Supplemental Material for van der Waals Bonding in Layered Compounds from Advanced Density-Functional First-Principles Calculations

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I. METHODS

A. Compound selection

We wish to identify layered compounds with interlayer bonding dominated by van der Waals (vdW) interactions and for computational reasons we wish these to have as high symmetry as possible. We selected the compounds in the study by successive filtering of all the compounds in the Inorganic Crystal Structure Database (ICSD). The strategy is to identify large deviations from the expected behaviour of covalently, ionically or metallically bonded solids, and a primary tool is the set of covalent radii of the compounds. We choose to simplify the problem by restricting the search to layered compounds where the layers are perpendicular to the crystallographic c axis, since the compounds we are interested in have a unique crystallographic axis and high in-plane symmetry perpendicular to this axis, and such compounds are conventionally chosen to have the c axis as the unique axis. Compounds that do not conform to this symmetry criterion are discarded. In a second coarse step, we filter out compounds based on the packing ratio, defined as the covalent volume divided by the total cell volume. This filters out systems such as close-packed metallic systems and very open molecular solids. In the third step we identify large gaps in along the crystallographic c axis, indicating that there may be layers bonded primarily by vdW forces. In the fourth and last step we select only those structures with a gap such that the distance between neighbouring atoms across the gap is significantly larger than the sum of their covalent radii. Several different sets of covalent radii were tested and the precise choice was found not to be important for the identification of the very overstretched bonds of primarily vdW bonded solids.

For computational reasons we also need to remove all non-stoichiometric compounds and compounds with overly large unit cells. We also remove any compound containing f-electron elements, since for the present purposes we wish to avoid all additional complications arising from the strong-correlation physics involved in these compounds. The study of binding energies also includes any of the layered transition metal dichalcogenides, also those previously discarded by the symmetry criteria.

B. Electronic structure calculations

We used the projector-augmented wave (PAW) potentials from the library distributed with the VASP code[1]. The plane wave cutoff was initially selected as 1.5 times the default cutoff, which was subsequently increased in individual cases if there were apparent convergence problems. The convergence was also more carefully tested for a small subset of compounds. Compounds containing elements in the $3d$ series from Cr to Ni were calculated in the ferromagnetic mode. Brillouin zone integrations were performed using the Gaussian smearing method with a smearing width of 0.1eV, using a uniform Monkhorst-Pack k-point mesh with the number of points selected to give a distance of 0.2Å^{-1} between the mesh points for non-magnetic calculations and 0.15Å^{-1} for magnetic calculations.

The RPA correlation energy was calculated using the adiabatic connection-fluctuation dissipation theorem. We used the standard VASP implementation[2], where the density-response function is represented in the plane-wave basis. The size of the basis is characterized by the energy cut-off, which has a strong influence on the correlation energy. In particular, Harl and Kresse have suggested that the correlation energy converges as

$$E_{\mathrm{c}}^{\mathrm{RPA}}(q) = E_{\mathrm{c}}^{\mathrm{RPA}}(q=\infty) + A/q^3, \tag{1}$$

where A is a constant and q is the cut-off wavenumber that can be related to the cut-off energy through the relation $E_{\mathrm{cut-off}} = q^2/2$. However, it can be shown[3] that Eq. 1 can be extended to

$$E_{\mathrm{c}}^{\mathrm{RPA}}(q) = E_{\mathrm{c}}^{\mathrm{RPA}}(q=\infty) + A/q^3 + B/q^5 + C/q^6 + \cdots, \tag{2}$$

where A, B and C are constants. However, we find numerically that when the energy differences involved in the vdW binding energies are calculated, the terms containing q^{-3} and q^{-6} vanish. Then, for energy differences the following relation holds

$$\delta E_{\mathrm{c}}^{\mathrm{RPA}}(q) \approx \delta E_{\mathrm{c}}^{\mathrm{RPA}}(q=\infty) + \alpha/q^5 + \beta/q^7 + \cdots, \tag{3}$$

where α and β are constants. In practical calculations, we have calculated RPA correlation energies using different cut-off energies and have used them for fitting of Equation 3. This procedure allowed us to obtain accurate estimates of the complete basis limit with cut-off energies as low as 100–150 eV, which are significantly lower than those previously used in Refs. 2 and 3. Translated into computational effort, this procedure allows us to obtain the binding energies cheaper by an order of magnitude without sacrificing the accuracy.

