6	0.0084	1	1
Bi ₂	6	0.4473	1	1
GeTe	6	0.0025	1	1
S ₂	6	0.001	1	1
CaCl	6	0.1363	1	1
IrTe ₂	7	0.0016	1	1
CdCl ₂	7	0.0036	1	1
Cl ₂ Mn	7	1.5537	1	1
MoTe ₂	7	0.2759	1	1
ReSe ₂	7	0.255	1	1
CaI ₂	7	0.4995	1	1
InSe ₂	7	0.0032	1	1
GeTe ₂	7	0.0045	1	1
HfTe ₂	7	0.0068	1	1
I ₂ Mn	7	0.0034	1	1
NSr ₂	7	0.0068	1	1
I ₂ Yb	7	0.4927	1	1
LiO ₂	7	0.0685	1	1
Cl ₂ Zn	7	0.1489	1	1
FeI ₂	7	0.0056	1	1
I ₂ Ni	7	0.0044	1	1
S ₂ Ti	7	0.247	1	1
NbS ₂	7	1.5654	1	1
CrI ₂	7	0.006	1	1
Te ₂ Zn	7	0.2757	1	1
BiBrTe	7	0.4561	1	1
Bi ₂ Pd	7	0.113	1	1
Cl ₂ Ni	7	0.2563	1	1
Cl ₂ Co	7	0.2465	1	1
CrTe ₂	7	0.2648	1	1
PtS ₂	7	0.2741	1	1
Br ₂ V	7	0.2539	1	1
ClN ₂ Zr	7	1.6288	1	1
Cl ₂ Fe	7	1.5973	1	1
S ₂ Ta	7	1.5283	1	1
Ba ₂ N	7	0.0084	1	1
Se ₂ Ti	7	0.2702	1	1
Br ₂ Ti	7	0.2639	1	1
Te ₂ Zr	7	0.0073	1	1
AsSe ₂	7	0.2583	1	1
I ₂ Tm	7	0.4963	1	1
BiTe	7	0.4725	1	1
CdO ₂	7	0.2463	1	1
BrN ₂ Zr	7	0.2601	1	1
NbSe ₂	7	0.2568	1	1
CoI ₂	7	0.008	1	1
GeS ₂	7	0.1274	1	1
MnSe ₂	7	0.1362	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

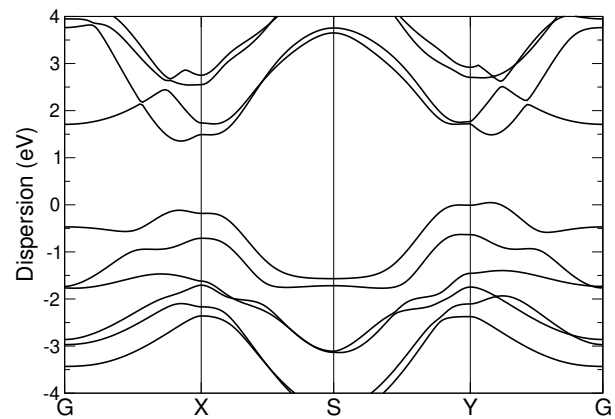
Formula	N° atoms	strain	cell size 1	cell size 2
Br ₂ Cr	565	0.0	73	91
Br ₂ H ₂ Zr ₂	838	0.0001	73	91
GeI ₂ La ₂	501	0.0001	64	49
I ₂ La ₂ P	805	0.0001	100	81
F ₂ Se ₂ Yb ₂	10	0.0001	1	1
Br ₂ Hf ₂	580	0.0001	64	81
Dy ₂ I ₂ S ₂	486	0.0002	57	43
Cl ₂ Sc ₂	656	0.0002	73	91
Br ₂ Ti	565	0.0003	73	91
CrO ₂	393	0.0003	39	79
CrTe ₂	565	0.0003	73	91
ReSe ₂	447	0.0003	57	73
I ₂ Tm	403	0.0003	64	49
S ₂ Zn ₂	8	0.0004	1	1
FKO ₂ Se	870	0.0004	135	66
O ₂ Zn	439	0.0004	49	81
NbSe ₂	499	0.0005	64	81
Ge ₂ I ₂ La ₂	634	0.0005	73	57
BrN ₂ Zr	499	0.0006	64	81
Cl ₂ Ni	447	0.0006	57	73
LiOS ₂ Ti	389	0.0006	36	49
I ₂ S ₂ Sm ₂	412	0.0006	49	36
Cl ₂ Fe	343	0.0007	43	57
C ₂ F ₂	52	0.0007	4	9
AsSe ₂	499	0.0008	64	81
Ni ₂ SbTe ₂	9	0.0008	1	1
Cl ₂ H ₂ Sc ₂	838	0.0008	73	91
Sm	25	0.0008	4	9
GdI ₂	643	0.0008	100	81
DyI ₂	357	0.0009	57	43
C ₂ Br ₂ La ₂	616	0.0009	67	58
Cl ₂ Mn	291	0.0009	36	49
S ₂	6	0.001	1	1
K	232	0.001	49	36
NbSe ₂	447	0.001	57	73
I ₂ Yb	403	0.001	64	49
PbS ₂ Sn	656	0.001	94	70
Cu ₂ Sr ₂	724	0.001	100	81
Se ₂ Ta	565	0.001	73	91
O ₂ Zn	331	0.001	37	61
Cl ₂ Zr	343	0.0011	43	57
AlLiTe ₂	656	0.0011	91	73
Se ₂ Ta	447	0.0011	57	73
Ba ₂ H ₂ I ₂	978	0.0011	126	79
Br ₂ V	447	0.0011	57	73
Cd ₂ I ₃	577	0.0012	73	57
Cl ₂ N ₂ Ti ₂	356	0.0012	35	36
Ba ₂ Cu ₂	452	0.0012	64	49
AsI ₂ La ₂	577	0.0012	73	57
H ₂ MnO ₂	116	0.0013	9	16

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

SnPbS₂ (Pm)

Structural and electronic properties

	Formula	SnPbS ₂
	Spacegroup	Pm
	Prototype	PbS ₂ Sn
	Parent 3D	Pb ₂ S ₄ Sn ₂
	Source DB	ICSD
	DB ID	156131
DF2-C09	Binding energy [meV/ Å²]	39.03
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	1.31

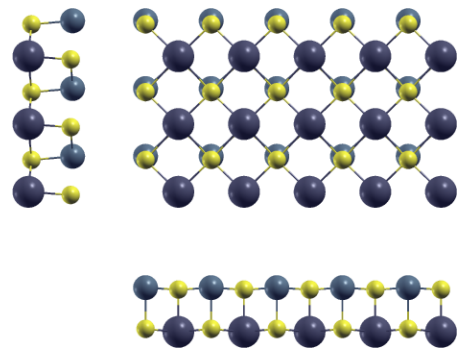


Band structure: Electronic band structure of SnPbS₂ (Pm) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of SnPbS₂ (Pm) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		0.00000000	-4.15643372	0.00000000
a₂		4.28535467	0.00000000	0.00000000
a₃		0.00000000	0.00000000	17.92145297
		x [Å]	y [Å]	z [Å]
●	Sn	3.68274503	0.00000000	-1.37979996
●	Pb	1.43769639	-2.07821686	1.41554830
●	S	1.24037037	-2.07821686	-1.26043362
●	S	3.45674470	0.00000000	1.22468528



Orthographic projections: views of SnPbS₂ (Pm) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.0134	1	1
K	5	0.1449	1	1
AgTl	6	0.0254	1	1
Ag ₂	6	0.15	1	1
Sb ₂	6	0.1124	1	1
CaCl	6	0.5747	1	1
Nd	7	0.1559	1	3
Ba ₂ Pt	7	0.1497	1	1
CaI ₂	7	0.137	1	1
Br ₂ Cu	7	0.328	1	1
Ca ₂ Si	7	0.1541	1	1
I ₂ Yb	7	0.135	1	1
AuTe ₂	7	0.1098	1	1
Cl ₂ Zn	7	0.2033	1	1
I ₂ Zn	7	0.1112	1	1
Ba ₂ Hg	7	0.0082	1	1
I ₂ Tm	7	0.1361	1	1
I ₂ Pb	7	0.1515	1	1
GeS ₂	7	0.5401	1	1
MnSe ₂	7	0.5744	1	1
DyI ₂	7	0.1394	1	1
F ₂ Ni	7	0.6061	1	1
PtTe ₂	7	0.1097	1	1
F ₂ Zn	7	0.2354	1	1
Ba ₂ Cd	7	0.0073	1	1
Bi ₂ Te ₂	8	0.1676	1	1
Fe ₂ Te ₂	8	0.2246	1	1
Li ₂ Tl ₂	8	0.1976	1	1
Bi ₂ In ₂	8	0.3637	1	1
Ca ₂ Cl ₂	8	0.2251	1	1
InSe	8	0.9356	1	2
Cu ₂ I ₂	8	0.0156	1	1
Bi ₂ Mn ₂	8	0.1555	1	1
Br ₂ Er ₂	8	0.11	1	1
Cu ₂ S ₂	8	0.2314	1	1
Au ₂ Br ₂	8	0.011	1	1
Br ₂ Cu ₂	8	0.2337	1	1
Fe ₂ Se ₂	8	0.6045	1	1
Cu ₂ Te ₂	8	0.2061	1	1
AgBrO ₂	8	0.1335	1	1
Cl ₂ La ₂	8	0.1105	1	1
As ₄	8	0.3385	1	1
Br ₂ Gd ₂	8	0.1101	1	1
O ₂ Sn ₂	8	0.2321	1	1
P ₂ Rh ₂	8	0.2306	1	1
Fe ₂ S ₂	8	0.5687	1	1
F ₂ Tl ₂	8	0.2308	1	1
Br ₂ Ho ₂	8	0.1095	1	1
Au ₂ I ₂	8	0.0272	1	1
Sb ₂ Te ₂	8	0.1528	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

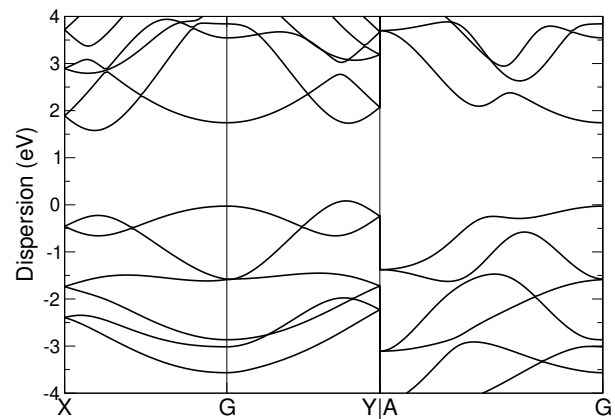
Formula	N° atoms	strain	cell size 1	cell size 2
NbS ₂	782	0.0005	83	150
Sn	296	0.0005	49	100
Br ₂ Ho ₂	708	0.0005	78	99
H ₂ Li ₂ O ₂	372	0.0006	30	42
S ₂ Ta	782	0.0006	83	150
LiNbS ₂	932	0.0007	83	150
As ₂ Fe ₂	488	0.0007	50	72
Hf ₂ Se ₂ Si ₂	632	0.0007	50	72
C ₂ Cl ₂ Y ₂	888	0.0007	72	100
Ga ₂ Se ₂	848	0.0008	86	126
As ₂ Fe ₂ Li ₂	742	0.0008	64	81
Br ₂ H ₂ Yb ₂	742	0.0008	64	81
Ge ₂ Hf ₂ Te ₂	732	0.0008	63	80
Cl ₂ Zn	873	0.0009	111	143
NS ₂ Ta	460	0.0009	35	80
ClNZr	185	0.0009	20	35
Cl ₂ Y ₂	848	0.001	86	126
K ₂ PdSe ₂	280	0.001	45	20
Fe ₂ SeTe	580	0.001	64	81
Cl ₂ OOs	872	0.001	94	124
P ₂ Sn ₂	656	0.001	70	94
Ag ₂ F ₄	686	0.001	92	53
F ₂ Se ₂ Yb ₂	844	0.001	70	94
FHOZn	144	0.0011	12	24
CrSe ₂	120	0.0011	12	24
CoI ₂	588	0.0011	72	100
I ₂ Ti	588	0.0011	72	100
S ₂ Zn ₂	656	0.0011	70	94
AuTe ₂	327	0.0012	42	53
AsSb	488	0.0012	72	100
H ₂ Li ₂ Pt	901	0.0012	69	125
Br ₂ Er ₂	380	0.0012	42	53
Ni ₂ SbTe ₂	750	0.0012	70	94
Cl ₂ Y ₂	788	0.0012	72	100
PtTe ₂	327	0.0013	42	53
GeS ₂	416	0.0013	50	72
Se ₂ Ta ₄	642	0.0013	48	75
Ca ₂ O ₂	292	0.0013	28	45
As ₂ Co ₂ Li ₂	732	0.0013	63	80
S ₂	468	0.0013	70	94
Se ₂ Sn	588	0.0014	72	100
As ₂ Fe ₂ Li ₂	732	0.0014	63	80
C	110	0.0014	10	70
I ₂ S ₂ Tl ₂	570	0.0014	48	63
Br ₂ H ₂ Yb ₂	732	0.0014	63	80
Cu ₂ Se ₂	444	0.0014	48	63
Cl ₂ ORu	376	0.0014	40	54
I ₂ N ₂ Zr ₂	76	0.0014	7	8
K ₂ O ₂ Tl ₂	204	0.0014	24	18
F ₂ Ni	381	0.0014	48	63

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

SnS (P1 (1))

Structural and electronic properties

	Formula	SnS
	Spacegroup	P1 (1)
	Prototype	FeSe
	Parent 3D	Sn ₄ S ₄
	Source DB	COD
	DB ID	9008785
DF2-C09	Binding energy [meV/ Å²]	36.2
RVV10	Binding energy [meV/ Å²]	36.52
	Band gap (PBE) [eV]	1.49

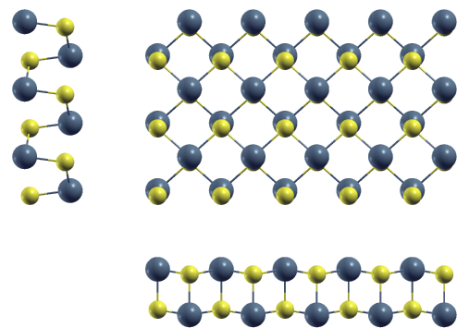


Band structure: Electronic band structure of SnS (P1 (1)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of SnS (P1 (1)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		4.05488851	−0.00004431	0.00000000
a₂		−0.00002695	4.29903287	0.00000000
a₃		0.00000000	0.00000000	22.92226541
		x [Å]	y [Å]	z [Å]
●	Sn	1.01428697	0.46973889	10.01048709
●	Sn	3.04071446	2.62130075	12.91174774
●	S	3.04190474	2.27872580	10.34100791
●	S	1.01323725	0.13138501	12.58133568



Orthographic projections: views of SnS (P1 (1)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.0223	1	1
Bi ₂	6	0.1265	1	1
PbTe	6	0.124	1	1
CdI ₂	7	0.1251	1	1
Nd	7	0.162	1	3
Br ₂ Ca	7	0.1258	1	1
Br ₂ Cu	7	0.1022	1	1
BiClTe	7	0.1253	1	1
Cl ₂ Zn	7	0.2218	1	1
HgI ₂	7	0.3358	1	1
BiBrTe	7	0.1289	1	1
GeI ₂	7	0.1241	1	1
GdI ₂	7	0.1309	1	1
CNNa	7	0.2303	1	1
CdI ₂	7	0.1248	1	1
F ₂ Zn	7	0.2471	1	1
I ₂ Pr	7	0.1253	1	1
Bi ₂ Te ₂	8	0.1743	1	1
Fe ₂ Te ₂	8	0.2356	1	1
Li ₂ Tl ₂	8	0.2055	1	1
Bi ₂ In ₂	8	0.3683	1	1
Ca ₂ Cl ₂	8	0.2361	1	1
Cu ₂ I ₂	8	0.016	1	1
Cu ₂ Sr ₂	8	0.1296	1	1
Cl ₂ OOs	8	0.1956	1	1
LiMnTe ₂	8	0.1243	1	1
O ₂ Sn ₂	8	0.2103	1	1
Cu ₂ S ₂	8	0.2428	1	1
Au ₂ Br ₂	8	0.019	1	1
AlLiTe ₂	8	0.1328	1	1
Br ₂ Cu ₂	8	0.2453	1	1
Cl ₂ ORu	8	0.6001	1	1
N ₃ Na	8	0.0545	1	1
Cu ₂ Te ₂	8	0.2249	1	1
O ₂ Pb ₂	8	0.0178	1	1
Ge ₂ S ₂	8	0.0301	1	1
O ₂ Sn ₂	8	0.2436	1	1
P ₂ Rh ₂	8	0.242	1	1
F ₂ Tl ₂	8	0.2421	1	1
BN	8	0.1466	1	2
Au ₂ I ₂	8	0.0344	1	1
Ge ₂ Se ₂	8	0.0095	1	1
Ag ₂ Te ₂	8	0.2436	1	1
As ₂ Ru ₂	8	0.2364	1	1
Bi ₂ O ₂	8	0.017	1	1
C ₂	8	0.1434	1	2
Fe ₂ SeTe	8	0.2287	1	1
Ag ₂ I ₂	8	0.3378	1	1
Se ₂ Sn ₂	8	0.0203	1	1
Br ₂ CsF	8	0.3642	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

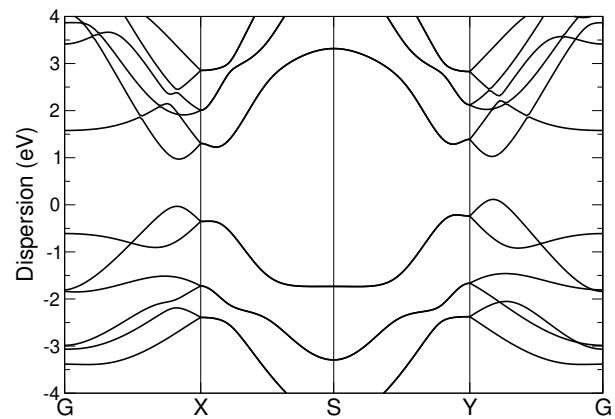
Formula	N° atoms	strain	cell size 1	cell size 2
NbSe ₂	378	0.0001	42	70
AsSe ₂	378	0.0002	42	70
Dy ₂ I ₂ S ₂	994	0.0004	100	99
Hf ₂ Se ₂ Si ₂	734	0.0004	59	83
Nd	81	0.0005	12	33
Hg ₃ N ₂	511	0.0005	84	35
Ga ₂ S ₃	840	0.0006	70	112
AsI ₂ La ₂	879	0.0006	96	99
Cd ₂ I ₃	879	0.0006	96	99
N ₄	380	0.0006	32	63
AlH ₄ Na	678	0.0006	78	61
MoSe ₂	342	0.0007	36	66
Br ₂ Hf ₂	448	0.0007	42	70
DyI ₂	697	0.0007	100	99
As ₂ Fe ₂	568	0.0008	59	83
Ca ₂ Cl ₂	872	0.0008	94	124
Se ₂ W	342	0.0008	36	66
BiBrTe	390	0.0008	54	58
As ₂ Co ₂	872	0.0008	94	124
C ₄ Ca ₂	732	0.0008	72	74
Cu ₂ Se ₂	556	0.001	61	78
Br ₂ O ₂ V ₂	444	0.001	36	50
I ₂ S ₂ Tb ₂	994	0.0011	100	99
Gd ₂ I ₂ S ₂	524	0.0011	53	52
BrNZr	378	0.0011	42	70
Se ₂ Ta	378	0.0011	42	70
I ₂ S ₂ Tl ₂	712	0.0012	61	78
Tl	210	0.0012	36	66
Ge ₂ I ₂ La ₂	526	0.0012	52	53
NbSe ₂	378	0.0012	42	70
I ₂ S ₂ Tb ₂	524	0.0013	53	52
Br ₂ Ca ₃ Si	524	0.0013	53	52
Sb ₂ Te ₃	574	0.0014	61	66
Cu ₄ Te ₂	564	0.0014	54	58
Cu ₂ Sr ₂	448	0.0014	54	58
Hf ₃ Te ₂	634	0.0015	61	78
F ₂ Ni	478	0.0015	61	78
Si ₂ Te ₂ Zr ₂	712	0.0015	61	78
CuO ₂	171	0.0015	18	33
GeS ₂	485	0.0015	59	83
O ₂ Sn ₂	384	0.0016	40	56
AgClO ₄	456	0.0016	54	40
Cl ₂ Fe ₂ O ₂	592	0.0016	46	68
MnSe ₂	322	0.0016	40	54
Cl ₂ Ni	378	0.0017	42	70
CaCl	268	0.0017	40	54
DyI ₂	368	0.0017	53	52
Cl ₂ Rb ₂	136	0.0017	24	10
O ₂ Sn ₂	384	0.0018	40	56
Bi ₂ SeTe ₂	574	0.0018	61	66

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

SnSe (P1 (1))

Structural and electronic properties

	Formula	SnSe
	Spacegroup	P1 (1)
	Prototype	FeSe
	Parent 3D	Sn ₄ Se ₄
	Source DB	COD
	DB ID	9008786
DF2-C09	Binding energy [meV/ Å²]	35.34
RVV10	Binding energy [meV/ Å²]	35.72
	Band gap (PBE) [eV]	0.86

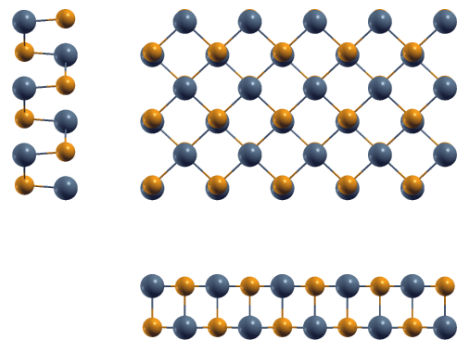


Band structure: Electronic band structure of SnSe (P1 (1)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of SnSe (P1 (1)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		4.28231716	−0.00004396	0.00000000
a₂		0.00003196	4.38199632	0.00000000
a₃		0.00000000	0.00000000	23.00657950
		x [Å]	y [Å]	z [Å]
●	Sn	3.21218968	4.00404113	12.87044108
●	Sn	1.07121773	1.81341842	10.13606196
●	Se	1.07114166	2.01407134	12.85324653
●	Se	3.21228547	4.20514670	10.15326238