The total RPA energy was evaluated as a sum of the correlation energy and the total energy from a non-self-consistent exact exchange calculation. In both cases, PBE orbitals were used.

All systems were studied at their experimental in-plane lattice constant, but at the equilibrium interlayer spacing for the different methods, with the exception of the hypothetical compounds presented in Section III, where the in-plane lattice constant was relaxed using the VV10 functional. The input structure to the electronic structure program was generated by stretching of the c-axis with the layers intact. The atoms were then allowed to relax to their equilibrium positions with a fixed unit cell so that the intralayer geometry was automatically relaxed, and the interlayer geometry was relaxed by hand, so as to obtain a binding energy curve as a function of the c-axis length as shown in Figure 1 (b) of the main paper. By fitting the total energy points closest to the minimum to a polynomial, we obtained values for the equilibrium length and the C_{33} elastic constant. RPA calculations were done with fixed layers, only varying the interlayer distance. The effect of this approximation on the binding energy was found to be negligible, but there is a softening of the C_{33} elastic constant of about 10% when the layers are relaxed. Supercells for calculation of exfoliation energies were constructed by stacking 6 layers of the compound and then adding 6 layers of vacuum. Layers were then removed one by one and the energy difference between 6 and 5+1 layers were calculated. Supercell convergence was tested with respect to the number of layers and the size of the vacuum region.

II. INVESTIGATION OF NON-LOCAL CORRELATION FUNCTIONALS

In addition to the functional listed in the main paper, we investigated the Perdew-Burke-Enzerhof (PBE)[4] GGA functional and the effect of applying the NLCF of Dion et al. on top of the PBE exchange functional (vdW-DF1 (PBE)). The functionals were tested in two different ways, by comparison of relaxed geometry to experiment and by comparison of interlayer binding energies to RPA.