Orthographic projections: views of SnSe (P1 (1)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	5	0.0056	1	1
K	5	0.1345	1	1
Na	5	0.1108	1	1
Ag ₂	6	0.1389	1	1
As ₂	6	0.1091	1	1
CaCl	6	0.536	1	1
Cl ₂ Zn	7	0.1093	1	1
MoTe ₂	7	0.1103	1	1
Nd	7	0.144	1	3
Ba ₂ Pt	7	0.1386	1	1
CaI ₂	7	0.1278	1	1
Te ₂ V	7	0.1099	1	1
I ₂ Pr	7	0.2239	1	1
Ca ₂ Si	7	0.1425	1	1
Br ₂ Co	7	0.1092	1	1
Ca ₂ N	7	0.109	1	1
Cl ₂ Zn	7	0.5772	1	1
Br ₂ Mn	7	0.1095	1	1
CrTe ₂	7	0.1121	1	1
PtS ₂	7	0.1106	1	1
CNRb	7	0.302	1	1
CdClO	7	0.11	1	1
Se ₂ Ti	7	0.1112	1	1
Br ₂ Ti	7	0.1122	1	1
Te ₂ W	7	0.1102	1	1
I ₂ Nd	7	0.2251	1	1
I ₂ Tm	7	0.127	1	1
I ₂ Pb	7	0.1402	1	1
OTl ₂	7	0.1099	1	1
Br ₂ Fe	7	0.1092	1	1
MnSe ₂	7	0.5357	1	1
Br ₂ Cr	7	0.1122	1	1
DyI ₂	7	0.1298	1	1
CeI ₂	7	0.223	1	1
F ₂ Ni	7	0.5655	1	1
I ₂ La	7	0.2309	1	1
F ₂ Zn	7	0.2193	1	1
Ba ₂ Cd	7	0.0144	1	1
Bi ₂ Te ₂	8	0.1544	1	1
Fe ₂ Te ₂	8	0.6115	1	1
Li ₂ Tl ₂	8	0.1815	1	1
Ca ₂ Cl ₂	8	0.2037	1	1
NS ₂ Zr	8	0.1107	1	1
Ir ₂ P ₂	8	0.2248	1	1
Ag ₂ Br ₂	8	0.2315	1	1
S ₂ Sn ₂	8	0.0183	1	1
Cu ₂ S ₂	8	0.2092	1	1
Au ₂ Br ₂	8	0.0109	1	1
Ge ₂ Te ₂	8	0.0077	1	1
Br ₂ Cu ₂	8	0.2178	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

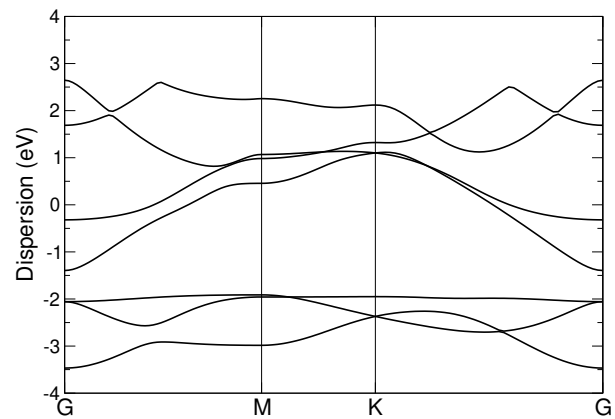
Formula	N° atoms	strain	cell size 1	cell size 2
Ni ₂ Se ₂	724	0.0002	81	100
CeI ₂	624	0.0002	81	100
Cl ₂ Zn	582	0.0002	72	98
Br ₂ Eu ₂ O ₂	924	0.0003	81	100
Ba ₂ N	599	0.0004	74	101
Br ₂ Ca ₃ Si	814	0.0005	79	83
Gd ₂ I ₂ S ₂	814	0.0005	79	83
Hf ₂ I ₂ N ₂	810	0.0005	60	95
CdClHO	620	0.0005	60	95
Cu ₃ Se ₃	902	0.0005	74	101
Ba ₂ Pt	528	0.0006	75	76
Br ₂ Mn	398	0.0006	44	74
Cl ₂ La ₂	668	0.0006	72	95
TaTe ₂	525	0.0006	60	95
Ca ₂ Cl ₂ H ₂	876	0.0007	72	98
Br ₂ Lu ₂ O ₂	514	0.0007	43	57
As ₂ Fe ₂ Li ₂	504	0.0007	42	56
Br ₂ H ₂ Yb ₂	504	0.0007	42	56
Ag ₂	452	0.0007	75	76
Br ₂ Cr ₂ O ₂	868	0.0008	67	100
Ge ₂ Te ₂ Zr ₂	514	0.0008	43	57
Se ₂ Zr	204	0.0008	24	36
KS ₂ Ti	472	0.0009	44	74
As ₂ Sn ₂	668	0.0009	72	95
Ge ₂ S ₂	52	0.0009	6	7
Cl ₂ Er ₂ O ₂	312	0.0009	24	36
I ₂ V	204	0.0009	24	36
I ₂ Pr	624	0.0009	81	100
Fe ₂ SeTe	400	0.0009	43	57
AgNO ₂	540	0.0009	63	72
Fe ₂ SeTe	392	0.0009	42	56
Cl ₂ OOs	584	0.0009	61	85
CrTe ₂	528	0.001	57	100
I ₂ Zn	656	0.001	83	108
Li ₂ Tl ₂	148	0.001	20	17
H ₂ Li ₂ Pd	490	0.001	35	70
Cl ₂ Sc ₂	628	0.0011	57	100
SiTe ₂	204	0.0011	24	36
AuTe ₂	511	0.0011	64	85
AsSn ₂	525	0.0011	60	95
O ₂ Sn ₂	580	0.0011	64	81
SbSe ₂ Tl	236	0.0012	32	27
Cl ₂ Ho ₂ O ₂	312	0.0012	24	36
Cu ₂ S ₂	580	0.0012	64	81
C ₂ Br ₂ La ₂	576	0.0012	51	62
Hf ₃ Te ₂	778	0.0012	72	98
Br ₂ O ₂ Sc ₂	606	0.0012	51	67
Br ₂ O ₂ Y ₂	742	0.0012	64	81
F ₂ Tl ₂	572	0.0012	63	80
C ₂ I ₂ Y ₂	606	0.0012	51	67

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Sr₂N (P3m1 (156))

Structural and electronic properties

	Formula	Sr ₂ N
	Spacegroup	P3m1 (156)
	Prototype	CdI2
	Parent 3D	Sr ₂ N
	Source DB	ICSD
	DB ID	69016
DF2-C09	Binding energy [meV/ Å²]	57.22
RVV10	Binding energy [meV/ Å²]	57.1
	Band gap (PBE) [eV]	0.0

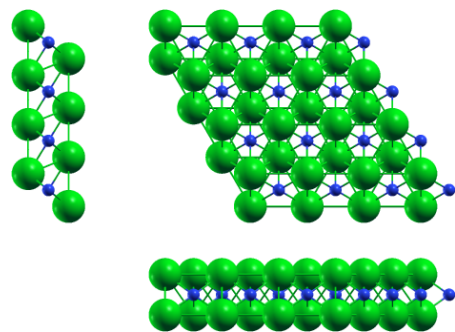


Band structure: Electronic band structure of Sr₂N (P3m1 (156)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Sr₂N (P3m1 (156)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.85694209	0.00000000	0.00000000
a₂		-1.92847105	3.34020983	0.00000000
a₃		0.00000000	0.00000000	22.76196333
		x [Å]	y [Å]	z [Å]
●	Sr	0.00000000	2.22680656	12.75556913
●	Sr	0.00000000	0.00000000	10.00638820
•	N	1.92847105	1.11340328	11.38098766



Orthographic projections: views of Sr₂N (P3m1 (156)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	4	0.4245	1	1
Tl	4	1.5624	1	1
InSe	5	0.4501	1	1
HgO	5	0.112	1	1
AsSb	5	0.0016	1	1
Bi ₂	5	0.4645	1	1
GeTe	5	0.0045	1	1
S ₂	5	0.0061	1	1
P ₂	5	1.5247	1	1
PbTe	5	0.4545	1	1
CaCl	5	0.1421	1	1
IrTe ₂	6	0.0054	1	1
CdCl ₂	6	0.0034	1	1
Cl ₂ Mn	6	0.2469	1	1
CdI ₂	6	0.4587	1	1
AgTe ₂	6	0.4313	1	1
MoSe ₂	6	1.557	1	1
ReSe ₂	6	0.2647	1	1
S ₂ Ta	6	0.2496	1	1
Br ₂ Ca	6	0.4618	1	1
CaI ₂	6	2.98	1	1
InSe ₂	6	0.0038	1	1
GeTe ₂	6	0.0024	1	1
SiTe ₂	6	0.0076	1	1
I ₂ Mn	6	0.0035	1	1
PbS ₂	6	0.0042	1	1
BiClTe	6	0.4596	1	1
Cl ₂ Ti	6	1.5258	1	1
LiO ₂	6	0.0657	1	1
FeI ₂	6	0.0013	1	1
I ₂ Ni	6	0.0026	1	1
S ₂ Ti	6	0.2562	1	1
NbS ₂	6	0.249	1	1
CrI ₂	6	0.0009	1	1
BiBrTe	6	0.4736	1	1
Bi ₂ Pd	6	0.1159	1	1
Cl ₂ Ni	6	0.266	1	1
Cl ₂ Co	6	0.2558	1	1
CrTe ₂	6	0.2749	1	1
Br ₂ V	6	0.2635	1	1
ClNZr	6	0.2606	1	1
Cl ₂ Fe	6	0.2548	1	1
Br ₂ Ti	6	0.274	1	1
AsSe ₂	6	0.2681	1	1
NiTe ₂	6	0.0082	1	1
I ₂ Tm	6	2.9644	1	1
I ₂ V	6	0.0063	1	1
GeI ₂	6	0.455	1	1
Se ₂ Zr	6	0.0072	1	1
BiTe	6	2.8457	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

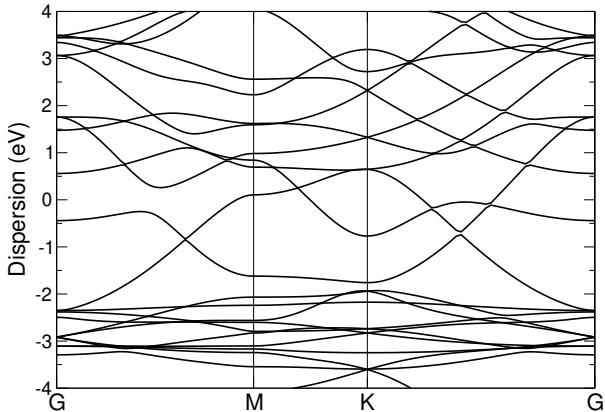
Formula	N° atoms	strain	cell size 1	cell size 2
Cl ₂ V	183	0.0001	25	36
Cu ₂ Sr ₂	499	0.0001	81	64
Pd ₂ S ₄	471	0.0001	85	36
CdO ₂	390	0.0001	57	73
Ag ₂	158	0.0001	36	25
Cl ₂ Zr	390	0.0001	57	73
LiOS ₂ Ti	414	0.0001	43	57
Ba ₂ Pt	183	0.0002	36	25
F ₄ Sn	435	0.0002	65	48
NbS ₂	339	0.0002	49	64
Cl ₂ Co	390	0.0002	57	73
NS ₂ Ta	355	0.0002	37	61
Br ₂ Ca	543	0.0002	100	81
Se ₂ Sn	6	0.0002	1	1
S ₂ Ta	339	0.0002	49	64
ReSe ₂	492	0.0003	73	91
Br ₂ Ca ₃ Si	315	0.0003	43	31
Cl ₂ Cr ₂ O ₂	306	0.0003	32	35
LiNbS ₂	403	0.0003	49	64
AsSe ₂	543	0.0003	81	100
Bi ₂ SeTe ₂	638	0.0004	91	73
Cl ₂ Y ₂	8	0.0004	1	1
Cl ₂ Fe	390	0.0005	57	73
Nd	196	0.0005	39	79
I ₂ Pr	543	0.0005	100	81
Br ₂ V	492	0.0006	73	91
S ₂ Ti	390	0.0006	57	73
C ₂ Cl ₂ Y ₂	522	0.0006	58	58
Ga ₂ I ₂ Tb ₂	786	0.0006	100	81
NbSe ₂	543	0.0006	81	100
Se ₂ Ta	543	0.0006	81	100
BiClTe	543	0.0006	100	81
Ge ₂ I ₂ La ₂	429	0.0007	57	43
NbSe ₂	543	0.0007	81	100
Ba ₂ Hg	339	0.0007	65	48
Ag ₂ F ₄	792	0.0007	144	60
Sb ₂ Te ₃	638	0.0007	91	73
Cl ₂ H ₂ Zr ₂	471	0.0008	43	57
O ₂ Sn ₂	357	0.0008	55	48
I ₂ Pr ₂ S ₂	258	0.0008	36	25
I ₂ Ti	6	0.0008	1	1
Gd ₂ GeI ₂	705	0.0009	100	81
Ga ₂ Gd ₂ I ₂	786	0.0009	100	81
Dy ₂ I ₂ S ₂	363	0.0009	49	36
GdI ₂	390	0.0009	73	57
CrI ₂	6	0.0009	1	1
ClNZr	435	0.0009	64	81
N ₄	212	0.0009	24	35
BiBrTe	435	0.001	81	64
Br ₂ Ca ₃ Si	483	0.001	65	48

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

SrCu (P6/mmm (191))

Structural and electronic properties

	Formula	SrCu
	Spacegroup	P6/mmm (191)
	Prototype	CuSr
	Parent 3D	Sr ₄ Cu ₄
	Source DB	ICSD
	DB ID	629306
DF2-C09	Binding energy [meV/ Å²]	44.63
RVV10	Binding energy [meV/ Å²]	46.51
	Band gap (PBE) [eV]	0.0

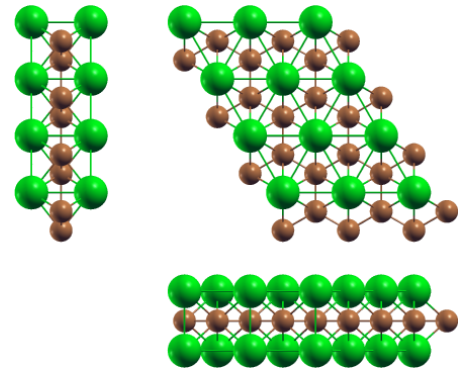


Band structure: Electronic band structure of SrCu (P6/mmm (191)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of SrCu (P6/mmm (191)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.33961415	0.00000000	0.00000000
a₂	−2.16980708	3.75821610	0.00000000
a₃	0.00000000	0.00000000	24.04327184
	x [Å]	y [Å]	z [Å]
● Sr	0.00000000	2.50547740	13.98484070
● Sr	0.00000000	2.50547740	10.05843114
● Cu	0.00000000	0.00000000	12.02163592
● Cu	2.16980708	1.25273870	12.02163592



Orthographic projections: views of SrCu (P6/mmm (191)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
AsSb	6	0.257	1	1
Bi ₂	6	0.0046	1	1
GeTe	6	0.2655	1	1
As ₂	6	1.4473	1	1
S ₂	6	0.2677	1	1
PbTe	6	0.0085	1	1
IrTe ₂	7	0.2668	1	1
CdCl ₂	7	0.2639	1	1
CdI ₂	7	0.0068	1	1
S ₂ Ta	7	4.8792	1	1
Br ₂ Zn	7	1.5852	1	1
Br ₂ Ca	7	0.0056	1	1
InSe ₂	7	0.2645	1	1
AsSn ₂	7	1.5353	1	1
GeTe ₂	7	0.2625	1	1
SiTe ₂	7	0.2488	1	1
I ₂ Pr	7	0.1287	1	1
I ₂ Mn	7	0.2641	1	1
Br ₂ Cu	7	0.6817	1	1
NSr ₂	7	0.2592	1	1
PbS ₂	7	0.2535	1	1
BiClTe	7	0.0065	1	1
Cl ₂ Zn	7	0.1151	1	1
FeI ₂	7	0.261	1	1
I ₂ Ni	7	0.2628	1	1
Te ₂ Ti	7	1.5874	1	1
NbS ₂	7	4.8694	1	1
CrI ₂	7	0.2604	1	1
BiBrTe	7	0.001	1	1
RhTe ₂	7	1.5556	1	1
I ₂ Nd	7	0.1294	1	1
NiTe ₂	7	0.248	1	1
Cl ₂ Cu	7	0.0711	1	1
I ₂ V	7	0.2506	1	1
GeI ₂	7	0.0082	1	1
Se ₂ Zr	7	0.2493	1	1
PtSe ₂	7	1.54	1	1
BiTe	7	0.0056	1	1
CoI ₂	7	0.2576	1	1
CeI ₂	7	0.1282	1	1
Br ₂ Mg	7	0.2608	1	1
I ₂ Ti	7	0.258	1	1
GdI ₂	7	0.0018	1	1
F ₂ Ni	7	0.1134	1	1
I ₂ La	7	0.1328	1	1
CdI ₂	7	0.0072	1	1
Se ₂ Sn	7	0.2589	1	1
F ₂ Zn	7	0.126	1	1
Gd	7	0.1757	1	3
I ₂ Pr	7	0.0064	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

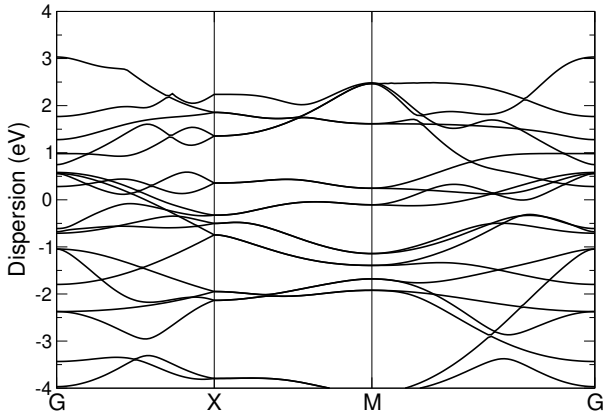
Formula	N° atoms	strain	cell size 1	cell size 2
Cl ₂ Er ₂ H ₂	838	0.0	73	91
NSr ₂	499	0.0001	64	81
Se ₂ Zr	388	0.0001	49	64
S ₂	524	0.0001	81	100
Cl ₂ Er ₂ O ₂	580	0.0001	49	64
InSe ₂	565	0.0001	73	91
Br ₂ Hf ₂ N ₂	316	0.0001	25	36
I ₂ Mn	565	0.0002	73	91
S ₂ Ta	439	0.0002	49	81
Br ₂ Pr ₂	400	0.0002	43	57
Ni ₂ SbTe ₂	824	0.0002	81	100
LiNbS ₂	520	0.0003	49	81
AsSe ₂	139	0.0003	16	25
NbS ₂	439	0.0003	49	81
CdCl ₂	565	0.0003	73	91
Se ₂ Sn	499	0.0003	64	81
C ₂ F ₂	136	0.0003	9	25
SiTe ₂	388	0.0003	49	64
Br ₂ Hg ₃	241	0.0004	49	9
LiNbS ₂	392	0.0004	37	61
Ga ₂ Se ₂	724	0.0004	81	100
As ₂ O ₃	180	0.0004	25	16
PTe ₂ Zr ₂	593	0.0004	57	73
ReS ₂	247	0.0004	25	49
H ₂ Si ₂	656	0.0004	73	91
CdClHO	340	0.0004	36	49
S ₂ Ta	331	0.0004	37	61
Ca ₂ N	208	0.0005	25	36
Cl ₂ Y ₂	661	0.0005	64	81
Ni ₂ Te ₂	656	0.0005	73	91
NbSe ₂	139	0.0005	16	25
IrTe ₂	624	0.0006	81	100
CoH ₂ O ₂	345	0.0006	25	49
O ₂ Zn	496	0.0006	49	100
F ₂ Se ₂ Y ₂	802	0.0006	91	73
HfSe ₂	343	0.0007	43	57
Se ₂ Ta	139	0.0007	16	25
Te ₂ Ti	343	0.0007	43	57
Cl ₂ N ₂ Zr ₂	316	0.0007	25	36
Cl ₂ Hf ₂	392	0.0008	37	61
NbSe ₂	139	0.0008	16	25
Ag ₂ F ₄	746	0.0008	104	55
GeTe	474	0.0008	73	91
CrI ₂	499	0.0008	64	81
Sn	411	0.0009	70	131
NbS ₂	331	0.0009	37	61
I ₂ Ti	499	0.0009	64	81
I ₂ La ₂ P	9	0.0009	1	1
CaH ₂ O ₂	280	0.0009	25	36
Nd	164	0.0009	25	64

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

SrMnGe (P4/nmm (129))

Structural and electronic properties

	Formula	SrMnGe
	Spacegroup	P4/nmm (129)
	Prototype	PbClF
	Parent 3D	Ge ₂ Mn ₂ Sr ₂
	Source DB	COD
	DB ID	1539720
DF2-C09	Binding energy [meV/ Å²]	46.9
RVV10	Binding energy [meV/ Å²]	50.41
	Band gap (PBE) [eV]	0.0

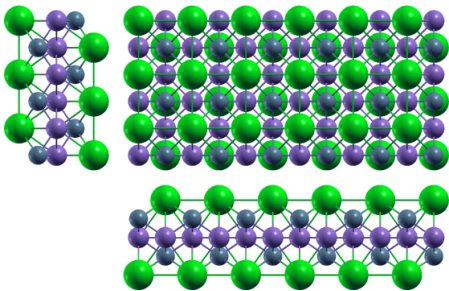


Band structure: Electronic band structure of SrMnGe (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of SrMnGe (P4/nmm (129)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.97079074	0.00000000	0.00000000
a₂		0.00000000	3.97079074	0.00000000
a₃		0.00000000	0.00000000	25.59356211
		x [Å]	y [Å]	z [Å]
●	Sr	0.00000000	1.98539537	15.55651498
●	Ge	1.98539537	0.00000000	14.17369469
●	Sr	1.98539537	0.00000000	10.03704713
●	Mn	1.98539537	1.98539537	12.79678105
●	Mn	0.00000000	0.00000000	12.79678105
●	Ge	0.00000000	1.98539537	11.41986742



Orthographic projections: views of SrMnGe (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	7	0.1746	1	1
InSe	8	0.1388	1	1
Bi ₂	8	0.1438	1	1
AgTl	8	0.0162	1	1
Ag ₂	8	0.1812	1	1
LiO	8	0.1115	1	1
P ₂	8	0.1097	1	1
PbTe	8	0.1403	1	1
I ₂ Mg	9	0.1308	1	1
CdI ₂	9	0.1418	1	1
Nd	9	0.1888	1	3
MoSe ₂	9	0.1088	1	1
Ba ₂ Pt	9	0.1809	1	1
Br ₂ Zn	9	0.1085	1	1
Br ₂ Ca	9	0.1429	1	1
CaI ₂	9	0.1641	1	1
I ₂ Pr	9	0.0076	1	1
Br ₂ La	9	0.1311	1	1
Br ₂ Cu	9	0.1024	1	1
Ca ₂ Si	9	0.1865	1	1
I ₂ Yb	9	0.1614	1	1
BiClTe	9	0.1421	1	1
Cl ₂ Ti	9	0.1097	1	1
BrCdI	9	0.1332	1	1
HgI ₂	9	0.3975	1	1
Te ₂ Ti	9	0.1086	1	1
BaF ₂	9	0.1357	1	1
BiBrTe	9	0.1471	1	1
GeI ₂	9	0.1295	1	1
AsKSn	9	0.1346	1	1
PbTe ₂	9	0.1324	1	1
I ₂ Nd	9	0.0067	1	1
Cl ₂ Cu	9	0.0972	1	1
I ₂ Tm	9	0.1628	1	1
GeI ₂	9	0.1405	1	1
I ₂ Pb	9	0.1831	1	1
STl ₂	9	0.1365	1	1
BiTe	9	0.1534	1	1
GeS ₂	9	0.2097	1	1
DyI ₂	9	0.1673	1	1
CeI ₂	9	0.0084	1	1
Se ₂ Yb	9	0.1297	1	1
BiTe ₂	9	0.1299	1	1
GdI ₂	9	0.1498	1	1
I ₂ La	9	0.002	1	1
CdI ₂	9	0.1414	1	1
I ₂ Pr	9	0.1422	1	1
HfSe ₂	9	0.1086	1	1
Se ₂ W	9	0.1088	1	1
Bi ₂ Te ₂	10	0.7683	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

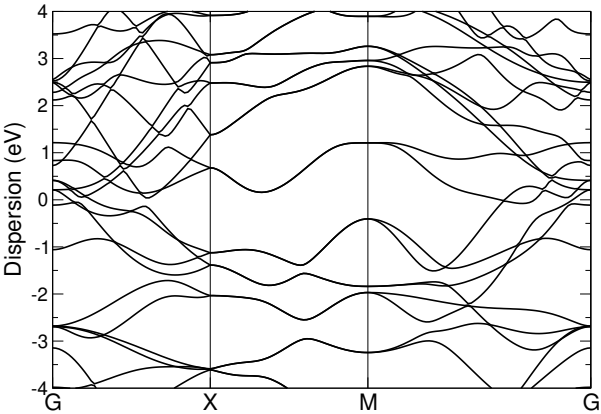
Formula	N° atoms	strain	cell size 1	cell size 2
AgClO ₄	612	0.0001	61	41
I ₂ N ₂ Ti ₂	102	0.0001	8	9
Cu ₂ Rb ₂ Te ₂	510	0.0001	49	36
Bi ₂ In ₂	438	0.0002	49	36
H ₄ Ti	833	0.0002	58	97
Cl ₄ Mn	815	0.0003	85	61
Ag ₂ K ₂ Se ₂	882	0.0003	82	65
As ₂ Cd ₂ K ₂	678	0.0003	64	49
H ₂ Li ₂ Pd	833	0.0003	58	97
Bi ₂ Pd	258	0.0004	25	36
NbTe ₂	483	0.0004	48	65
Ag ₂ K ₂ Se ₂	870	0.0005	81	64
In	70	0.0005	9	16
Ba ₂ F ₂ I ₂	690	0.0006	65	50
Ag ₂ K ₂ Te ₂	366	0.0006	36	25
Pb ₂ Se ₂	602	0.0006	65	53
Br ₂ OV	782	0.0006	71	89
S ₂ Zr	483	0.0006	48	65
Se ₂ Ti	840	0.0006	81	118
Br ₂ Zr ₂	958	0.0007	81	118
CBr ₂ Lu ₂	613	0.0008	48	65
As ₂ Ir ₂	10	0.0009	1	1
Fe ₂ S ₂	896	0.0009	82	101
Br ₂ N ₂ Zr ₂	678	0.0009	48	65
S ₂ Sn	483	0.0009	48	65
Bi ₂ Se ₂	86	0.0009	9	8
O ₄ PTl	690	0.0009	65	50
Bi ₂ Se ₄	318	0.001	36	17
AgTe ₂	171	0.001	16	25
LiNbS ₂	978	0.0011	79	126
Br ₂ O ₂ Pr ₂	12	0.0011	1	1
S ₂ Ta	852	0.0011	79	126
HgI ₂	678	0.0011	81	64
Br ₂ O ₂ Sc ₂	114	0.0011	9	10
Cu ₂ F ₄	150	0.0011	16	9
Cl ₂ S ₂ Tl ₂	246	0.0012	25	16
CNRb	516	0.0012	64	44
CrS ₂	237	0.0012	20	39
Ho ₂ S ₂	866	0.0012	85	89
Cl ₂ Er ₂ S ₂	42	0.0012	4	3
Br ₂ Lu ₂ S ₂	42	0.0013	4	3
Br ₂ Lu ₂ S ₂	42	0.0013	4	3
NbS ₂	852	0.0013	79	126
O ₄ PSn	678	0.0013	64	49
P ₄	354	0.0014	35	36
PSn ₂	483	0.0014	48	65
Fe ₂ S ₂	886	0.0014	81	100
O ₂ Sn ₂	840	0.0014	76	96
Hf ₂ Se ₂ Si ₂	870	0.0014	64	81
Cl ₂ Zn	531	0.0015	52	73

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Ta₂Se (P4/nmm (129))

Structural and electronic properties

Formula	Ta ₂ Se
Spacegroup	P4/nmm (129)
Prototype	SeTa ₂
Parent 3D	Ta ₄ Se ₂
Source DB	ICSD
DB ID	65739
DF2-C09 Binding energy [meV/ Å²]	33.41
RVV10 Binding energy [meV/ Å²]	37.86
Band gap (PBE) [eV]	0.0

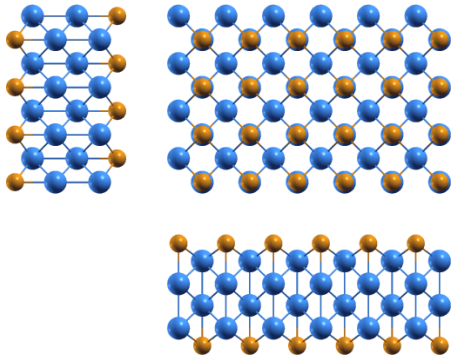


Band structure: Electronic band structure of Ta₂Se (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Ta₂Se (P4/nmm (129)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.38413406	0.00000000	0.00000000
a₂		0.00000000	3.38413406	0.00000000
a₃		0.00000000	0.00000000	27.34365722
		x [Å]	y [Å]	z [Å]
●	Ta	1.69206703	0.00000000	11.27782081
●	Ta	0.00000000	1.69206703	12.90504145
●	Se	0.00000000	1.69206703	10.02728905
●	Ta	0.00000000	1.69206703	16.06583641
●	Ta	1.69206703	0.00000000	14.43861577
●	Se	1.69206703	0.00000000	17.31636817



Orthographic projections: views of Ta₂Se (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Sn	7	0.5913	1	1
Na	7	0.1317	1	1
In	7	0.2082	1	1
AsSb	8	0.1667	1	1
GeTe	8	0.1736	1	1
As ₂	8	0.1379	1	1
S ₂	8	0.1755	1	1
Mg ₂	8	0.2212	1	1
Sb ₂	8	0.7745	1	1
IrTe ₂	9	0.1747	1	1
Cl ₂ Zn	9	0.137	1	1
CdCl ₂	9	0.1724	1	1
MoTe ₂	9	0.1334	1	1
PSn ₂	9	0.1455	1	1
Br ₂ Zn	9	0.1558	1	1
HfS ₂	9	0.1401	1	1
InSe ₂	9	0.1728	1	1
AsSn ₂	9	0.1491	1	1
GeTe ₂	9	0.1712	1	1
SiTe ₂	9	0.1601	1	1
HfTe ₂	9	0.1849	1	1
Te ₂ V	9	0.1348	1	1
I ₂ Mn	9	0.1725	1	1
CuTe ₂	9	0.1398	1	1
S ₂ Zr	9	0.1449	1	1
NSr ₂	9	0.1685	1	1
NiO ₂	9	0.1089	1	1
PbS ₂	9	0.1638	1	1
Br ₂ Co	9	0.1375	1	1
Ca ₂ N	9	0.1383	1	1
AuTe ₂	9	0.195	1	1
LiO ₂	9	0.1048	1	1
PdTe ₂	9	0.1917	1	1
FeI ₂	9	0.17	1	1
I ₂ Ni	9	0.1714	1	1
Te ₂ Ti	9	0.1561	1	1
CrI ₂	9	0.1694	1	1
Te ₂ Zn	9	0.1332	1	1
RhTe ₂	9	0.1518	1	1
GeI ₂	9	0.7894	1	1
Br ₂ Mn	9	0.136	1	1
PtS ₂	9	0.1324	1	1
CoTe ₂	9	0.1404	1	1
CdClO	9	0.1345	1	1
Ba ₂ N	9	0.1868	1	1
Se ₂ Ti	9	0.1305	1	1
Te ₂ Zr	9	0.1855	1	1
Te ₂ W	9	0.1335	1	1
NiTe ₂	9	0.1594	1	1
S ₂ Sn	9	0.1451	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

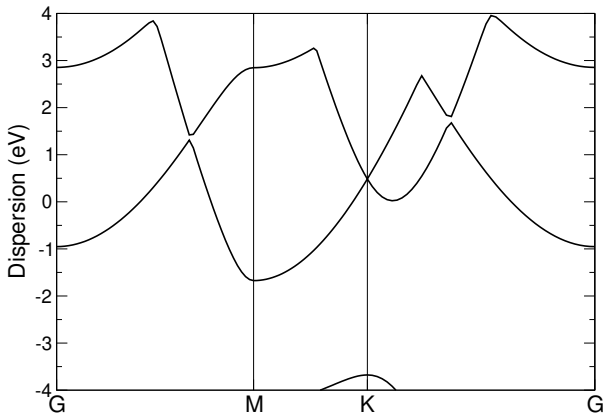
Formula	N° atoms	strain	cell size 1	cell size 2
H ₂ I ₂ Yb ₂	510	0.0	49	36
As ₂ Ru ₂	742	0.0	81	64
Br ₂ F ₂ Yb ₂	678	0.0001	64	49
Br ₂ O ₂ Tb ₂	690	0.0001	65	50
K ₂ Mn ₂ Sb ₂	876	0.0001	85	61
F ₂ I ₂ Sm ₂	366	0.0001	36	25
Br ₂ Ce ₂ O ₂	876	0.0001	85	61
Cu ₂ Na ₂ Te ₂	780	0.0001	81	49
Fe ₂ Te ₂	752	0.0001	82	65
Ca ₂ Cl ₂	742	0.0002	81	64
Nd	281	0.0002	36	65
Fe ₂ SeTe	934	0.0002	101	82
Br ₂ O ₂ Tm ₂	870	0.0002	81	64
CeI ₂	933	0.0003	113	85
O ₂ Pb ₂	316	0.0003	36	25
Br ₂ O ₂ Yb ₂	882	0.0003	82	65
C ₂ F ₂	276	0.0003	20	39
Fe ₂ SeTe	924	0.0003	100	81
Br ₂ Ca ₂ F ₂	678	0.0003	64	49
Eu ₂ I ₂ O ₂	876	0.0004	85	61
K	701	0.0004	106	65
Br ₂ Cu ₂	590	0.0005	65	50
I ₂ Pr	933	0.0005	113	85
LiO ₂	75	0.0005	8	9
Fe ₂ Te ₂	742	0.0006	81	64
Br ₂ Cu ₂	580	0.0006	64	49
BiTe	951	0.0006	118	81
I ₂ La	402	0.0006	49	36
F ₂ Zn	531	0.0007	64	49
Br ₂ Nd ₂ O ₂	510	0.0008	49	36
O ₂ Sn ₂	590	0.0008	65	50
AgClO ₄	972	0.0009	109	53
As ₂ Rh ₂	438	0.0009	49	36
AgClO ₄	894	0.0009	100	49
In	823	0.001	113	145
Ca ₂ H ₂ I ₂	876	0.001	85	61
I ₂ O ₂ Y ₂	510	0.001	49	36
Br ₂ Gd ₂ O ₂	678	0.001	64	49
O ₄ PTl	150	0.001	16	9
I ₂ O ₂ Pr ₂	366	0.001	36	25
Mg ₂	694	0.001	82	101
Br ₂ O ₂ Tb ₂	678	0.001	64	49
Ba ₂ F ₂ I ₂	150	0.001	16	9
Eu ₂ F ₂ I ₂	366	0.001	36	25
Br ₂ O ₂ Yb ₂	870	0.0011	81	64
Br ₂ La ₂ O ₂	366	0.0011	36	25
Ag ₂ Br ₂	438	0.0012	49	36
Sn	358	0.0012	49	64
N ₂ W	840	0.0012	81	118
Ho ₂ S ₂	874	0.0012	97	73

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Tl (P6/mmm (191))

Structural and electronic properties

Formula	Tl
Spacegroup	P6/mmm (191)
Prototype	In
Parent 3D	CrTlTe ₂
Source DB	ICSD
DB ID	79007
DF2-C09 Binding energy [meV/ Å ²]	41.14
RVV10 Binding energy [meV/ Å ²]	43.8
Band gap (PBE) [eV]	0.0

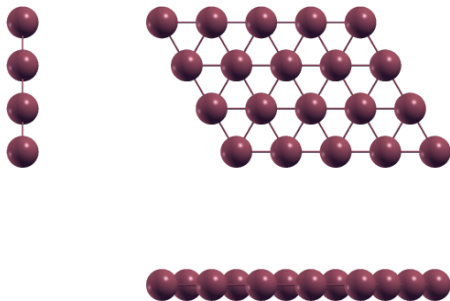


Band structure: Electronic band structure of Tl (P6/mmm (191)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Tl (P6/mmm (191)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.32104917	−0.00000000	0.00000000
a₂	−1.66052458	2.87611295	0.00000000
a₃	0.00000000	0.00000000	20.00000000
	x [Å]	y [Å]	z [Å]
● Tl	1.66052458	2.87611295	10.00000000



Orthographic projections: views of Tl (P6/mmm (191)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	2	0.1509	1	1
Sn	2	0.125	1	1
In	2	0.1278	1	1
GeTe	3	3.0274	1	1
P ₂	3	0.0052	1	1
Mg ₂	3	0.1365	1	1
IrTe ₂	4	3.0397	1	1
CdCl ₂	4	3.013	1	1
Cl ₂ Mn	4	0.0058	1	1
CdI ₂	4	13.647	1	1
AgTe ₂	4	0.1538	1	1
PSn ₂	4	0.4571	1	1
MoSe ₂	4	0.0007	1	1
S ₂ Ta	4	0.0079	1	1
Br ₂ Zn	4	0.4842	1	1
InSe ₂	4	3.018	1	1
AsSn ₂	4	0.4666	1	1
HgO	4	0.2298	2	1
SiTe ₂	4	0.4951	1	1
I ₂ Mn	4	3.0146	1	1
S ₂ Zr	4	0.4553	1	1
NSr ₂	4	2.9681	1	1
BiClTe	4	13.6681	1	1
Cl ₂ Ti	4	0.005	1	1
FeI ₂	4	2.9851	1	1
I ₂ Ni	4	3.0021	1	1
Mg ₃	4	0.1453	1	1
Te ₂ Ti	4	0.485	1	1
NbS ₂	4	0.0075	1	1
RhTe ₂	4	0.4737	1	1
N ₂ W	4	0.2746	1	1
NbS ₂	4	0.0031	1	1
S ₂ Ta	4	0.0022	1	1
Se ₂ V	4	0.0009	1	1
NiTe ₂	4	0.4935	1	1
Cl ₂ Cu	4	0.1222	1	1
S ₂ Sn	4	0.4559	1	1
I ₂ V	4	0.4986	1	1
Se ₂ Zr	4	0.4962	1	1
PtSe ₂	4	0.4682	1	1
GeS ₂	4	0.2098	1	1
TaTe ₂	4	0.4651	1	1
FeSe ₂	4	0.121	1	1
Br ₂ Mg	4	2.9833	1	1
NbTe ₂	4	0.4547	1	1
N ₂ Re	4	1.5635	1	1
Se ₂ Sn	4	2.9649	1	1
I ₂ Pr	4	13.6731	1	1
HfSe ₂	4	0.485	1	1
Se ₂ W	4	0.0006	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

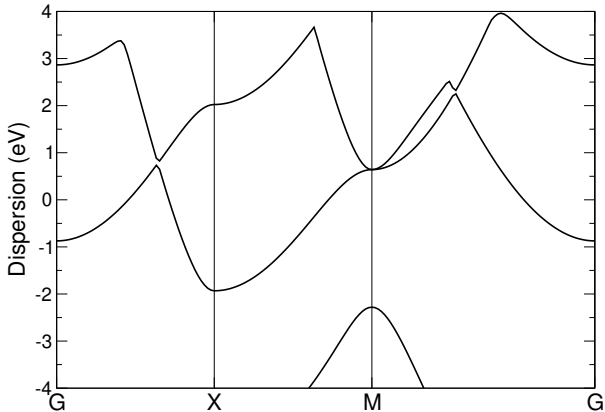
Formula	N° atoms	strain	cell size 1	cell size 2
Ce ₂ I ₂ Si ₂	121	0.0	25	16
Cl ₂ Er ₂ O ₂	358	0.0001	64	49
Bi ₂ STe ₂	326	0.0001	81	49
PbS ₂	186	0.0001	57	43
GeI ₂	172	0.0001	61	37
AsSn ₂	310	0.0001	91	73
SiTe ₂	211	0.0001	64	49
LiMnTe ₂	209	0.0002	61	37
As ₂ Mg ₂ Na ₂	159	0.0002	39	20
I ₂ N ₂ Zr ₂	465	0.0002	81	64
GeTe ₂	157	0.0002	49	36
Ba ₂ N	111	0.0002	36	25
I ₂ Mg	73	0.0003	25	16
CCL ₂ Gd ₂	358	0.0003	73	57
K	59	0.0003	39	20
Se ₂ Zr	211	0.0003	64	49
CdI ₂	228	0.0003	81	49
Sb ₂ Se ₂ Te	105	0.0003	25	16
CBr ₂ Y ₂	358	0.0003	73	57
As ₂ CeLi ₂	246	0.0003	61	37
Br ₂ Y ₂	229	0.0004	57	43
PbTe	135	0.0004	61	37
HNiO ₂	437	0.0004	73	91
Br ₂ Zn	244	0.0004	73	57
H ₂ Li ₂ Pt	735	0.0004	125	122
I ₂ Ni	157	0.0004	49	36
MnSe ₂	209	0.0004	65	48
Br ₂ La ₂ P	326	0.0004	81	49
I ₂ Pb	124	0.0005	49	25
CaCl	161	0.0005	65	48
Cu ₃ Se ₃	186	0.0005	36	25
Bi ₂ STe ₂	246	0.0005	61	37
PtSe ₂	310	0.0005	91	73
Se ₂ W	4	0.0006	1	1
Br ₂ La	73	0.0006	25	16
Bi ₂ Se ₃	105	0.0007	25	16
Ge ₂ I ₂ La ₂	70	0.0007	16	9
Te ₂ Ti	244	0.0007	73	57
Cu ₂ Te ₂	442	0.0007	118	81
HfSe ₂	244	0.0007	73	57
Ga ₂ Se ₂	229	0.0007	57	43
TaTe ₂	310	0.0007	91	73
NiTe ₂	211	0.0007	64	49
CdI ₂	228	0.0007	81	49
MoSe ₂	4	0.0007	1	1
Sb ₂ Se ₂ Te	105	0.0008	25	16
Te ₄ TiZr	157	0.0008	49	18
Gd ₂ GeI ₂	326	0.0009	81	49
Se ₂ V	4	0.0009	1	1
Cl ₂ Y ₂	301	0.0009	73	57

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Tl (P4/mmm (123))

Structural and electronic properties

	Formula	Tl
	Spacegroup	P4/mmm (123)
	Prototype	Sn
	Parent 3D	Co ₂ TlSe ₂
	Source DB	COD
	DB ID	1531163
DF2-C09	Binding energy [meV/ Å ²]	46.9
RVV10	Binding energy [meV/ Å ²]	49.38
	Band gap (PBE) [eV]	0.0

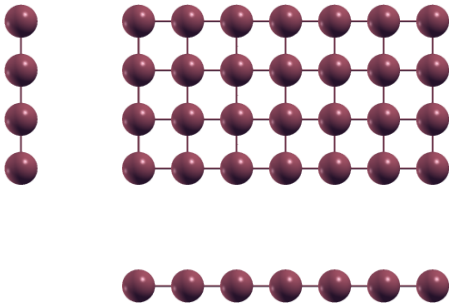


Band structure: Electronic band structure of Tl (P4/mmm (123)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Tl (P4/mmm (123)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	3.16324135	0.00000000	0.00000000
a₂	0.00000000	3.16324135	0.00000000
a₃	0.00000000	0.00000000	20.00000000
	x [Å]	y [Å]	z [Å]
● Tl	1.58162068	1.58162068	10.00000000



Orthographic projections: views of Tl (P4/mmm (123)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	2	0.1321	1	1
Na	2	0.1603	1	1
Sm	2	0.1098	1	1
AsSb	3	0.7781	1	1
As ₂	3	0.169	1	1
CaCl	3	0.4073	1	1
Cl ₂ Zn	4	0.1679	1	1
Cl ₂ Mn	4	0.1366	1	1
MoTe ₂	4	0.1627	1	1
AgTe ₂	4	0.003	1	1
PSn ₂	4	0.1795	1	1
MoSe ₂	4	0.1316	1	1
ReSe ₂	4	0.1479	1	1
S ₂ Ta	4	0.1382	1	1
Br ₂ Zn	4	0.1931	1	1
HfS ₂	4	0.1722	1	1
AsSn ₂	4	0.1842	1	1
SiTe ₂	4	0.7548	1	1
Te ₂ V	4	0.1648	1	1
CuTe ₂	4	0.1718	1	1
S ₂ Zr	4	0.1786	1	1
NSr ₂	4	0.7845	1	1
PbS ₂	4	0.7681	1	1
Br ₂ Co	4	0.1686	1	1
Ca ₂ N	4	0.1696	1	1
LiO ₂	4	0.1242	1	1
FeI ₂	4	0.7895	1	1
S ₂ Ti	4	0.1425	1	1
Mg ₃	4	0.0058	1	1
Te ₂ Ti	4	0.1935	1	1
NbS ₂	4	0.1379	1	1
CrI ₂	4	0.7878	1	1
Te ₂ Zn	4	0.1625	1	1
RhTe ₂	4	0.1878	1	1
Br ₂ Mn	4	0.1665	1	1
Cl ₂ Ni	4	0.1488	1	1
Cl ₂ Co	4	0.1422	1	1
CrTe ₂	4	0.1548	1	1
PtS ₂	4	0.1614	1	1
NbS ₂	4	0.1344	1	1
CoTe ₂	4	0.1726	1	1
Br ₂ V	4	0.1472	1	1
ClNZr	4	0.1453	1	1
Cl ₂ Fe	4	0.1415	1	1
CdClO	4	0.1643	1	1
S ₂ Ta	4	0.1338	1	1
Se ₂ V	4	0.1328	1	1
Se ₂ Ti	4	0.1586	1	1
Br ₂ Ti	4	0.1542	1	1
Te ₂ W	4	0.1629	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

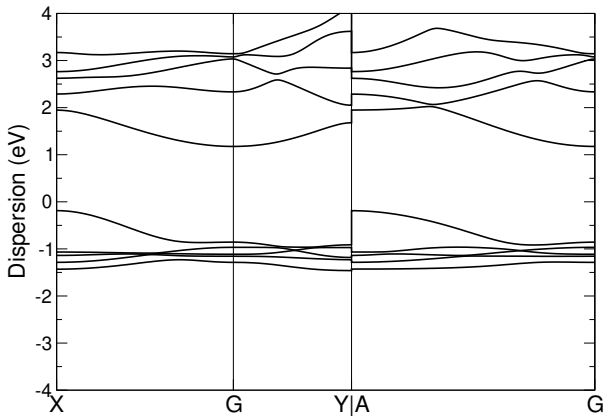
Formula	N° atoms	strain	cell size 1	cell size 2
I ₂ La	73	0.0001	25	16
As ₂ Fe ₂	424	0.0001	100	81
Br ₂ O ₂ Tb ₂	307	0.0001	61	41
I ₂ O ₂ Yb ₂	670	0.0001	136	89
Fe ₂ S ₂	597	0.0001	145	113
Ag ₂ I ₂	445	0.0001	149	74
Cu ₂ I ₂	329	0.0001	97	58
Cu ₂ Te ₂	329	0.0002	85	61
Co ₂ Se ₂	453	0.0002	113	85
As ₂ Rh ₂	89	0.0002	25	16
Co ₂ S ₂	265	0.0002	65	50
AlLiTe ₂	368	0.0002	108	65
As ₂ Co ₂ Li ₂	451	0.0002	85	61
GeS ₂	347	0.0002	101	82
Ir ₂ P ₂	492	0.0002	136	89
Ba ₂ F ₂ I ₂	394	0.0003	100	49
Mg ₄	5	0.0003	1	1
I ₂ O ₂ Sm ₂	859	0.0003	181	113
Br ₂ O ₂ Yb ₂	186	0.0003	36	25
Eu ₂ F ₂ I ₂	375	0.0003	81	49
Br ₂ La ₂ O ₂	375	0.0004	81	49
Br ₂ O ₂ Sm ₂	670	0.0004	136	89
O ₂ Pb ₂	277	0.0004	81	49
Br ₂ OV	373	0.0004	89	71
I ₂ Nd	403	0.0005	136	89
Se ₂ Si ₂ Zr ₂	472	0.0005	82	65
Ag ₂ Br ₂	89	0.0005	25	16
As ₂ Cd ₂ K ₂	427	0.0005	109	53
I ₂ Pr	403	0.0005	136	89
O ₄ PTl	394	0.0005	100	49
Br ₂ H ₂ Sr ₂	445	0.0006	97	58
Hf ₂ Se ₂ Si ₂	586	0.0006	100	81
I ₂ Nd ₂ O ₂	496	0.0006	106	65
CuO ₂	249	0.0006	60	63
F ₂ I ₂ Sm ₂	375	0.0006	81	49
Eu ₂ I ₂ O ₂	859	0.0006	181	113
Br ₂ La ₂	442	0.0006	118	81
Sb ₂	280	0.0006	118	81
Eu ₂ H ₂ I ₂	859	0.0007	181	113
Cu ₂ Se ₂	193	0.0007	49	36
H ₂ I ₂ Yb ₂	121	0.0007	25	16
Fe ₂ O ₄	380	0.0007	56	54
Cu ₂ Se ₂ Tl ₂	445	0.0007	97	58
F ₄ Nb	570	0.0008	145	85
Fe ₂ Te ₂	136	0.0008	36	25
GeS ₂	343	0.0008	100	81
Hf ₂ Si ₂ Te ₂	623	0.0008	113	85
Br ₂ Lu ₂ S ₂	97	0.0008	25	12
Ge ₂ Hf ₂ Te ₂	451	0.0008	85	61
Br ₂ Lu ₂ S ₂	97	0.0008	25	12

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Tl₂CS₃ (P1 (1))

Structural and electronic properties







	Formula	Tl ₂ CS ₃
	Spacegroup	P1 (1)
	Prototype	CS3Tl2
	Parent 3D	Tl ₄ C ₂ S ₆
	Source DB	ICSD
	DB ID	420223
DF2-C09	Binding energy [meV/ Å²]	N/A
RVV10	Binding energy [meV/ Å²]	43.5
	Band gap (PBE) [eV]	1.27

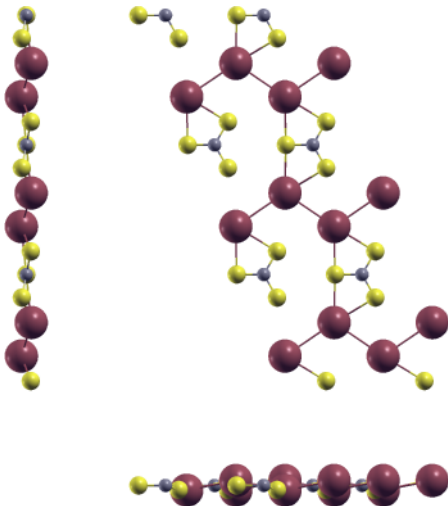


Band structure: Electronic band structure of Tl₂CS₃ (P1 (1)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Tl₂CS₃ (P1 (1)) in Cartesian coordinates.

		<i>x</i> [Å]	<i>y</i> [Å]	<i>z</i> [Å]
a₁		6.25052303	0.00000064	0.00000000
a₂		−3.12526067	8.23594995	0.00000000
a₃		0.00000000	0.00000000	20.63432624
		<i>x</i> [Å]	<i>y</i> [Å]	<i>z</i> [Å]
	Tl	1.07958918	2.22220260	10.62836507
	S	0.57560058	5.93784317	10.60053978
	Tl	4.20484795	4.35355864	10.00596379
	C	−0.27207769	7.40584424	10.31716082
	S	−1.99251879	7.40585376	10.31716264
	S	3.70085947	0.63791267	10.03378662



Orthographic projections: views of Tl₂CS₃ (P1 (1)) as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
IrTe ₂	9	0.1598	1	1
HfTe ₂	9	0.1609	1	1
Te ₂ Zr	9	0.1609	1	1
NaPSn	9	0.1607	1	1
AgTl	10	0.1072	1	2
S ₂ Zn ₂	10	0.16	1	1
P ₂ Sn ₂	10	0.16	1	1
LiMnSe ₂	10	0.1604	1	1
Ga ₂ Se ₂	10	0.1598	1	1
Pt ₂ Te ₂	10	0.1607	1	1
Cl ₂ Tb ₂	10	0.1602	1	1
K ₂ PdS ₂	11	2.2275	1	1
In ₂ Se ₃	11	0.1609	1	1
Hg ₃ S ₂	11	0.574	1	1
K ₂ PtS ₂	11	2.216	1	1
Ni ₂ SbTe ₂	11	0.1599	1	1
BrKO ₃	11	0.0875	1	1
Au ₂ K ₂ S ₂	12	0.0998	1	1
Tl	12	0.0595	1	6
GeNi ₃ Te ₂	12	0.1606	1	1
I ₄ Sr ₂	12	0.0884	1	1
Bi ₂ Te ₂	14	0.0881	1	2
Cu ₂ I ₂	14	0.103	1	2
Pb ₂ Se ₂	14	0.2521	1	2
O ₂ Pb ₂	14	0.1035	1	2
Bi ₂ O ₂	14	0.1033	1	2
PbS ₂ Sn	14	0.0989	1	2
S ₂ V	15	0.1844	1	3
MoS ₂	15	0.1849	1	3
S ₂ W	15	0.1849	1	3
MoS ₂	15	0.185	1	3
F ₄ Nb	16	0.1024	1	2
ClH ₃ O	16	0.0882	1	2
K ₂ PdSe ₂	16	2.7715	1	2
Br ₂ In ₂ O ₂	18	0.1146	1	2
Br ₂ F ₂ Sr ₂	18	0.1027	1	2
Eu ₂ F ₂ I ₂	18	0.1034	1	2
Br ₂ N ₂ Zr ₂	18	0.1153	1	2
I ₂ N ₂ Zr ₂	18	0.112	1	2
F ₂ I ₂ Sm ₂	18	0.1036	1	2
Br ₂ F ₂ Pb ₂	18	0.1027	1	2
AsCuLi ₂	18	0.4656	1	3
Cu ₂ Se ₂ Tl ₂	18	0.1031	1	2
I ₂ Pb	18	0.4884	1	4
P ₂	18	0.0557	1	6
Br ₂ H ₂ Sr ₂	18	0.1029	1	2
Ho ₂ S ₂	18	0.0375	1	3
Ga ₂ Te ₂	18	0.4662	1	3
SbSe ₂ Tl	18	0.3262	1	3
Cl ₂ Hg ₂ N ₂	18	0.1199	1	2

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

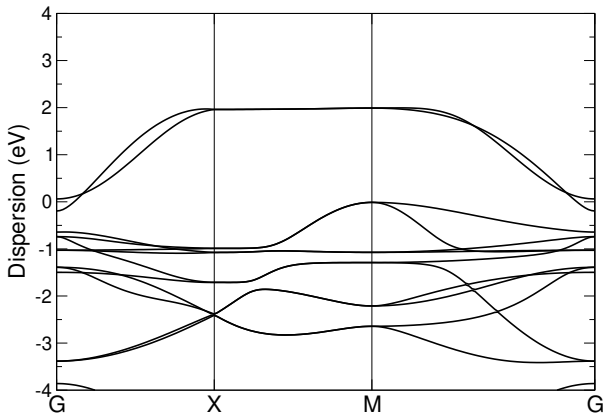
Formula	N° atoms	strain	cell size 1	cell size 2
I ₂ V	513	0.0001	28	115
Br ₂ Hf ₂ N ₂	216	0.0004	8	28
Te ₂ Zn	480	0.0007	24	112
Se ₂ Zr	513	0.0008	28	115
DyI ₂	870	0.001	59	172
CNNa	243	0.001	16	49
Ho ₂ S ₂	294	0.001	15	51
Hf ₂ Se ₂ Si ₂	834	0.0011	27	112
Au ₂ I ₂	786	0.0011	47	126
Cl ₂ O ₂ Y ₂	858	0.0012	28	115
Cl ₄ Mn	212	0.0012	12	28
SiTe ₂	513	0.0012	28	115
As ₂ Fe ₂	610	0.0014	27	112
C ₂ Br ₂ La ₂	312	0.0014	12	40
O ₄ PTl	762	0.0015	36	91
Br ₂ In ₂ O ₂	186	0.0017	7	24
Sn ₂ Te ₂	636	0.0017	40	99
Ga ₂ Se ₂	628	0.0017	28	115
Br ₃ Cs	726	0.0017	65	84
Cl ₂ ORu	348	0.0017	16	63
I ₂ N ₂ Zr ₂	156	0.0018	6	20
NiTe ₂	513	0.0018	28	115
Cl ₄ Mg ₂	810	0.0019	63	72
Hg ₃ N ₂	681	0.0019	56	69
Ba ₂ F ₂ I ₂	762	0.002	36	91
Cl ₄ Mg ₂	792	0.002	62	70
GeS ₂	498	0.0021	27	112
AlH ₄ Na	240	0.0021	12	28
Ag ₂ F ₄	402	0.0021	25	42
Ho ₂ S ₂	276	0.0021	14	48
IKO ₃	568	0.0022	48	56
O ₄ PSn	834	0.0022	40	99
Mo ₂ Te ₄	696	0.0022	35	81
ClKO ₃	745	0.0023	60	77
Br ₂ F ₂ Pb ₂	876	0.0023	36	110
Br ₂ F ₂ Sr ₂	876	0.0023	36	110
Br ₂ Ca ₃ Si	834	0.0023	47	92
Cu ₂ O ₂	708	0.0023	36	123
Cu ₂ K ₂ Te ₂	834	0.0024	40	99
I ₃ Sn	942	0.0024	77	120
Ga ₂ S ₃	704	0.0024	24	112
BaF ₂	690	0.0024	43	144
CaClHO	628	0.0024	28	115
Br ₂ H ₂ Sr ₂	876	0.0025	36	110
As ₂ O ₃	896	0.0025	56	112
STl ₂	690	0.0025	43	144
AgNO ₃	802	0.0026	47	104
PbS ₂	291	0.0026	16	65
Cu ₂ I ₂	656	0.0026	36	110
Br ₂ F ₂ Sr ₂	558	0.0026	23	70

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Tl₂S₂Cl₂ (P4/nmm)

Structural and electronic properties







	Formula	Tl ₂ S ₂ Cl ₂
	Spacegroup	P4/nmm
	Prototype	LiOH
	Parent 3D	Cl ₂ S ₂ Tl ₂
	Source DB	MPDS
	DB ID	S545242
DF2-C09	Binding energy [meV/ Å²]	40.94
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

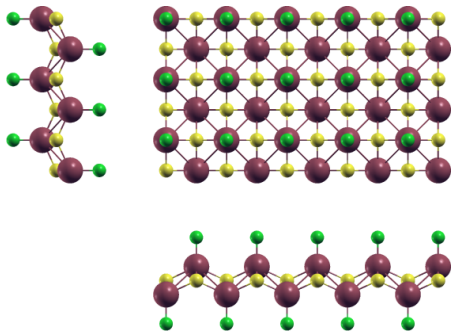


Band structure: Electronic band structure of Tl₂S₂Cl₂ (P4/nmm) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Tl₂S₂Cl₂ (P4/nmm) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		4.97601527	0.00000000	0.00000000
a₂		0.00000000	4.97601527	0.00000000
a₃		0.00000000	0.00000000	26.12943567
		x [Å]	y [Å]	z [Å]
	Tl	1.24400382	-1.24400382	1.14440712
	Cl	1.24400382	-1.24400382	3.54587407
	Tl	-1.24400382	-3.73201145	-1.14440712
	S	-1.24400382	-1.24400382	0.00000000
	S	1.24400382	-3.73201145	0.00000000
	Cl	-1.24400382	-3.73201145	-3.54587407



Orthographic projections: views of Tl₂S₂Cl₂ (P4/nmm) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	7	0.5831	1	1
Sb ₂	8	0.11	1	1
I ₂ Mg	9	0.1089	1	1
Br ₂ La	9	0.1088	1	1
HgI ₂	9	0.2193	1	1
I ₂ Zn	9	0.1108	1	1
GeI ₂	9	0.1092	1	1
CNRb	9	0.0346	1	1
Se ₂ Yb	9	0.1092	1	1
BiTe ₂	9	0.1091	1	1
Au ₂ Br ₂	10	0.5788	1	1
Ge ₂ Te ₂	10	0.2091	1	1
Cl ₂ La ₂	10	0.1113	1	1
AsCuLi ₂	10	0.1093	1	1
In ₂ Se ₂	10	0.111	1	1
La ₂ S ₂	10	0.5982	1	1
Ga ₂ Te ₂	10	0.1093	1	1
Br ₂ La ₂	10	0.1101	1	1
Ag ₂ I ₂	10	0.2205	1	1
Se ₂ Sn ₂	10	0.5996	1	1
Br ₂ HLa	10	0.1094	1	1
As ₂ O ₃	11	0.1473	1	1
CeLi ₂ P ₂	11	0.1095	1	1
F ₄ Pb	11	0.6125	1	1
Ba ₂ Ni ₃	11	0.1093	1	1
Sb ₂ Se ₂ Te	11	0.1091	1	1
Li ₂ P ₂ Pr	11	0.1099	1	1
Sb ₂ Se ₂ Te	11	0.109	1	1
Bi ₂ Se ₃	11	0.1088	1	1
Ho ₂ I ₂ S ₂	12	0.2244	1	1
Br ₂ Cu	12	0.4104	1	2
NiO ₂	12	0.1444	1	2
Cu ₂ Na ₂ Te ₂	12	0.5936	1	1
BH ₄ Li	12	0.1096	1	1
Ga ₂ Ge ₂ Te ₂	12	0.1099	1	1
I ₂ Se ₂ Tb ₂	12	0.0624	1	1
Gd ₂ I ₂ Se ₂	12	0.0623	1	1
Pd ₂ S ₄	12	0.3844	1	1
Br ₂ Er ₂ Se ₂	12	0.3389	1	1
Tl	12	0.7917	1	6
Er ₂ I ₂ Se ₂	12	0.3438	1	1
I ₂ Se ₂ Tm ₂	12	0.3422	1	1
Ag ₂ K ₂ Se ₂	12	0.2175	1	1
LiO	12	0.1617	1	3
AuI ₄ Li	12	0.3094	1	1
Ce ₂ I ₂ Si ₂	12	0.1089	1	1
Ag ₂ F ₄	12	0.4204	1	1
I ₂ Se ₂ Yb ₂	12	0.3417	1	1
As ₂ Mg ₂ Na ₂	12	0.5821	1	1
N ₂ Re	12	0.1463	1	2

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

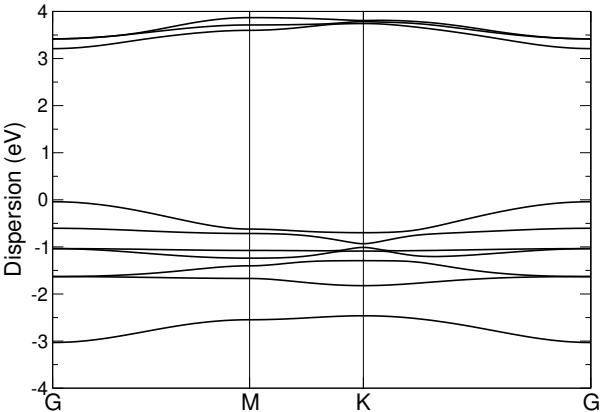
Formula	N° atoms	strain	cell size 1	cell size 2
Br ₂ Ca ₂ F ₂	780	0.0	49	81
Cu ₂ S ₂	736	0.0	58	97
Cu ₂ Te ₂	118	0.0001	9	16
HgI ₂	786	0.0001	81	100
Br ₂ O ₂ Y ₂	930	0.0001	58	97
Ni ₂ Se ₂	814	0.0001	65	106
Br ₂ Dy ₂ O ₂	930	0.0002	58	97
K	623	0.0002	85	113
Ho ₂ I ₂ Se ₂	660	0.0003	54	56
Cl ₂ Zr ₂	844	0.0003	54	130
GeS ₂	891	0.0003	74	149
As ₂ Ir ₂	196	0.0003	16	25
Ag ₂ I ₂	896	0.0004	82	101
CeI ₂	708	0.0004	65	106
F ₂ Zn	537	0.0004	49	81
Br ₂ F ₂ Yb ₂	780	0.0004	49	81
Bi ₂ Se ₂	208	0.0004	18	25
Cu ₂ Na ₂ Te ₂	678	0.0004	49	64
As ₂ Co ₂ Li ₂	150	0.0005	9	16
Pb ₂ Se ₂	278	0.0005	25	32
Cl ₂ O ₂ Sc ₂	468	0.0005	28	50
Ca ₂ O ₂	60	0.0005	4	9
O ₂ Sn ₂	736	0.0005	58	97
H ₄ Ti	649	0.0006	34	89
F ₂ Tl ₂	736	0.0006	58	97
Br ₂ V	714	0.0006	54	130
CCl ₂ Sc ₂	974	0.0006	54	130
Se ₂ Si ₂ Zr ₂	444	0.0006	25	49
Br ₂ Gd ₂ O ₂	780	0.0007	49	81
In	79	0.0007	9	25
Ca ₂ H ₂ I ₂	246	0.0007	16	25
P ₂ Rh ₂	736	0.0007	58	97
Bi ₂ Pd	51	0.0008	4	9
Au ₂ Br ₂	412	0.0008	36	49
PbS ₂	237	0.0008	20	39
F ₂ I ₂ Pb ₂	876	0.0009	61	85
CuGeO ₃	869	0.0009	64	97
Ag ₂ I ₂	886	0.0009	81	100
Br ₂ Cu ₂	618	0.001	49	81
ReSe ₂	633	0.001	48	115
Ba ₂ Cd	621	0.001	61	85
Br ₂ Y ₂	276	0.001	20	39
Ge ₂ Hf ₂ Te ₂	150	0.0011	9	16
PTe ₂ Zr ₂	315	0.0011	20	39
Br ₂ V	633	0.0011	48	115
H ₂ Li ₂ Pd	649	0.0011	34	89
In ₂ Se ₂	838	0.0011	81	88
I ₂ Pr	708	0.0011	65	106
Cl ₂ N ₂ Zr ₂	402	0.0012	25	42
Ge ₂ Mn ₂ Sr ₂	246	0.0012	16	25

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

TlO₃I (P3m1)

Structural and electronic properties

	Formula	TlO ₃ I
	Spacegroup	P3m1
	Prototype	KNO3
	Parent 3D	IO ₃ Tl
	Source DB	ICSD
	DB ID	62106
DF2-C09	Binding energy [meV/ Å²]	80.93
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	3.25

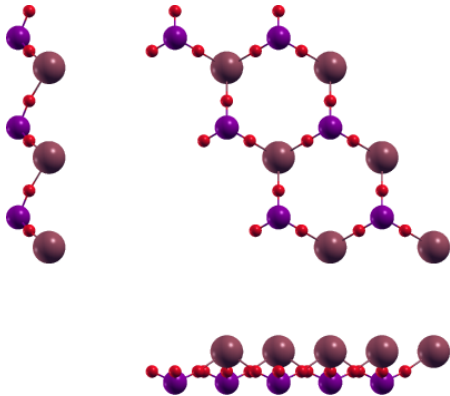


Band structure: Electronic band structure of TlO₃I (P3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of TlO₃I (P3m1) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		-3.36066293	-5.82083894	0.00000000
a₂		6.72132586	0.00000000	0.00000000
a₃		0.00000000	0.00000000	16.35795429
		x [Å]	y [Å]	z [Å]
●	I	3.36066293	-1.94027965	0.83103458
●	O	3.36066293	-0.21535577	0.11511908
●	O	1.86683503	-2.80274159	0.11511908
●	O	4.85449083	-2.80274159	0.11511908
●	Tl	0.00000000	-3.88055929	-1.17639183



Orthographic projections: views of TlO₃I (P3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
CKN	8	0.1162	1	1
Cl ₂ Rb ₂	9	0.1547	1	1
AgNO ₂	9	0.178	1	1
Tl	9	0.0055	1	4
Br ₃ Cs	9	0.0038	1	1
In	9	0.1242	1	4
SbSe ₂ Tl	9	0.1231	1	1
I ₃ Sn	9	0.1159	1	1
ClKO ₃	10	0.0073	1	1
Hg ₃ S ₂	10	0.4706	1	1
Cl ₄ Cu ₂	11	0.1371	1	1
H ₂ Na ₂ O ₂	11	0.1633	1	1
Se ₂ Ta ₄	11	0.1627	1	1
Sn	11	0.1469	1	6
I ₄ Sr ₂	11	0.2213	1	1
Ag ₂ F ₄	11	0.112	1	1
Br ₂ Ca ₃ Si	11	0.1128	1	1
S ₂	12	0.1632	2	1
Bi ₂ Mn ₂	13	0.1185	1	2
HfTe ₂	13	0.1638	2	1
Pb ₂ Se ₂	13	0.1391	1	2
Bi ₂ Se ₂	13	0.1244	1	2
Au ₂ Se ₂	13	0.1986	1	2
Ho ₂ S ₂	13	0.1918	1	2
SbSe ₂ Tl	13	0.0458	1	2
NaPSn	13	0.1637	2	1
Cl ₂ Gd ₂	14	0.1633	2	1
S ₂ Zn ₂	14	0.1633	2	1
P ₂ Sn ₂	14	0.1633	2	1
LiMnSe ₂	14	0.1635	2	1
Ga ₂ Se ₂	14	0.1632	2	1
Pt ₂ Te ₂	14	0.1637	2	1
I ₂ Y ₂	14	0.1634	2	1
Sn ₂ Te ₂	14	0.155	2	1
Cl ₂ Tb ₂	14	0.1634	2	1
In ₂ Se ₃	15	0.1638	2	1
ClH ₃ O	15	0.224	1	2
CuGeO ₃	15	0.1151	1	2
Ni ₂ SbTe ₂	15	0.1632	2	1
Ba ₂ H ₂ I ₂	16	0.1548	2	1
GeNi ₃ Te ₂	16	0.1637	2	1
Cl ₄ Mg ₂	16	0.124	2	1
F ₂ Se ₂ Tm ₂	16	0.1635	2	1
O ₄ PSn	16	0.155	2	1
Er ₂ F ₂ Se ₂	16	0.1638	2	1
F ₂ Se ₂ Yb ₂	16	0.1633	2	1
Cu ₂ K ₂ Te ₂	16	0.1549	2	1
Cl ₄ KTl	16	0.2305	2	1
Cl ₂ Mn	17	0.0001	1	4
MoSe ₂	17	0.0063	1	4

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

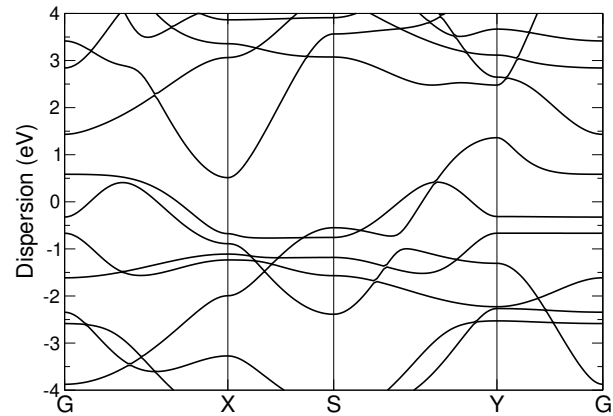
Formula	N° atoms	strain	cell size 1	cell size 2
PtTe ₂	120	0.0	9	25
Cl ₂ Mn	17	0.0001	1	4
Bi ₂ Te ₂	321	0.0002	25	49
AsKSn	317	0.0003	25	64
PTe ₂ Zr ₂	325	0.0003	16	49
AsSb	178	0.0004	16	49
AuTe ₂	120	0.0004	9	25
I ₂ Tm	47	0.0004	4	9
I ₂ N ₂ Zr ₂	611	0.0005	25	81
Sn ₂ Te ₂	626	0.0005	50	94
Cl ₂ NSc ₂	25	0.0006	1	4
RhTe ₂	368	0.0006	25	81
GeI ₂ La ₂	65	0.0007	4	9
CaI ₂	47	0.0007	4	9
CoI ₂	227	0.0008	16	49
AgClO ₄	973	0.0008	65	108
I ₂ La ₂	381	0.0008	25	64
Te ₄ TiZr	801	0.0009	57	86
Ga ₂ I ₂ Y ₂	509	0.0009	25	64
Br ₂ Er ₂	145	0.0009	9	25
Li ₂ Tl ₂	109	0.001	9	16
Br ₂ Ho ₂	145	0.001	9	25
GeI ₃ Rb	65	0.001	9	4
BaF ₂	317	0.0011	25	64
I ₂ Ti	227	0.0011	16	49
Bi ₂ S ₃	170	0.0012	9	25
Cu ₂ K ₂ Te ₂	684	0.0012	42	79
O ₄ PSn	684	0.0013	42	79
K ₂ PdS ₂	995	0.0013	99	100
CdClHO	449	0.0014	25	81
LiOS ₂ Ti	25	0.0014	1	4
Br ₂ Tb ₂	145	0.0015	9	25
Br ₂ Gd ₂	145	0.0015	9	25
Ga ₂ Se ₂	449	0.0015	25	81
Cl ₂ Y ₂	325	0.0016	16	49
Cl ₂ Cu	533	0.0016	37	116
As ₂ Sn ₂	145	0.0016	9	25
I ₂ Sb ₂ Te ₂	561	0.0016	45	56
Cl ₂ Rb ₂	989	0.0016	113	106
Se ₂ Sn	227	0.0017	16	49
NbS ₂	17	0.0018	1	4
I ₂ Yb	47	0.0018	4	9
Cl ₂ F ₂ Pb ₂	953	0.0018	49	118
Ge ₂ S ₂	485	0.0018	33	80
Bi ₂ I ₂ O ₂	953	0.0018	49	118
Cu ₂ Na ₂ Se ₂	953	0.0018	49	118
I ₂ Nd ₂ O ₂	953	0.0018	49	118
K ₂ PtS ₂	545	0.0018	54	55
Br ₂ Lu ₂ S ₂	554	0.0018	34	64
F ₂ I ₂ Tm ₂	953	0.0019	49	118

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

TlSbSe₂ (Pmmm (47))

Structural and electronic properties

	Formula	TlSbSe ₂
	Spacegroup	Pmmm (47)
	Prototype	VOC12
	Parent 3D	SbSe ₂ Tl
	Source DB	cod
	DB ID	1530590
DF2-C09	Binding energy [meV/ Å²]	56.45
RVV10	Binding energy [meV/ Å²]	58.33
	Band gap (PBE) [eV]	0.0

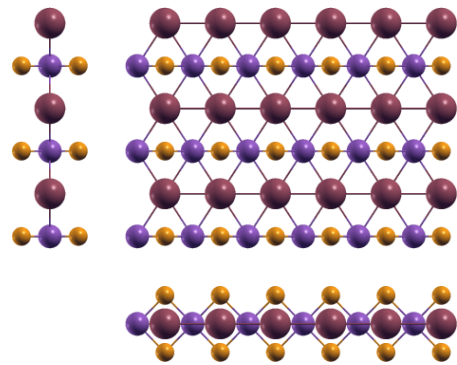


Band structure: Electronic band structure of TlSbSe₂ (Pmmm (47)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of TlSbSe₂ (Pmmm (47)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.79441322	0.00000000	0.00000000
a₂		0.00000000	5.85082211	0.00000000
a₃		0.00000000	0.00000000	24.30311868
		x [Å]	y [Å]	z [Å]
●	Tl	1.89720661	2.92541105	12.15155934
●	Sb	0.00000000	0.00000000	12.15155934
●	Se	1.89720661	0.00000000	14.10318595
●	Se	1.89720661	0.00000000	10.19993273



Orthographic projections: views of TlSbSe₂ (Pmmm (47)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
AgTl	6	0.2934	1	1
Tl	6	0.1325	1	2
In	6	0.1243	1	2
CKN	7	0.4412	1	1
CoO ₂	7	0.2109	1	1
In ₂ Se ₂	8	0.092	1	1
AgNO ₂	8	0.6823	1	1
Pb ₂ Se ₂	8	0.2149	1	1
P ₄	8	1.0501	1	1
Br ₃ Cs	8	0.4423	1	1
Sn	8	0.3045	1	4
S ₂	8	0.7286	1	2
Au ₂ Se ₂	8	0.0268	1	1
P ₂	8	0.1294	1	2
K ₂ PdS ₂	9	1.7446	1	1
IO ₃ Tl	9	0.4328	1	1
FKO ₂ Se	9	0.2483	1	1
ClKO ₃	9	0.451	1	1
NaO ₄	9	0.8671	1	1
AgNO ₃	9	0.8706	1	1
ClH ₃ O	9	0.722	1	1
K ₂ PdSe ₂	9	1.748	1	1
Br ₂ In ₂ O ₂	10	0.2725	1	1
Br ₂ Ho ₂ S ₂	10	0.4607	1	1
Cl ₂ Mn	10	0.0359	1	2
MoSe ₂	10	0.132	1	2
ReSe ₂	10	0.1458	1	2
Ho ₂ I ₂ S ₂	10	0.1789	1	1
S ₂ Ta	10	0.0347	1	2
Br ₂ Zn	10	0.0401	1	2
C ₂ I ₂ La ₂	10	0.1352	1	1
Br ₂ N ₂ Zr ₂	10	0.2714	1	1
GeTe ₂	10	0.7154	1	2
I ₂ N ₂ Zr ₂	10	0.2788	1	1
SiTe ₂	10	0.0436	1	2
Br ₂ Cu	10	0.1519	1	2
PbS ₂	10	0.692	1	2
Cl ₂ Rh ₂ Te ₂	10	0.679	1	1
Cl ₂ Ti	10	0.1295	1	2
K ₂ O ₂ Tl ₂	10	0.0222	1	1
S ₂ Ti	10	0.0321	1	2
I ₂ Se ₂ Tb ₂	10	0.2166	1	1
Te ₂ Ti	10	0.0403	1	2
Gd ₂ I ₂ Se ₂	10	0.2197	1	1
NbS ₂	10	0.0349	1	2
I ₄ Zr ₂	10	0.7501	1	1
Gd ₂ I ₂ S ₂	10	0.206	1	1
Cl ₂ Ni	10	0.1465	1	2
Cl ₂ Co	10	0.0322	1	2
NbS ₂	10	0.0375	1	2

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

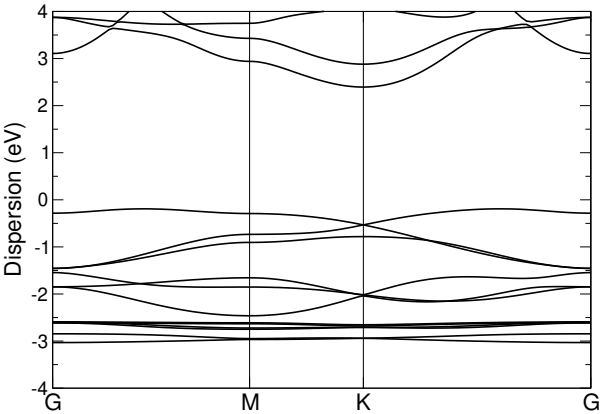
Formula	N° atoms	strain	cell size 1	cell size 2
STl ₂	416	0.0004	50	72
Hg ₃ S ₂	668	0.0004	107	48
Cl ₂ Er ₂ O ₂	132	0.0004	9	16
S ₂ Ta	86	0.0004	8	18
LiNbS ₂	104	0.0004	8	18
NbS ₂	86	0.0005	8	18
CuO ₂	330	0.0005	30	70
Br ₂ Hg ₃	126	0.0005	24	6
O ₄ PSn	438	0.0005	42	45
As ₂ Sn ₂	492	0.0006	48	75
Br ₂ Gd ₂	492	0.0007	48	75
Cl ₂ La ₂	492	0.0007	48	75
Nd	150	0.0007	20	70
O ₂ Zn	444	0.0007	36	100
Cl ₄ Mg ₂	244	0.0007	25	24
P ₄	728	0.0007	74	108
Hg ₃ S ₂	655	0.0009	105	47
HgO	246	0.0009	30	63
I ₂ S ₂ Tb ₂	974	0.001	98	97
BaF ₂	416	0.001	50	72
Hg ₃ S ₂	543	0.001	87	39
I ₂ Sb ₂ Te ₂	328	0.001	40	28
C ₂ Cl ₂ Y ₂	964	0.0011	67	116
Br ₂ Ca ₃ Si	54	0.0011	6	5
La ₂ S ₂	264	0.0011	30	36
As ₂ Cd ₂ K ₂	438	0.0011	42	45
Dy ₂ I ₂ S ₂	974	0.0011	98	97
In ₂ Te ₃	560	0.0012	50	72
Se ₂ Sn ₂	236	0.0012	27	32
Li ₂ Tl ₂	96	0.0012	12	12
Br ₂ Er ₂	492	0.0012	48	75
I ₄ Sr ₂	260	0.0012	35	20
Sb ₂ SeTe ₂	560	0.0012	50	72
Ga ₂ I ₂ Y ₂	632	0.0012	50	72
AuI ₄ Li	362	0.0012	44	31
Au ₂ Br ₂	668	0.0013	75	92
Au ₂ Br ₂	640	0.0013	72	88
Cl ₂ Ho ₂ O ₂	132	0.0014	9	16
Br ₃ Cs	892	0.0014	143	80
Cl ₂ Hf ₂	104	0.0014	8	18
Al ₂ Cl ₂ O ₂	388	0.0014	25	48
Br ₃ Cs	780	0.0015	125	70
Cl ₂ NSc ₂	122	0.0015	8	18
H ₂ MnO ₂	608	0.0015	32	96
Bi ₂ Se ₂ Te	560	0.0016	50	72
Cu ₂ K ₂ Te ₂	438	0.0016	42	45
As ₂ O ₃	335	0.0016	40	35
Br ₃ Cs	680	0.0016	109	61
Hg ₃ S ₂	530	0.0016	85	38
H ₂ Na ₂ O ₂	914	0.0016	59	113

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

Y₂Se₂F₂ (P-3m1)

Structural and electronic properties

	Formula	Y ₂ Se ₂ F ₂
	Spacegroup	P-3m1
	Prototype	SmSI
	Parent 3D	F ₂ Se ₂ Y ₂
	Source DB	MPDS
	DB ID	S307725
DF2-C09	Binding energy [meV/ Å²]	124.79
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	2.59

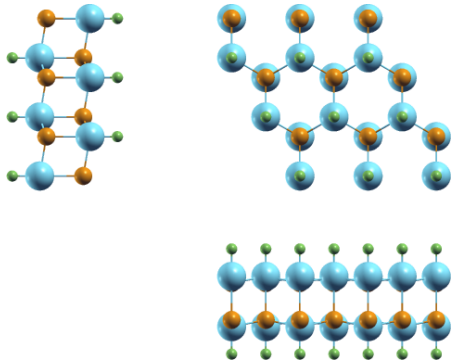


Band structure: Electronic band structure of Y₂Se₂F₂ (P-3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of Y₂Se₂F₂ (P-3m1) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		2.42586402	-4.20171974	0.00000000
a₂		2.42586402	4.20171974	0.00000000
a₃		0.00000000	0.00000000	27.93680946
		x [Å]	y [Å]	z [Å]
•	F	3.63879603	0.70028662	-3.74045294
•	Y	3.63879603	0.70028662	-1.78878459
•	Y	1.21293201	-0.70028662	1.78878459
•	Se	3.63879603	0.70028662	1.31060307
•	Se	1.21293201	-0.70028662	-1.31060307
•	F	1.21293201	-0.70028662	3.74045294



Orthographic projections: views of Y₂Se₂F₂ (P-3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	7	0.1251	1	1
InSe	8	0.2492	1	1
Bi ₂	8	0.257	1	1
AgTl	8	0.1113	1	1
CdI ₂	9	0.2539	1	1
Br ₂ Ca	9	0.2555	1	1
BiClTe	9	0.2544	1	1
HgI ₂	9	0.1376	1	1
BiBrTe	9	0.262	1	1
Ba ₂ Hg	9	0.1168	1	1
CNRb	9	0.1268	1	1
PbTe ₂	9	1.5583	1	1
Cl ₂ Cu	9	0.2778	1	1
BiTe	9	0.2714	1	1
GdI ₂	9	0.266	1	1
CdI ₂	9	0.2533	1	1
Ba ₂ Cd	9	0.1181	1	1
I ₂ Pr	9	0.2545	1	1
Bi ₂ Te ₂	10	0.0051	1	1
Bi ₂ In ₂	10	0.1522	1	1
Cu ₂ I ₂	10	0.1124	1	1
Cu ₂ Sr ₂	10	0.2634	1	1
Br ₂ Pr ₂	10	4.8681	1	1
AgCuTe ₂	10	0.1136	1	1
AsLi ₃	10	0.2496	1	1
S ₂ Sn ₂	10	0.1172	1	1
Au ₂ Br ₂	10	0.1148	1	1
AlLiTe ₂	10	0.2697	1	1
Ge ₂ Te ₂	10	0.1262	1	1
N ₃ Na	10	0.1386	1	1
As ₂ Ir ₂	10	0.4242	1	1
O ₂ Pb ₂	10	0.1113	1	1
Ge ₂ Se ₂	10	0.115	1	1
Bi ₂ O ₂	10	0.1117	1	1
AgClO ₂	10	0.2414	1	1
PbS ₂ Sn	10	0.1191	1	1
Gd ₂ I ₂	10	1.5473	1	1
SbSe ₂ Tl	10	0.2177	1	1
Ag ₂ I ₂	10	0.1384	1	1
Se ₂ Sn ₂	10	0.1263	1	1
Br ₂ CsF	10	0.1503	1	1
Sn ₂ Te ₂	10	0.1451	1	1
As ₂ O ₃	11	0.4696	1	1
F ₄ Pb	11	0.1318	1	1
SSb ₂ Te ₂	11	1.565	1	1
As ₂ Li ₂ Nd	11	0.2484	1	1
F ₄ Sn	11	0.1164	1	1
Bi ₂ STe ₂	11	0.2505	1	1
AsI ₂ La ₂	11	0.2758	1	1
Bi ₂ Te ₃	11	0.2713	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

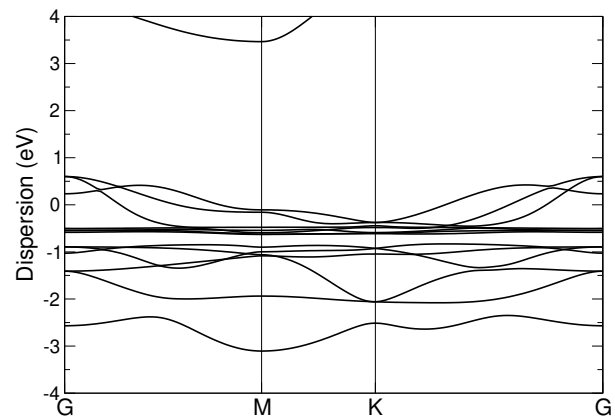
Formula	N° atoms	strain	cell size 1	cell size 2
InSe	422	0.0	49	64
CdO ₂	471	0.0	39	79
As ₂ Li ₂ Pr	614	0.0	49	64
Br ₂ Ca	561	0.0001	57	73
Sb ₂ Te ₃	789	0.0001	64	81
Gd ₂ I ₂	412	0.0001	36	49
NbSe ₂	297	0.0001	25	49
I ₂ La ₂ Si ₂	678	0.0001	49	64
Cl ₂ Co	471	0.0001	39	79
Bi ₂ Se ₃	461	0.0002	36	49
Se ₂ Ta	297	0.0002	25	49
H ₂ Na ₂ Pd	930	0.0002	65	108
Ni ₂ Te ₂	196	0.0002	16	25
F ₂ Na	405	0.0002	37	61
Cl ₂ Zr	471	0.0002	39	79
Br ₂ La	363	0.0002	36	49
Cl ₂ O ₂ Yb ₂	588	0.0002	37	61
Br ₂ Er ₂	294	0.0003	25	36
AsLi ₃	550	0.0003	49	64
I ₂ La ₂ P	893	0.0003	73	91
Br ₂ Gd ₂	294	0.0003	25	36
N ₃ W ₂	179	0.0003	9	25
Ga ₂ S ₂	118	0.0003	9	16
Br ₂ Pr ₂	618	0.0003	49	81
Cl ₂ Ni	297	0.0003	25	49
BaF ₂	429	0.0004	43	57
Cu ₂ I ₂	412	0.0004	36	49
Br ₂ Gd ₂ Ge	461	0.0004	36	49
As ₂ Sn ₂	294	0.0004	25	36
CdCl ₂	171	0.0004	16	25
LiO	42	0.0004	4	9
Ga ₂ I ₂ Tb ₂	780	0.0004	57	73
I ₂ Ni	171	0.0004	16	25
S ₂ Ti	471	0.0005	39	79
I ₂ Mn	171	0.0005	16	25
Er ₂ I ₂ Se ₂	312	0.0005	28	24
I ₂ Mg	363	0.0006	36	49
STl ₂	429	0.0006	43	57
Ga ₂ I ₂ Y ₂	600	0.0006	43	57
Cl ₂ Fe	471	0.0006	39	79
GeTe ₂	171	0.0006	16	25
Cl ₂ Er ₂ H ₂	246	0.0006	16	25
Cu ₄ Te ₂	870	0.0006	64	81
Cl ₂ O ₂ Tm ₂	588	0.0006	37	61
Cu ₂ Sr ₂	802	0.0006	73	91
PTe ₂ Ti ₂	134	0.0007	9	16
C ₄ Ca ₂	768	0.0007	58	70
As ₂ Li ₂ Nd	614	0.0007	49	64
Ga ₂ Gd ₂ I ₂	780	0.0007	57	73
Ga ₂ S ₂	118	0.0007	9	16

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

YbSe₂ (P-3m1 (164))

Structural and electronic properties

	Formula	YbSe ₂
	Spacegroup	P-3m1 (164)
	Prototype	CdI ₂
	Parent 3D	KYbSe ₂
	Source DB	COD
	DB ID	8100307
DF2-C09	Binding energy [meV/ Å²]	127.82
RVV10	Binding energy [meV/ Å²]	300.73
	Band gap (PBE) [eV]	0.0

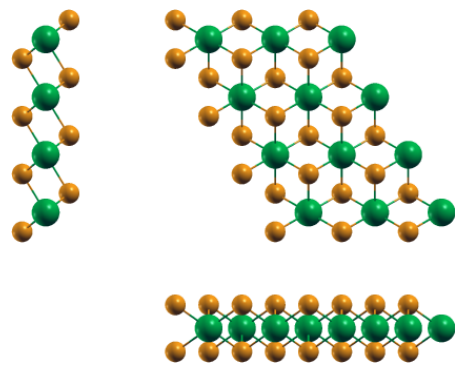


Band structure: Electronic band structure of YbSe₂ (P-3m1 (164)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of YbSe₂ (P-3m1 (164)) in Cartesian coordinates.

	x [Å]	y [Å]	z [Å]
a₁	4.13929987	0.00000000	0.00000000
a₂	−2.06964993	3.58473884	0.00000000
a₃	0.00000000	0.00000000	23.10127191
	x [Å]	y [Å]	z [Å]
● Yb	2.06964993	1.19491295	11.55063595
● Se	0.00000000	0.00000000	13.00848399
● Se	0.00000000	2.38982589	10.09278791



Orthographic projections: views of YbSe₂ (P-3m1 (164)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	4	0.4552	1	1
Na	4	1.5473	1	1
AgTl	5	0.1648	1	1
Ag ₂	5	0.4689	1	1
As ₂	5	0.247	1	1
Sb ₂	5	0.004	1	1
CaCl	5	0.1189	1	1
Cl ₂ Zn	6	1.5977	1	1
I ₂ Mg	6	0.0016	1	1
MoTe ₂	6	1.5636	1	1
PSn ₂	6	0.259	1	1
Ba ₂ Pt	6	0.4683	1	1
Br ₂ Zn	6	0.2742	1	1
HfS ₂	6	0.2506	1	1
AsSn ₂	6	0.2642	1	1
I ₂ Pr	6	0.1467	1	1
CuTe ₂	6	0.2501	1	1
S ₂ Zr	6	0.2579	1	1
Br ₂ La	6	0.002	1	1
Ca ₂ Si	6	0.4798	1	1
Br ₂ Co	6	0.2464	1	1
Ca ₂ N	6	0.2477	1	1
BrCdI	6	0.0048	1	1
Cl ₂ Zn	6	0.1275	1	1
Te ₂ Ti	6	0.2747	1	1
I ₂ Zn	6	0.0072	1	1
BaF ₂	6	0.0082	1	1
RhTe ₂	6	0.2683	1	1
GeI ₂	6	0.0002	1	1
Br ₂ Mn	6	1.5888	1	1
PtS ₂	6	1.5547	1	1
CoTe ₂	6	1.6283	1	1
Se ₂ Ti	6	1.5357	1	1
AsKSn	6	0.0067	1	1
Te ₂ W	6	1.5648	1	1
PbTe ₂	6	0.0038	1	1
I ₂ Nd	6	0.1476	1	1
S ₂ Sn	6	0.2583	1	1
SnTe ₂	6	0.0025	1	1
Sn	6	0.6327	1	3
Cl ₂ V	6	4.8598	1	1
I ₂ Pb	6	0.4729	1	1
STl ₂	6	0.0092	1	1
PtSe ₂	6	0.2652	1	1
Br ₂ Fe	6	0.2465	1	1
GeS ₂	6	0.1133	1	1
TaTe ₂	6	0.2634	1	1
MnSe ₂	6	0.1188	1	1
Br ₂ Ni	6	1.6409	1	1
CeI ₂	6	0.146	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

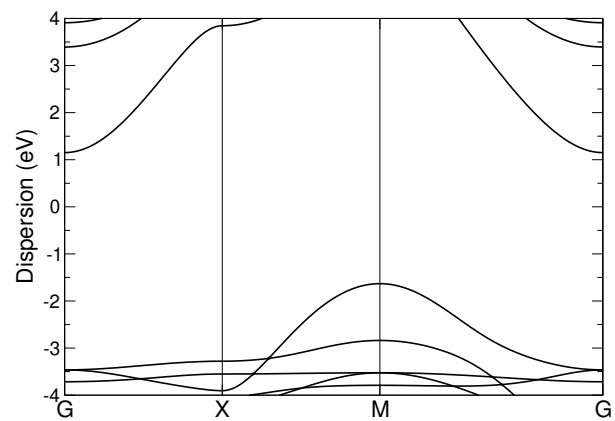
Formula	N° atoms	strain	cell size 1	cell size 2
Cl ₂ N ₂ Zr ₂	531	0.0	49	64
Na	157	0.0001	36	49
AsSn ₂	492	0.0001	73	91
ClH ₃ O	386	0.0001	57	43
KS ₂ Ti	357	0.0001	43	57
CrSe ₂	294	0.0001	37	61
Br ₂ V	183	0.0001	25	36
Sb ₂ Te ₂	499	0.0002	81	64
CaH ₂ O ₂	467	0.0002	49	64
GeI ₂	6	0.0002	1	1
PSn ₂	435	0.0002	64	81
BiTe ₂	6	0.0003	1	1
CdClHO	643	0.0003	81	100
Br ₂ N ₂ Zr ₂	609	0.0003	57	73
ReS ₂	75	0.0003	9	16
CBr ₂ Lu ₂	536	0.0003	57	73
MnO ₂	39	0.0003	4	9
Ga ₂ S ₃	353	0.0004	36	49
Ba ₂ Ni ₃	8	0.0004	1	1
Ga ₂ Te ₂	7	0.0004	1	1
NS ₂ Zr	304	0.0005	36	49
Br ₂ Mn	300	0.0005	43	57
RhTe ₂	543	0.0005	81	100
Ag ₂ I ₂	387	0.0005	65	48
Ba ₂ Pt	492	0.0005	91	73
I ₂ Pr ₂ Si ₂	9	0.0005	1	1
AgBrO ₂	291	0.0006	41	42
Br ₂ Hf ₂ N ₂	531	0.0006	49	64
HgI ₂	339	0.0006	65	48
PtSe ₂	492	0.0006	73	91
Sb ₂ Se ₂ Te	8	0.0006	1	1
MoSe ₂	123	0.0006	16	25
TaTe ₂	492	0.0006	73	91
Cl ₂ Zr ₂	219	0.0006	25	36
CuTe ₂	339	0.0006	49	64
AsCuLi ₂	7	0.0007	1	1
Cl ₂ Zn	300	0.0007	43	57
Cl ₂ V	390	0.0007	49	81
C ₂ Cl ₂ Y ₂	576	0.0007	58	67
S ₂ Sn	435	0.0007	64	81
N ₃ W ₂	512	0.0008	39	79
Se ₂ W	123	0.0008	16	25
Ag ₂	419	0.0008	91	73
I ₂ Nd ₂ S ₂	786	0.0009	100	81
ReSe ₂	183	0.0009	25	36
Au ₂ I ₂	639	0.001	105	81
AgNO ₃	155	0.001	25	16
S ₂ Zr	435	0.001	64	81
HfS ₂	339	0.001	49	64
CCl ₂ Sc ₂	255	0.001	25	36

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

ZnF₂ (P4/mmm)

Structural and electronic properties

	Formula	ZnF ₂
	Spacegroup	P4/mmm
	Prototype	F2Zn
	Parent 3D	F ₄ N ₂ Zn
	Source DB	MPDS
	DB ID	S1703458
DF2-C09	Binding energy [meV/ Å²]	65.11
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	2.78

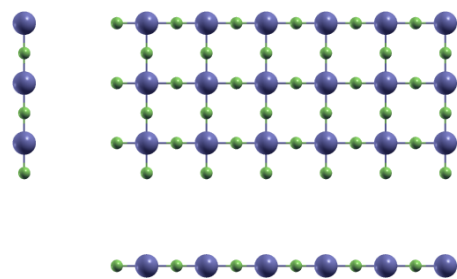


Band structure: Electronic band structure of ZnF₂ (P4/mmm) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of ZnF₂ (P4/mmm) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.87339484	0.00000000	0.00000000
a₂		0.00000000	3.87339484	0.00000000
a₃		0.00000000	0.00000000	12.00000000
		x [Å]	y [Å]	z [Å]
●	Zn	1.93669742	-1.93669742	0.00000000
●	F	1.93669742	0.00000000	0.00000000
●	F	0.00000000	-1.93669742	0.00000000



Orthographic projections: views of ZnF₂ (P4/mmm) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	4	0.3856	1	1
K	4	0.1891	1	1
In	4	0.1112	1	1
InSe	5	0.1493	1	1
Bi ₂	5	0.1549	1	1
AgTl	5	0.0261	1	1
Ag ₂	5	0.1963	1	1
LiO	5	0.1089	1	1
PbTe	5	0.151	1	1
Sb ₂	5	0.1354	1	1
I ₂ Mg	6	0.14	1	1
S ₂ V	6	0.1105	1	1
MoS ₂	6	0.1103	1	1
CdI ₂	6	0.1527	1	1
Nd	6	0.7711	1	3
PSn ₂	6	0.1087	1	1
Ba ₂ Pt	6	0.196	1	1
Br ₂ Ca	6	0.1539	1	1
CaI ₂	6	0.1776	1	1
I ₂ Pr	6	0.004	1	1
S ₂ Zr	6	0.1086	1	1
Br ₂ La	6	0.1403	1	1
Br ₂ Cu	6	0.1074	1	1
I ₂ Yb	6	0.1746	1	1
BiClTe	6	0.153	1	1
AuTe ₂	6	0.1295	1	1
BrCdI	6	0.1427	1	1
I ₂ Zn	6	0.1329	1	1
BaF ₂	6	0.1457	1	1
BiBrTe	6	0.1586	1	1
S ₂ W	6	0.1103	1	1
Bi ₂ Pd	6	0.5626	1	1
GeI ₂	6	0.1385	1	1
AsKSn	6	0.1444	1	1
PbTe ₂	6	0.1419	1	1
I ₂ Nd	6	0.005	1	1
Cl ₂ Cu	6	0.0994	1	1
I ₂ Tm	6	0.1762	1	1
S ₂ Sn	6	0.1086	1	1
SnTe ₂	6	0.1366	1	1
Cl ₂ V	6	0.1094	1	1
GeI ₂	6	0.1512	1	1
I ₂ Pb	6	0.7542	1	1
STl ₂	6	0.1466	1	1
BiTe	6	0.1657	1	1
DyI ₂	6	0.181	1	1
CeI ₂	6	0.0032	1	1
NbTe ₂	6	0.1085	1	1
Se ₂ Yb	6	0.1387	1	1
MoS ₂	6	0.1102	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

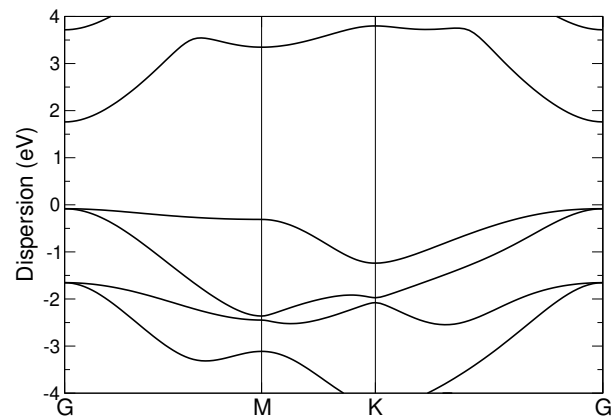
Formula	N° atoms	strain	cell size 1	cell size 2
Cu ₂ Na ₂ Te ₂	636	0.0001	82	65
Cl ₂ Rb ₂	111	0.0001	25	9
Ca ₂ O ₂	304	0.0001	36	49
CdClO	339	0.0002	48	65
OTl ₂	339	0.0002	48	65
Cl ₂ Hf ₂ N ₂	534	0.0002	48	65
AgClO ₄	171	0.0002	25	16
Cl ₄ Cu ₂	342	0.0003	64	25
Br ₂ Gd ₂ O ₂	9	0.0003	1	1
Pd ₂ S ₄	471	0.0003	79	39
Ba ₂ F ₂ I ₂	363	0.0003	49	36
Ag ₂ K ₂ Se ₂	849	0.0003	113	85
Br ₂ Ca ₂ F ₂	9	0.0004	1	1
Cl ₂ S ₂ Tl ₂	537	0.0004	81	49
Te ₂ V	339	0.0005	48	65
Cu ₂ K ₂ Te ₂	621	0.0005	85	61
O ₄ PTl	363	0.0005	49	36
Br ₂ V	597	0.0007	81	118
Se ₂ Ta ₄	531	0.0007	49	64
Mg ₂	701	0.0007	113	181
H ₂ I ₂ Sr ₂	795	0.0007	101	82
Br ₂ F ₂ Yb ₂	9	0.0008	1	1
Cl ₂ Zr ₂	715	0.0008	81	118
Cu ₂ Na ₂ Te ₂	627	0.0008	81	64
LiO ₂	363	0.0009	49	72
CdH ₂ O ₂	469	0.0009	48	65
I ₂ Lu ₂ O ₂	9	0.0009	1	1
Br ₂ F ₂ Tm ₂	9	0.001	1	1
CuGeO ₃	851	0.001	112	103
F ₄ Pb	445	0.001	65	50
Cl ₂ O ₂ V ₂	42	0.0011	4	5
K	688	0.0011	181	145
CCl ₂ Sc ₂	833	0.0011	81	118
HN ₃ OZn	993	0.0011	79	126
Ca ₂ Ge ₂ Mn ₂	9	0.0012	1	1
Br ₂ O ₂ V ₂	51	0.0012	5	6
Bi ₂ Pd	255	0.0012	36	49
HgI ₂	594	0.0012	113	85
As ₂ Mg ₂ Na ₂	786	0.0012	100	81
ReSe ₂	597	0.0012	81	118
H ₂ I ₂ Sr ₂	786	0.0013	100	81
FeSe ₂	75	0.0013	9	16
Br ₂ Cu ₂	7	0.0013	1	1
HNiO ₂	216	0.0013	20	39
Te ₂ W	339	0.0013	48	65
Bi ₂ In ₂	208	0.0014	36	25
MoS ₂	519	0.0014	64	109
Mg ₃	675	0.0014	89	136
I ₂ Tm	576	0.0014	103	89
S ₂ W	519	0.0014	64	109

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

ZnN₃OH (P3m1)

Structural and electronic properties

	Formula	ZnN ₃ OH
	Spacegroup	P3m1
	Prototype	HN3OZn
	Parent 3D	H ₂ N ₆ O ₂ Zn ₂
	Source DB	ICSD
	DB ID	196345
DF2-C09	Binding energy [meV/ Å²]	62.34
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	1.84

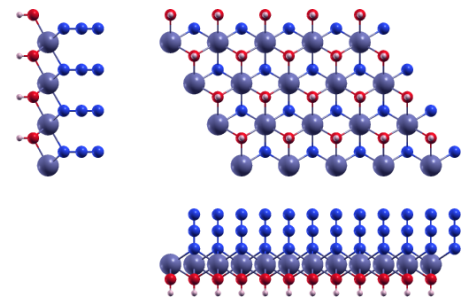


Band structure: Electronic band structure of ZnN₃OH (P3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of ZnN₃OH (P3m1) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		-1.64615811	-2.85122949	0.00000000
a₂		3.29231623	0.00000000	0.00000000
a₃		0.00000000	0.00000000	22.94264110
		x [Å]	y [Å]	z [Å]
●	Zn	0.00000000	0.00000000	0.64739816
*	H	1.64615811	-0.95040983	2.64128000
●	N	0.00000000	-1.90081966	-0.44577803
●	N	0.00000000	-1.90081966	-1.68649704
●	N	0.00000000	-1.90081966	-2.82885687
●	O	1.64615811	-0.95040983	1.67245379



Orthographic projections: views of ZnN₃OH (P3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	7	0.0041	1	1
Sn	7	0.1276	1	1
In	7	0.1307	1	1
AsSb	8	3.0011	1	1
LiO	8	0.0086	1	1
P ₂	8	0.0011	1	1
Mg ₂	8	0.1398	1	1
PSn ₂	9	0.4674	1	1
MoSe ₂	9	0.0034	1	1
Br ₂ Zn	9	0.495	1	1
HfS ₂	9	0.452	1	1
AsSn ₂	9	0.477	1	1
CuTe ₂	9	0.4512	1	1
S ₂ Zr	9	0.4655	1	1
Cl ₂ Ti	9	0.001	1	1
Mg ₃	9	0.1492	1	1
Te ₂ Ti	9	0.4958	1	1
CrI ₂	9	3.0343	1	1
RhTe ₂	9	0.4843	1	1
NbS ₂	9	0.0072	1	1
CoTe ₂	9	0.4528	1	1
S ₂ Ta	9	0.0064	1	1
Se ₂ V	9	0.005	1	1
S ₂ Sn	9	0.4661	1	1
PtSe ₂	9	0.4787	1	1
TaTe ₂	9	0.4755	1	1
Br ₂ Ni	9	0.4569	1	1
FeSe ₂	9	0.1234	1	1
NbTe ₂	9	0.465	1	1
Cl ₂ Mg	9	0.4571	1	1
I ₂ La	9	0.3141	1	1
F ₂ Na	9	0.5003	1	1
HfSe ₂	9	0.4959	1	1
Se ₂ W	9	0.0035	1	1
CdClHO	10	0.4741	1	1
Br ₂ Pr ₂	10	0.4982	1	1
HNiO ₂	10	0.2697	1	1
Ag ₂ Br ₂	10	0.3151	1	1
CdClHO	10	0.4823	1	1
As ₂ Ir ₂	10	0.32	1	1
Mg ₄	10	0.1546	1	1
Ga ₂ S ₂	10	0.4532	1	1
CaClHO	10	2.9049	1	1
AgClO ₂	10	1.8044	1	1
As ₂ Rh ₂	10	0.3146	1	1
Ga ₂ S ₂	10	0.4558	1	1
O ₂ Sn ₂	10	0.2984	1	1
CS ₂ Ta ₂	11	0.0009	1	1
PTe ₂ Ti ₂	11	0.4566	1	1
H ₂ MnO ₂	11	0.2596	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

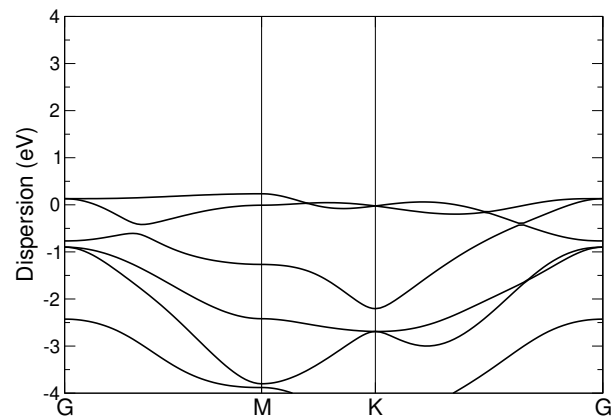
Formula	N° atoms	strain	cell size 1	cell size 2
Bi ₂ Se ₂ Te	731	0.0	81	49
Bi ₂ Te ₃	141	0.0	16	9
BiTe	123	0.0001	16	9
NiTe ₂	471	0.0001	57	43
I ₂ Nd ₂ S ₂	444	0.0001	49	25
Te ₂ Ti	531	0.0001	64	49
Br ₂ Zn	531	0.0002	64	49
N ₂ Re	429	0.0002	43	57
HfSe ₂	531	0.0002	64	49
CoO ₂	363	0.0002	36	49
TaTe ₂	678	0.0002	81	64
In ₂ Te ₃	551	0.0002	61	37
PSn ₂	765	0.0002	91	73
H ₂ MnO ₂	789	0.0002	64	81
SnTe ₂	198	0.0002	25	16
H ₂ Li ₂ O ₂	678	0.0002	65	48
Sb ₂ SeTe ₂	551	0.0003	61	37
CCL ₂ Gd ₂	629	0.0003	64	49
S ₂ Sn	765	0.0003	91	73
AsSb	366	0.0003	49	36
CdClHO	666	0.0003	73	57
NiO ₂	363	0.0004	36	49
PTe ₂ Zr ₂	474	0.0004	49	36
AsSn ₂	678	0.0004	81	64
RhTe ₂	609	0.0004	73	57
I ₂ N ₂ Zr ₂	636	0.0004	66	40
GeI ₂ Y ₂	731	0.0004	81	49
SiTe ₂	471	0.0005	57	43
Br ₂ In ₂ O ₂	798	0.0005	82	51
BH ₄ Li	246	0.0005	25	16
S ₂ Zr	765	0.0006	91	73
Bi ₂ Se ₂ Te	551	0.0006	61	37
N ₃ W ₂	707	0.0006	57	73
C ₂	86	0.0006	9	16
Ga ₂ Ge ₂ Te ₂	246	0.0006	25	16
As ₂ Li ₂ Nd	731	0.0007	81	49
Cl ₂ Er ₂ O ₂	600	0.0007	57	43
CaClHO	514	0.0007	57	43
Hf ₂ I ₂ N ₂	870	0.0007	81	64
CdClHO	742	0.0007	81	64
Li ₂ P ₂ Pr	230	0.0007	25	16
CoI ₂	402	0.0008	49	36
NbTe ₂	765	0.0008	91	73
Br ₂ O ₂ Sc ₂	906	0.0008	91	60
CrO ₂	258	0.0008	25	36
GeNi ₃ Te ₂	366	0.0008	36	25
CBr ₂ Y ₂	629	0.0008	64	49
Cl ₂ O ₂ Tm ₂	600	0.0009	57	43
KNO ₃	29	0.0009	4	1
Se ₂ Zr	471	0.0009	57	43

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

ZnO₂ (P-3m1)

Structural and electronic properties

	Formula	ZnO ₂
	Spacegroup	P-3m1
	Prototype	CdI2
	Parent 3D	O ₂ Zn
	Source DB	COD
	DB ID	1529590
DF2-C09	Binding energy [meV/ Å ²]	63.89
RVV10	Binding energy [meV/ Å ²]	N/A
	Band gap (PBE) [eV]	0.0

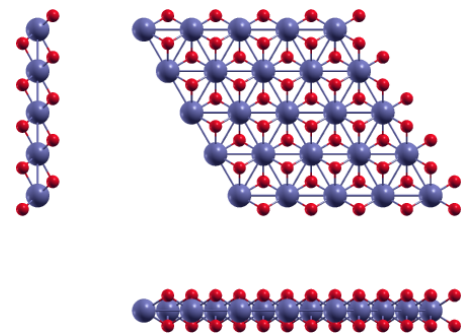


Band structure: Electronic band structure of ZnO₂ (P-3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of ZnO₂ (P-3m1) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		1.52085237	−2.63419358	0.00000000
a₂		1.52085237	2.63419358	0.00000000
a₃		0.00000000	0.00000000	15.84774912
		x [Å]	y [Å]	z [Å]
•	O	0.76042619	−2.19516131	−0.96548488
•	Zn	−0.76042619	−1.31709679	0.00000000
•	O	0.76042619	−0.43903226	0.96548488



Orthographic projections: views of ZnO₂ (P-3m1) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Nd	4	0.2601	1	1
CrS ₂	6	0.0034	1	1
Cl ₂ Mn	6	0.4549	1	1
S ₂ Ta	6	0.4601	1	1
ReS ₂	6	0.0095	1	1
CrO ₂	6	0.2703	1	1
LiO ₂	6	13.5029	1	1
MnO ₂	6	0.2736	1	1
S ₂ Ti	6	0.4726	1	1
NbS ₂	6	0.459	1	1
Te ₂ Zn	6	3.0243	1	1
N ₂ W	6	0.0034	1	1
Cl ₂ Co	6	0.4717	1	1
NbS ₂	6	0.4483	1	1
Br ₂ V	6	0.4861	1	1
ClNZr	6	0.4807	1	1
Cl ₂ Fe	6	0.4699	1	1
AsSe ₂	6	0.4945	1	1
CdO ₂	6	0.4713	1	1
BrNZr	6	0.498	1	1
Cl ₂ Zr	6	0.4709	1	1
FeSe ₂	6	0.1534	1	1
NbSe ₂	6	0.4952	1	1
Cl ₂ Hf ₂	7	0.4631	1	1
Br ₂ Hf ₂	7	0.4969	1	1
Cl ₂ Zr ₂	7	0.4841	1	1
C ₂ F ₂	7	1.5447	1	1
LiNbS ₂	7	0.4603	1	1
In	7	0.2313	2	1
NS ₂ Ta	7	0.0056	1	1
Bi ₂	8	0.2216	2	1
CoH ₂ O ₂	8	0.0084	1	1
Cl ₂ NSc ₂	8	0.4561	1	1
CCl ₂ Sc ₂	8	0.4831	1	1
Sn	8	0.2992	2	2
LiOS ₂ Ti	8	0.4512	1	1
FeH ₂ O ₂	8	0.0022	1	1
Ga ₂ S ₃	8	3.001	1	1
CdI ₂	9	0.2187	2	1
C ₂ Br ₂ Y ₂	9	0.7276	1	1
Br ₂ Ca	9	0.2202	2	1
Br ₂ H ₂ Zr ₂	9	2.9199	1	1
BiClTe	9	0.2191	2	1
Cl ₂ H ₂ Zr ₂	9	0.449	1	1
Br ₂ H ₂ Zr ₂	9	0.4821	1	1
Cl ₂ Cu	9	0.106	2	1
CNNa	9	0.568	2	1
I ₂ Sb ₂ Te ₂	9	3.118	1	1
C ₂ I ₂ Y ₂	9	1.8609	1	1
F ₂ Se ₂ Yb ₂	9	13.6366	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

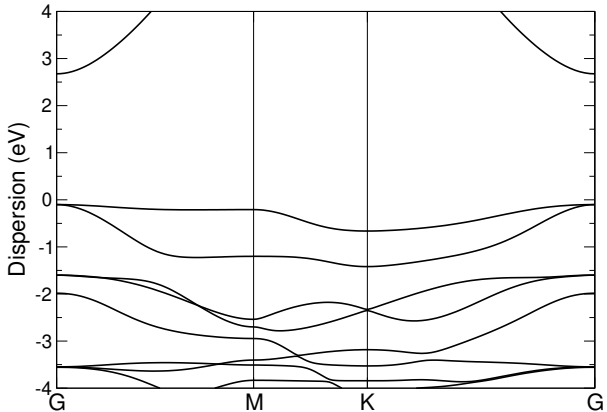
Formula	N° atoms	strain	cell size 1	cell size 2
Cl ₂ La ₂	84	0.0	16	9
Na	183	0.0	49	36
CCl ₂ Sc ₂	504	0.0001	73	57
NbSe ₂	339	0.0001	64	49
S ₂	257	0.0001	61	37
BiBrTe	354	0.0001	79	39
I ₂ La	177	0.0002	39	20
Br ₂ Ti	300	0.0002	57	43
Br ₂ Hg ₃	345	0.0002	100	9
Fe ₂ Te ₂	339	0.0002	65	36
Ni ₂ SbTe ₂	368	0.0003	61	37
PbTe	197	0.0003	49	25
C ₂ F ₂	304	0.0003	36	49
I ₂ La ₂ P	545	0.0003	100	49
Cl ₂ H ₂ Lu ₂	258	0.0003	36	25
Cl ₂ H ₂ Sc ₂	429	0.0003	57	43
Ca ₂ Cl ₂	339	0.0003	65	36
Ga ₂ S ₃	327	0.0003	49	36
As ₂ CeLi ₂	272	0.0003	49	25
Cl ₂ Zr ₂	447	0.0003	73	57
AsSe ₂	339	0.0003	64	49
LiNbS ₂	624	0.0004	100	81
NS ₂ Zr	291	0.0004	49	36
I ₂ V	123	0.0004	25	16
Ga ₂ Se ₂	331	0.0004	61	37
As ₂ Rh ₂	197	0.0004	39	20
P ₂ Sn ₂	439	0.0004	81	49
Br ₂ H ₂ Zr ₂	429	0.0004	57	43
Br ₂ H ₂ Zr ₂	561	0.0004	73	57
S ₂ Ta	543	0.0004	100	81
As ₂ Ru ₂	339	0.0005	65	36
GeI ₂	222	0.0005	49	25
Br ₂ Cr	300	0.0005	57	43
Se ₂ Ta	300	0.0005	57	43
Bi ₂ STe ₂	272	0.0005	49	25
C ₂ Br ₂ Gd ₂	594	0.0005	92	53
Se ₂ Zr	123	0.0005	25	16
F ₂ Se ₂ Yb ₂	537	0.0005	81	49
IKO ₃	192	0.0005	49	9
Nd	273	0.0006	64	81
Br ₂ Hf ₂	388	0.0006	64	49
IrTe ₂	294	0.0006	61	37
H ₂ I ₂ Yb ₂	237	0.0006	39	20
Cl ₂ Mg	183	0.0006	36	25
Cu ₂ Sr ₂	496	0.0006	100	49
Br ₂ O ₂ Yb ₂	411	0.0006	65	36
Ag ₂ Br ₂	197	0.0006	39	20
Br ₂ Ni	183	0.0007	36	25
SbSe ₂ Tl	444	0.0007	100	36
Br ₂ O ₂ Tm ₂	411	0.0007	65	36

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

ZnOHF (P3m1)

Structural and electronic properties





	Formula	ZnOHF
	Spacegroup	P3m1
	Prototype	FHOZn
	Parent 3D	FHOZn
	Source DB	MPDS
	DB ID	S1621908
DF2-C09	Binding energy [meV/ Å²]	80.55
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	2.78

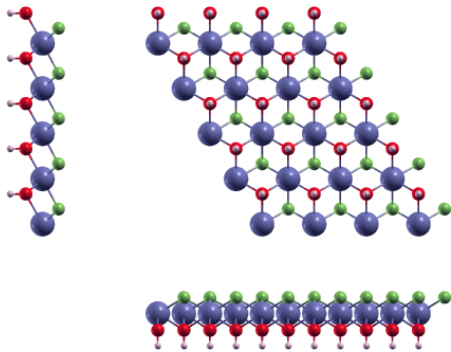


Band structure: Electronic band structure of ZnOHF (P3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of ZnOHF (P3m1) in Cartesian coordinates.

		<i>x</i> [Å]	<i>y</i> [Å]	<i>z</i> [Å]
a₁		−1.60355876	−2.77744524	0.00000000
a₂		3.20711751	0.00000000	0.00000000
a₃		0.00000000	0.00000000	18.10006679
		<i>x</i> [Å]	<i>y</i> [Å]	<i>z</i> [Å]
	Zn	0.00000000	0.00000000	−0.50864845
	H	1.60355876	−0.92581508	1.48437602
	O	1.60355876	−0.92581508	0.51700514
	F	0.00000000	−1.85163016	−1.49273271



Orthographic projections: views of ZnOHF (P3m1) as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Sn	5	0.1368	1	1
Na	5	0.4562	1	1
In	5	0.1405	1	1
In	5	0.0068	1	1
As ₂	6	0.4762	1	1
LiO	6	0.0036	1	1
Mg ₂	6	0.151	1	1
Cl ₂ Zn	7	0.4735	1	1
S ₂ V	7	0.0037	1	1
MoS ₂	7	0.003	1	1
MoTe ₂	7	0.4618	1	1
PSn ₂	7	0.4996	1	1
HfS ₂	7	0.4833	1	1
Te ₂ V	7	0.4666	1	1
I ₂ Pr	7	0.3278	1	1
CuTe ₂	7	0.4823	1	1
S ₂ Zr	7	0.4975	1	1
Br ₂ Co	7	0.4751	1	1
Ca ₂ N	7	0.4776	1	1
Te ₂ Zn	7	0.4614	1	1
S ₂ W	7	0.0029	1	1
Br ₂ Mn	7	0.4705	1	1
PtS ₂	7	0.4587	1	1
CoTe ₂	7	0.4841	1	1
CdClO	7	0.4654	1	1
Se ₂ Ti	7	0.4522	1	1
Te ₂ W	7	0.4622	1	1
I ₂ Nd	7	0.3298	1	1
S ₂ Sn	7	0.4982	1	1
Cl ₂ V	7	0.0011	1	1
OTl ₂	7	0.4659	1	1
Br ₂ Fe	7	0.4753	1	1
CeI ₂	7	0.3262	1	1
FeSe ₂	7	0.1318	1	1
NbTe ₂	7	0.497	1	1
MoS ₂	7	0.0028	1	1
CrSe ₂	7	0.0001	1	1
CrSe ₂	7	0.0024	1	1
O ₂ Pt	7	0.0083	1	1
N ₂ Re	7	0.2616	1	1
F ₂ Zn	7	0.3196	1	1
NS ₂ Zr	8	0.4572	1	1
Ir ₂ P ₂	8	0.3294	1	1
CdClHO	8	2.9656	1	1
Cu ₂ S ₂	8	0.3131	1	1
Br ₂ Cu ₂	8	0.3169	1	1
Br ₂ Zr ₂	8	0.4513	1	1
O ₂ Sn ₂	8	0.3143	1	1
KS ₂ Ti	8	0.4715	1	1
Ga ₂ S ₂	8	0.4845	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

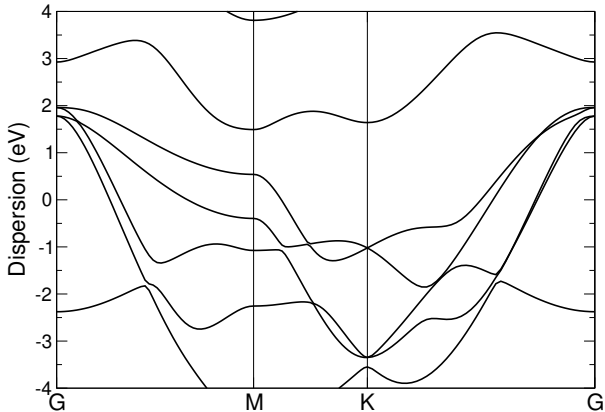
Formula	N° atoms	strain	cell size 1	cell size 2
HfS ₂	463	0.0	73	57
CdI ₂	91	0.0	16	9
CCl ₂ Lu ₂	644	0.0	81	64
SnTe ₂	355	0.0001	61	37
Te ₂ Zn	643	0.0001	100	81
As ₂	452	0.0001	81	64
CrO ₂	291	0.0001	36	49
Te ₂ V	583	0.0001	91	73
CrSe ₂	7	0.0001	1	1
CoI ₂	219	0.0002	36	25
Gd ₂ GeI ₂	109	0.0002	16	9
Br ₂ Cd	148	0.0002	25	16
I ₂ Ti	219	0.0002	36	25
Cu ₂ Rb ₂ Te ₂	844	0.0002	130	54
HfLiS ₂	724	0.0002	100	81
BH ₄ Li	466	0.0002	61	37
I ₂ La ₂ Sb	645	0.0002	100	49
CaI ₂	271	0.0002	49	25
CeLi ₂ P ₂	569	0.0003	81	49
MoTe ₂	643	0.0003	100	81
Br ₂ La ₂ P	109	0.0003	16	9
Br ₂ Fe	516	0.0003	81	64
I ₂ N ₂ Ti ₂	860	0.0003	110	70
CuTe ₂	463	0.0003	73	57
Br ₂ Co	516	0.0003	81	64
CoTe ₂	463	0.0004	73	57
Br ₂ PY ₂	180	0.0004	25	16
Pb ₂ Se ₂	992	0.0004	170	78
CdI ₂	91	0.0004	16	9
Cl ₂ Hf ₂ N ₂	802	0.0004	91	73
BiClTe	91	0.0004	16	9
OTl ₂	583	0.0004	91	73
Te ₂ W	643	0.0004	100	81
Bi ₂ In ₂	736	0.0004	130	54
C ₂ Br ₂ Gd ₂	526	0.0005	67	43
C ₂ Br ₂ Tb ₂	526	0.0005	67	43
I ₂ N ₂ Zr ₂	412	0.0005	49	36
I ₂ Pr	91	0.0005	16	9
Ga ₂ S ₂	520	0.0005	73	57
Ga ₂ Se ₂	340	0.0005	49	36
K	449	0.0006	100	49
NbTe ₂	403	0.0006	64	49
CdClO	583	0.0006	91	73
AsSb	194	0.0006	36	25
Cl ₂ Y ₂	269	0.0006	36	25
Ca ₂ N	516	0.0006	81	64
Au ₂ I ₂	480	0.0006	82	38
CBr ₂ Lu ₂	501	0.0006	64	49
Br ₂ HLa	520	0.0006	81	49
CaCl	634	0.0007	118	81

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

ZnTe₂ (P-3m1)

Structural and electronic properties

	Formula	ZnTe ₂
	Spacegroup	P-3m1
	Prototype	CdI2
	Parent 3D	Te ₂ Zn
	Source DB	MPDS
	DB ID	S1404529
DF2-C09	Binding energy [meV/ Å²]	84.44
RVV10	Binding energy [meV/ Å²]	N/A
	Band gap (PBE) [eV]	0.0

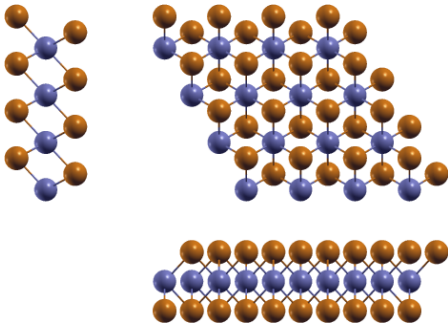


Band structure: Electronic band structure of ZnTe₂ (P-3m1) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of ZnTe₂ (P-3m1) in Cartesian coordinates.

	<i>x</i> [Å]	<i>y</i> [Å]	<i>z</i> [Å]
a₁	1.78204686	−3.08659570	0.00000000
a₂	1.78204686	3.08659570	0.00000000
a₃	0.00000000	0.00000000	17.98385579
	<i>x</i> [Å]	<i>y</i> [Å]	<i>z</i> [Å]
● Te	1.78204686	−1.02886523	−1.92117098
● Zn	−0.00000000	0.00000000	0.00000000
● Te	1.78204686	1.02886523	1.92117098



Orthographic projections: views of ZnTe₂ (P-3m1) as seen from the *x* axis (left), the *y* axis (bottom) and the *z* axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	4	0.1243	1	1
Na	4	0.0021	1	1
In	4	0.1111	1	1
In	4	0.2577	1	1
Gd	4	0.1143	1	1
HgO	5	0.1327	1	1
As ₂	5	0.0059	1	1
LiO	5	0.2727	1	1
Mg ₂	5	0.1156	1	1
Cl ₂ Zn	6	0.0049	1	1
S ₂ V	6	0.2621	1	1
MoS ₂	6	0.2632	1	1
MoTe ₂	6	0.0002	1	1
AgTe ₂	6	0.1263	1	1
HfS ₂	6	0.0088	1	1
HfTe ₂	6	0.4642	1	1
Te ₂ V	6	0.0021	1	1
CuTe ₂	6	0.0084	1	1
Br ₂ Co	6	0.0055	1	1
Ca ₂ N	6	0.0065	1	1
AuTe ₂	6	0.484	1	1
PdTe ₂	6	0.4777	1	1
Mg ₃	6	0.1209	1	1
I ₂ Zn	6	0.4961	1	1
S ₂ W	6	0.2633	1	1
Bi ₂ Pd	6	0.1403	1	1
Br ₂ Mn	6	0.0036	1	1
CrTe ₂	6	0.0073	1	1
PtS ₂	6	0.0011	1	1
CoTe ₂	6	0.0091	1	1
CdClO	6	0.0016	1	1
Ba ₂ N	6	0.4681	1	1
Se ₂ Ti	6	0.0037	1	1
Br ₂ Ti	6	0.0079	1	1
Te ₂ Zr	6	0.4654	1	1
Te ₂ W	6	0.0003	1	1
PbTe ₂	6	3.0187	1	1
Cl ₂ Cu	6	0.5976	1	1
SnTe ₂	6	2.9354	1	1
Cl ₂ V	6	0.269	1	1
OTl ₂	6	0.0018	1	1
Br ₂ Fe	6	0.0056	1	1
O ₂ Zn	6	1.5322	1	1
Br ₂ Cr	6	0.0076	1	1
CuO ₂	6	2.7288	1	1
MoS ₂	6	0.2635	1	1
CrSe ₂	6	0.2673	1	1
Se ₂ Ta	6	0.0087	1	1
PtTe ₂	6	0.483	1	1
Br ₂ Cd	6	0.4753	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

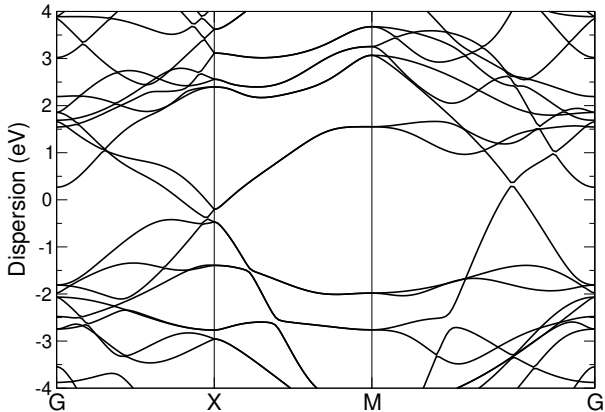
Formula	N° atoms	strain	cell size 1	cell size 2
CoH ₂ O ₂	414	0.0	43	57
K	220	0.0	61	37
CdI ₂	183	0.0	36	25
Sb ₂	257	0.0	57	43
PtTe ₂	390	0.0001	73	57
FHOZn	643	0.0001	81	100
Gd ₂ GeI ₂	233	0.0001	36	25
O ₂ Pt	390	0.0001	57	73
Bi ₂ Se ₃	327	0.0001	49	36
Gd ₂ I ₂	291	0.0001	49	36
MoTe ₂	6	0.0002	1	1
Cu ₂ Rb ₂ Te ₂	237	0.0002	39	20
Br ₂ La ₂	343	0.0002	57	43
Br ₂ La	255	0.0002	49	36
Br ₂ O ₂ Tb ₂	483	0.0002	65	48
CrSe ₂	543	0.0002	81	100
Cu ₃ Se ₃	711	0.0002	91	73
Br ₂ Cd	435	0.0003	81	64
Cl ₂ OV	519	0.0003	77	72
I ₂ Zn	339	0.0003	64	49
GeNi ₃ Te ₂	786	0.0003	100	81
HfLiS ₂	7	0.0003	1	1
I ₂ La ₂ Sb	488	0.0003	81	49
AuTe ₂	390	0.0003	73	57
NaPSn	543	0.0003	100	81
BiClTe	183	0.0003	36	25
I ₂ La ₂ Sb	368	0.0003	61	37
Te ₂ W	6	0.0003	1	1
HNiO ₂	219	0.0003	25	36
Bi ₂ In ₂	197	0.0003	39	20
Br ₂ La ₂ P	233	0.0003	36	25
Br ₂ Cu ₂	387	0.0004	65	48
I ₂ S ₂ Sm ₂	405	0.0004	61	37
I ₂ Pr	183	0.0004	36	25
Cu ₂ I ₂	291	0.0004	49	36
Br ₂ Gd ₂ Ge	327	0.0004	49	36
Br ₂ PY ₂	563	0.0004	81	64
Ba ₂ N	492	0.0005	91	73
CdI ₂	183	0.0005	36	25
Br ₂ Lu ₂ S ₂	738	0.0005	120	63
Pt ₂ Te ₂	624	0.0005	100	81
Br ₂ Ho ₂ S ₂	582	0.0005	96	49
I ₂ Mg	255	0.0005	49	36
Br ₂ Lu ₂ S ₂	738	0.0005	120	63
H ₂ NiO ₂	674	0.0006	73	91
Te ₂ Zr	492	0.0006	91	73
MoS ₂	492	0.0006	73	91
Br ₂ Hf ₂ N ₂	30	0.0006	4	3
I ₄ Sr ₂	150	0.0006	32	9
Li ₂ P ₂ Pr	386	0.0006	57	43

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

ZrGeSe (P4/nmm (129))

Structural and electronic properties







	Formula	ZrGeSe
	Spacegroup	P4/nmm (129)
	Prototype	PbClF
	Parent 3D	Zr ₂ Ge ₂ Se ₂
	Source DB	COD
	DB ID	1527644
DF2-C09	Binding energy [meV/ Å²]	69.21
RVV10	Binding energy [meV/ Å²]	64.51
	Band gap (PBE) [eV]	0.0

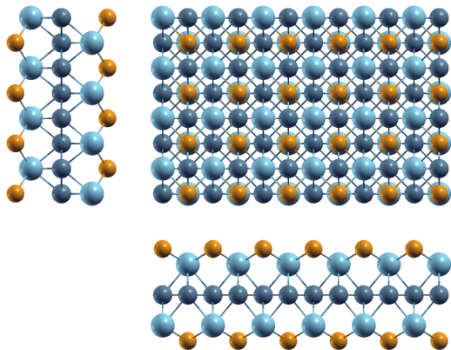


Band structure: Electronic band structure of ZrGeSe (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of ZrGeSe (P4/nmm (129)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.63283082	0.00000000	0.00000000
a₂		0.00000000	3.63283082	0.00000000
a₃		0.00000000	0.00000000	26.28566641
		x [Å]	y [Å]	z [Å]
	Zr	0.00000000	1.81641541	15.34810848
	Se	1.81641541	0.00000000	16.46853595
	Zr	1.81641541	0.00000000	10.93755793
	Ge	0.00000000	0.00000000	13.14283320
	Ge	1.81641541	1.81641541	13.14283320
	Se	0.00000000	1.81641541	9.81713045



Orthographic projections: views of ZrGeSe (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	7	0.588	1	1
InSe	8	0.1825	1	1
HgO	8	0.2153	1	1
AsSb	8	0.1349	1	1
Bi ₂	8	0.1899	1	1
GeTe	8	0.1398	1	1
AgTl	8	0.3994	1	1
S ₂	8	0.1411	1	1
PbTe	8	0.1847	1	1
Sb ₂	8	0.1639	1	1
CaCl	8	0.0042	1	1
IrTe ₂	9	0.1406	1	1
I ₂ Mg	9	0.1702	1	1
CdCl ₂	9	0.1389	1	1
CdI ₂	9	0.1869	1	1
AgTe ₂	9	0.5971	1	1
ReSe ₂	9	0.109	1	1
Br ₂ Ca	9	0.1885	1	1
InSe ₂	9	0.1392	1	1
GeTe ₂	9	0.1381	1	1
SiTe ₂	9	0.1303	1	1
HfTe ₂	9	0.148	1	1
I ₂ Mn	9	0.139	1	1
Br ₂ La	9	0.1706	1	1
Br ₂ Cu	9	0.1274	1	1
NSr ₂	9	0.1362	1	1
PbS ₂	9	0.1329	1	1
BiClTe	9	0.1874	1	1
AuTe ₂	9	0.1556	1	1
BrCdI	9	0.1739	1	1
LiO ₂	9	0.3412	1	1
PdTe ₂	9	0.1532	1	1
FeI ₂	9	0.1372	1	1
I ₂ Ni	9	0.1382	1	1
CrI ₂	9	0.1368	1	1
I ₂ Zn	9	0.1604	1	1
BaF ₂	9	0.1778	1	1
BiBrTe	9	0.1946	1	1
GeI ₂	9	0.1681	1	1
Ba ₂ Hg	9	1.1286	1	1
N ₂ W	9	0.1093	1	1
Br ₂ V	9	0.1088	1	1
Ba ₂ N	9	0.1495	1	1
AsKSn	9	0.1761	1	1
Te ₂ Zr	9	0.1485	1	1
PbTe ₂	9	0.1727	1	1
NiTe ₂	9	0.1299	1	1
SnTe ₂	9	0.1656	1	1
I ₂ V	9	0.1313	1	1
GeI ₂	9	0.185	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

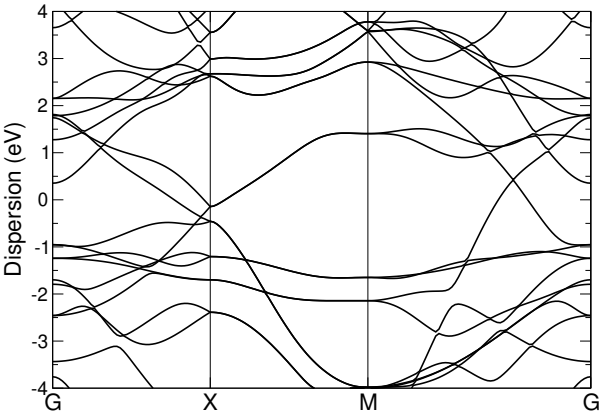
Formula	N° atoms	strain	cell size 1	cell size 2
Ca ₂ Cl ₂	10	0.0	1	1
As ₂ Cd ₂ K ₂	246	0.0	25	16
AgClO ₄	150	0.0	16	9
Pb ₂ Se ₂	628	0.0001	72	49
Cu ₂ Se ₂ Tl ₂	870	0.0003	81	64
AgTe ₂	495	0.0004	50	65
H ₂ I ₂ Sr ₂	876	0.0004	85	61
Bi ₂ In ₂	896	0.0005	106	65
LiOS ₂ Ti	613	0.0006	48	65
Cu ₂ I ₂	742	0.0006	81	64
Au ₂ I ₂	306	0.0006	35	24
Ba ₂ Hg	933	0.0006	113	85
Bi ₂ O ₂	752	0.0007	82	65
AgTe ₂	486	0.0007	49	64
As ₂ Co ₂	10	0.0007	1	1
LiO	722	0.0007	81	118
Cl ₄ Mn	872	0.0008	97	58
H ₄ Ti	791	0.0009	61	85
Br ₂ H ₂ Sr ₂	870	0.001	81	64
O ₄ PSn	246	0.001	25	16
Cl ₂ Mn	483	0.001	48	65
Cu ₂ Na ₂ Te ₂	366	0.001	36	25
Cl ₂ Rb ₂	944	0.001	130	41
I ₂ La ₂ O ₂	678	0.001	64	49
FeSe ₂	171	0.0011	16	25
Br ₂ La ₂ O ₂	882	0.0012	82	65
Eu ₂ F ₂ I ₂	882	0.0012	82	65
BN	584	0.0013	54	130
Br ₂ Ca ₃ Si	360	0.0013	40	20
H ₂ Li ₂ Pd	791	0.0014	61	85
Br ₂ In ₂ O ₂	90	0.0014	8	7
Bi ₂ O ₂	742	0.0014	81	64
Cl ₂ H ₂ Zr ₂	678	0.0014	48	65
AsKSn	885	0.0014	103	89
Cl ₂ NSc ₂	613	0.0015	48	65
Ge ₂ Te ₂	734	0.0015	83	59
Cu ₂ Te ₂	984	0.0015	98	99
Ba ₂ Pt	594	0.0015	73	52
Mg ₃	363	0.0015	36	49
Mg ₄	962	0.0015	85	113
HN ₃ OZn	750	0.0015	52	73
AsKSn	765	0.0016	89	77
Ag ₂	542	0.0016	73	52
Br ₂ Ti	603	0.0016	62	77
HgO	554	0.0016	65	82
Cl ₂ H ₂ Sc ₂	834	0.0016	62	77
Br ₂ Cr	603	0.0017	62	77
NbS ₂	483	0.0017	48	65
Cl ₂ Sc ₂	680	0.0017	62	77
Se ₂ Ta	603	0.0017	62	77

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

ZrGeTe (P4/nmm (129))

Structural and electronic properties







	Formula	ZrGeTe
	Spacegroup	P4/nmm (129)
	Prototype	PbClF
	Parent 3D	Zr ₂ Ge ₂ Te ₂
	Source DB	COD
	DB ID	1527645
DF2-C09	Binding energy [meV/ Å²]	57.98
RVV10	Binding energy [meV/ Å²]	36.76
	Band gap (PBE) [eV]	0.0

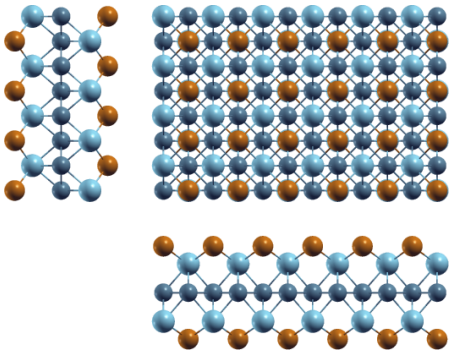


Band structure: Electronic band structure of ZrGeTe (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of ZrGeTe (P4/nmm (129)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.76533008	0.00000000	0.00000000
a₂		0.00000000	3.76533008	0.00000000
a₃		0.00000000	0.00000000	26.88739744
		x [Å]	y [Å]	z [Å]
	Zr	0.00000000	1.88266504	15.61714817
	Te	1.88266504	0.00000000	16.96023244
	Zr	1.88266504	0.00000000	11.27024927
	Ge	0.00000000	0.00000000	13.44369872
	Ge	1.88266504	1.88266504	13.44369872
	Te	0.00000000	1.88266504	9.92716500



Orthographic projections: views of ZrGeTe (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
K	7	1.1181	1	1
K	7	0.7784	1	1
InSe	8	0.1629	1	1
Bi ₂	8	0.1693	1	1
AgTl	8	0.3634	1	1
PbTe	8	0.1648	1	1
Sb ₂	8	0.1468	1	1
CrS ₂	9	0.1115	1	1
I ₂ Mg	9	0.1522	1	1
CdI ₂	9	0.1667	1	1
MoTe ₂	9	0.1084	1	1
Br ₂ Ca	9	0.1681	1	1
CaI ₂	9	0.1946	1	1
HfTe ₂	9	0.1337	1	1
Te ₂ V	9	0.1089	1	1
Br ₂ La	9	0.1526	1	1
Br ₂ Cu	9	0.115	1	1
I ₂ Yb	9	0.1912	1	1
BiClTe	9	0.1671	1	1
ReS ₂	9	0.1101	1	1
AuTe ₂	9	0.1399	1	1
BrCdI	9	0.1554	1	1
Cl ₂ Zn	9	0.0066	1	1
PdTe ₂	9	0.1379	1	1
I ₂ Zn	9	0.1439	1	1
BaF ₂	9	0.1588	1	1
BiBrTe	9	0.1734	1	1
Bi ₂ Pd	9	0.2073	1	1
GeI ₂	9	0.1504	1	1
Ba ₂ Hg	9	0.3821	1	1
CdClO	9	0.1088	1	1
Ba ₂ N	9	0.1348	1	1
AsKSn	9	0.1573	1	1
Te ₂ Zr	9	0.134	1	1
Te ₂ W	9	0.1085	1	1
PbTe ₂	9	0.1544	1	1
Cl ₂ Cu	9	0.1038	1	1
I ₂ Tm	9	0.193	1	1
SnTe ₂	9	0.1483	1	1
GeI ₂	9	0.165	1	1
STl ₂	9	0.1598	1	1
OTl ₂	9	0.1088	1	1
BiTe	9	0.1813	1	1
DyI ₂	9	0.754	1	1
Se ₂ Yb	9	0.1507	1	1
BiTe ₂	9	0.1509	1	1
GdI ₂	9	0.1768	1	1
PtTe ₂	9	0.1396	1	1
Br ₂ Cd	9	0.1371	1	1
CdI ₂	9	0.1662	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

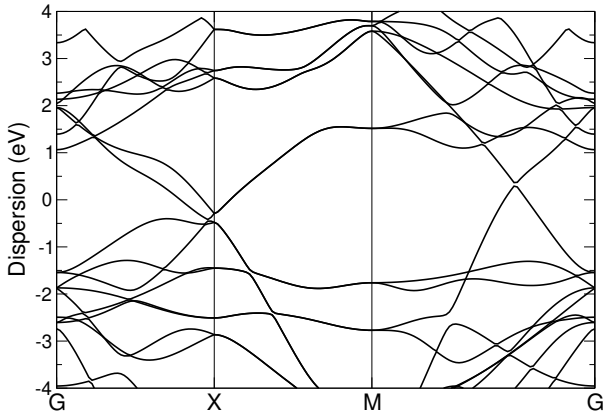
Formula	N° atoms	strain	cell size 1	cell size 2
Ba ₂ Hg	843	0.0001	100	81
H ₂ I ₂ Sr ₂	690	0.0001	65	50
FeSe ₂	639	0.0002	58	97
Br ₂ Lu ₂ O ₂	12	0.0002	1	1
NbSe ₂	483	0.0002	48	65
AgClO ₄	780	0.0003	81	49
Ba ₂ F ₂ I ₂	366	0.0004	36	25
AuI ₄ Li	912	0.0004	105	47
La ₂ S ₂	580	0.0005	64	49
AsSe ₂	483	0.0005	48	65
Br ₂ Hf ₂	548	0.0005	48	65
O ₄ PTl	366	0.0006	36	25
La ₂ S ₂	570	0.0007	63	48
Se ₂ Sn ₂	514	0.0008	57	43
Sn	496	0.0008	65	106
LiO ₂	366	0.0008	36	50
Cl ₄ KTl	390	0.0009	49	16
AlH ₄ Na	246	0.0009	25	16
BrNZr	483	0.0009	48	65
AgTe ₂	621	0.0009	61	85
Sm	403	0.001	48	115
C ₂ Br ₂ Y ₂	990	0.001	80	85
Fe ₂ SeTe	10	0.001	1	1
In	859	0.001	113	181
CrSe ₂	852	0.0011	79	126
AgClO ₂	928	0.0011	92	94
FHOZn	978	0.0011	79	126
H ₂ I ₂ Sr ₂	678	0.0012	64	49
C ₄ Ca ₂	870	0.0012	79	66
Br ₂ H ₂ Yb ₂	12	0.0013	1	1
As ₂ Mg ₂ Na ₂	678	0.0013	64	49
C ₂ Br ₂ La ₂	138	0.0013	12	11
C ₂ Br ₂ Y ₂	978	0.0013	79	84
C ₂ Br ₂ Y ₂	756	0.0013	61	65
As ₂ Fe ₂ Li ₂	12	0.0013	1	1
Bi ₂ Pd	495	0.0013	50	65
Se ₂ Ta	483	0.0014	48	65
Au ₂ I ₂	968	0.0014	108	80
ReS ₂	711	0.0014	64	109
Cl ₂ Mn	840	0.0015	81	118
NbSe ₂	483	0.0015	48	65
GdI ₂	885	0.0015	103	89
Gd	382	0.0015	46	106
Br ₂ Cr ₂ S ₂	558	0.0015	48	45
NbS ₂	840	0.0015	81	118
F ₄ Pb	474	0.0015	49	36
Ca ₂ Cl ₂ F ₂	12	0.0015	1	1
Mg ₂	806	0.0015	89	136
I ₂ Se ₂ Tb ₂	228	0.0015	24	14
S ₂ Ti	531	0.0016	52	73

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.

ZrSiSe (P4/nmm (129))

Structural and electronic properties







Formula	ZrSiSe
Spacegroup	P4/nmm (129)
Prototype	PbClF
Parent 3D	Zr ₂ Si ₂ Se ₂
Source DB	COD
DB ID	9008350
DF2-C09 Binding energy [meV/ Å²]	58.49
RVV10 Binding energy [meV/ Å²]	47.18
Band gap (PBE) [eV]	0.0

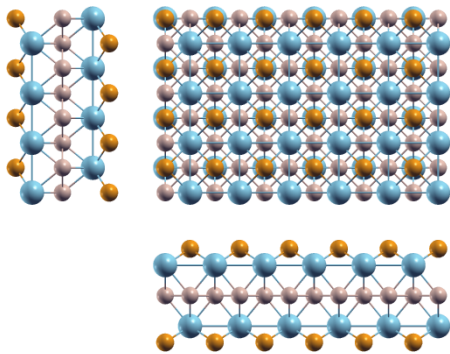


Band structure: Electronic band structure of ZrSiSe (P4/nmm (129)) in a representative window around the Fermi energy and along a high-symmetry path.

Optimized crystal structure

Structural parameters: relaxed cell (top) and atomic positions (bottom) of ZrSiSe (P4/nmm (129)) in Cartesian coordinates.

		x [Å]	y [Å]	z [Å]
a₁		3.54944270	0.00000000	0.00000000
a₂		0.00000000	3.54944270	0.00000000
a₃		0.00000000	0.00000000	26.49393366
		x [Å]	y [Å]	z [Å]
	Zr	1.77472135	0.00000000	15.41949334
	Se	0.00000000	1.77472135	16.58706286
	Zr	0.00000000	1.77472135	11.07444032
	Si	0.00000000	0.00000000	13.24696683
	Si	1.77472135	1.77472135	13.24696683
	Se	1.77472135	0.00000000	9.90687080



Orthographic projections: views of ZrSiSe (P4/nmm (129)) as seen from the x axis (left), the y axis (bottom) and the z axis (center).

Lattice matching - minimal size

Formula	N° atoms	strain	cell size 1	cell size 2
Tl	7	0.2141	1	1
InSe	8	0.1967	1	1
AsSb	8	0.1441	1	1
Bi ₂	8	0.7716	1	1
GeTe	8	0.1497	1	1
S ₂	8	0.1512	1	1
Sb ₂	8	0.1764	1	1
CaCl	8	0.0068	1	1
IrTe ₂	9	0.1505	1	1
I ₂ Mg	9	0.1834	1	1
CdCl ₂	9	0.1486	1	1
Cl ₂ Mn	9	0.1085	1	1
AgTe ₂	9	0.2175	1	1
S ₂ Ta	9	0.109	1	1
Br ₂ Zn	9	0.1355	1	1
Br ₂ Ca	9	0.7674	1	1
InSe ₂	9	0.149	1	1
AsSn ₂	9	0.1303	1	1
GeTe ₂	9	0.1477	1	1
SiTe ₂	9	0.1388	1	1
HfTe ₂	9	0.1589	1	1
I ₂ Mn	9	0.1488	1	1
Br ₂ La	9	0.1838	1	1
NSr ₂	9	0.1455	1	1
PbS ₂	9	0.1418	1	1
AuTe ₂	9	0.1673	1	1
BrCdI	9	0.1873	1	1
PdTe ₂	9	0.1646	1	1
FeI ₂	9	0.1467	1	1
I ₂ Ni	9	0.1479	1	1
Mg ₃	9	0.2077	1	1
Te ₂ Ti	9	0.1357	1	1
NbS ₂	9	0.1089	1	1
CrI ₂	9	0.1463	1	1
I ₂ Zn	9	0.1726	1	1
BaF ₂	9	0.1916	1	1
BiBrTe	9	0.7855	1	1
RhTe ₂	9	0.1324	1	1
GeI ₂	9	0.1811	1	1
Ba ₂ N	9	0.1605	1	1
AsKSn	9	0.1898	1	1
Te ₂ Zr	9	0.1594	1	1
PbTe ₂	9	0.1861	1	1
NiTe ₂	9	0.1383	1	1
SnTe ₂	9	0.1783	1	1
I ₂ V	9	0.1399	1	1
Se ₂ Zr	9	0.1392	1	1
STl ₂	9	0.1929	1	1
PtSe ₂	9	0.1308	1	1
CoI ₂	9	0.1445	1	1

Table showing the first 50 lattice matching combinations with the smallest number of atoms in the supercell.

Lattice matching - minimal strain

Formula	N° atoms	strain	cell size 1	cell size 2
Ca ₂ H ₂ I ₂	882	0.0	82	65
Pb ₂ Se ₂	860	0.0	100	65
Br ₂ Ce ₂ O ₂	870	0.0001	81	64
K ₂ Mn ₂ Sb ₂	870	0.0001	81	64
Mg ₄	718	0.0001	65	82
Cu ₂ K ₂ Te ₂	780	0.0004	81	49
Tl	472	0.0005	65	82
CNb ₂ S ₂	613	0.0005	48	65
I ₂ O ₂ Pr ₂	678	0.0005	64	49
Br ₂ Ca ₃ Si	876	0.0005	85	61
Eu ₂ I ₂ O ₂	870	0.0006	81	64
Ba ₂ H ₂ I ₂	930	0.0006	97	58
F ₂ I ₂ Sm ₂	678	0.0006	64	49
In	604	0.0006	81	118
Cl ₂ S ₂ Tl ₂	444	0.0006	49	25
Sn	186	0.0007	25	36
Gd ₂ I ₂ S ₂	168	0.0007	18	10
Ba ₂ Hg	693	0.0008	85	61
Ca ₂ H ₂ I ₂	870	0.0008	81	64
O ₂ Pb ₂	580	0.0008	64	49
Mg ₄	708	0.0009	64	81
Cu ₄ Te ₂	972	0.0009	90	72
Cl ₂ N ₂ Zr ₂	78	0.0009	7	6
P ₂	418	0.001	48	65
C ₂	518	0.001	48	115
As ₂ Ir ₂	752	0.001	82	65
N ₂ W	852	0.001	79	126
CKN	684	0.0011	88	52
Cl ₂ Ti	483	0.0011	48	65
Pb ₂ Se ₂	422	0.0011	49	32
I ₂ La	843	0.0012	100	81
CS ₂ Ta ₂	613	0.0012	48	65
Tl	465	0.0012	64	81
Cl ₄ Cu ₂	390	0.0013	49	16
AgTl	528	0.0013	70	54
Sb ₂	796	0.0014	103	89
Br ₂ La ₂	974	0.0014	103	89
O ₄ PSn	780	0.0014	81	49
I ₂ Nd ₂ O ₂	690	0.0014	65	50
As ₂ Rh ₂	924	0.0014	100	81
I ₂ S ₂ Tb ₂	750	0.0015	73	52
Cu ₂ F ₄	78	0.0015	9	4
Au ₂ Br ₂	316	0.0015	36	25
I ₂ O ₂ Sm ₂	870	0.0016	81	64
I ₂ S ₂ Yb ₂	198	0.0016	21	12
Br ₂ La ₂	842	0.0016	89	77
Br ₂ Ca ₃ Si	984	0.0016	96	68
Eu ₂ F ₂ I ₂	678	0.0016	64	49
F ₄ Sn	815	0.0016	85	61
DyI ₂	594	0.0016	73	52

Table showing the first 50 lattice matching combinations with the smallest strain needed to build the supercell.