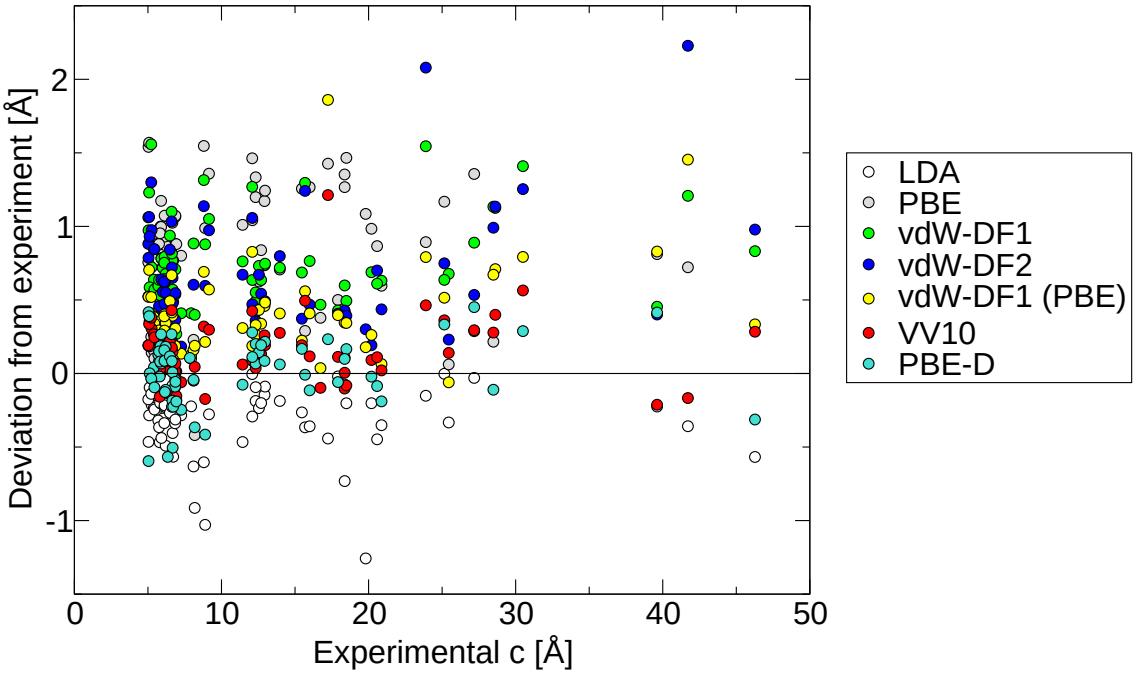

FIG. 1. Deviations (Å) of the calculated c-axis values from the experimentally reported value.

A. Geometrical considerations

For the structural benchmarks, structures of 72 compounds were calculated using various NLCF's, and 28 compounds were calculated with RPA. Figure 1 shows the deviations from the experimental c-axis length for all NLCF and standard LDA/GGA functionals tested. Table I summarizes the deviations from the experimental c-axis lengths in terms of: mean relative deviation (MRD), mean absolute relative deviation (MARD), maximal absolute relative deviation (Max. ARD) and one standard deviation (Sigma RD). It can immediately be seen that RPA performs significantly better than any other method for the smaller set of compounds where it was applied. The VV10 functional performs significantly better than other density functionals. The PBE-D functional reproduces well geometrical properties, but it shows large maximal deviations, illustrating a tendency of sometimes failing badly for no obvious reason, and for 6 systems it completely failed to give a sensible binding energy curve. The failures are mostly for systems that contain heavier elements, which are likely to have the least well-tested parameters. It seems probable that suitable refitting of the empirical parameters of PBE-D for layered systems would yield much better results. LDA

also performs rather well for structural properties, giving numbers that are in line with the normal LDA overbinding for covalent bonds. The two functionals vdW-DF1 and vdW-DF2 are barely improvements over the PBE result for the c-axis lengths, but the shape of the binding energy curves are very different, and so are the C_{33} elastic constants. Applying the original van der Waals density functional on top of PBE instead of RPBE gives a significant improvement of the structural properties. The reason for this is that the spurious LDA binding remains to a larger extent in the PBE functional than in RPBE and this improves the van der Waals bond lengths.

TABLE I. Deviations from experimental values of the different functionals investigated.

Method	MRD [%]	MARD [%]	Max dev. [%]	σ [%]
RPA	1.0	1.5	4.5	1.6
VV10	1.5	2.0	7.3	2.2
vdW-DF1	8.5	8.5	29.8	5.5
vdW-DF2	7.2	7.2	24.9	5.5
vdW-DF1 (PBE)	3.9	3.9	13.9	3.0
PBE-D	0.1	2.1	11.8	3.1
LDA	-3.5	3.5	11.6	2.6
GGA	9.5	9.6	30.9	6.5

B. Energy considerations

To get a high-quality energy benchmark, RPA calculations of binding energies were performed for 28 materials, in addition to the previously published value of graphite by Lebègue et al.[5]. The results of the comparison with the other functionals, shown in Figure 1 of the main paper, demonstrates that the vdW-DF type of functionals follows the trends of the RPA calculations well. The VV10 functional follows the trends of the RPA calculations particularly well. If rescaled by a factor of about 2/3, the VV10 energies very closely follow the RPA energies, as shown in Figure 2 for all compounds investigated by RPA in the present study. In view of Figure 1 of the main paper, one could argue that the Langreth-Lundqvist

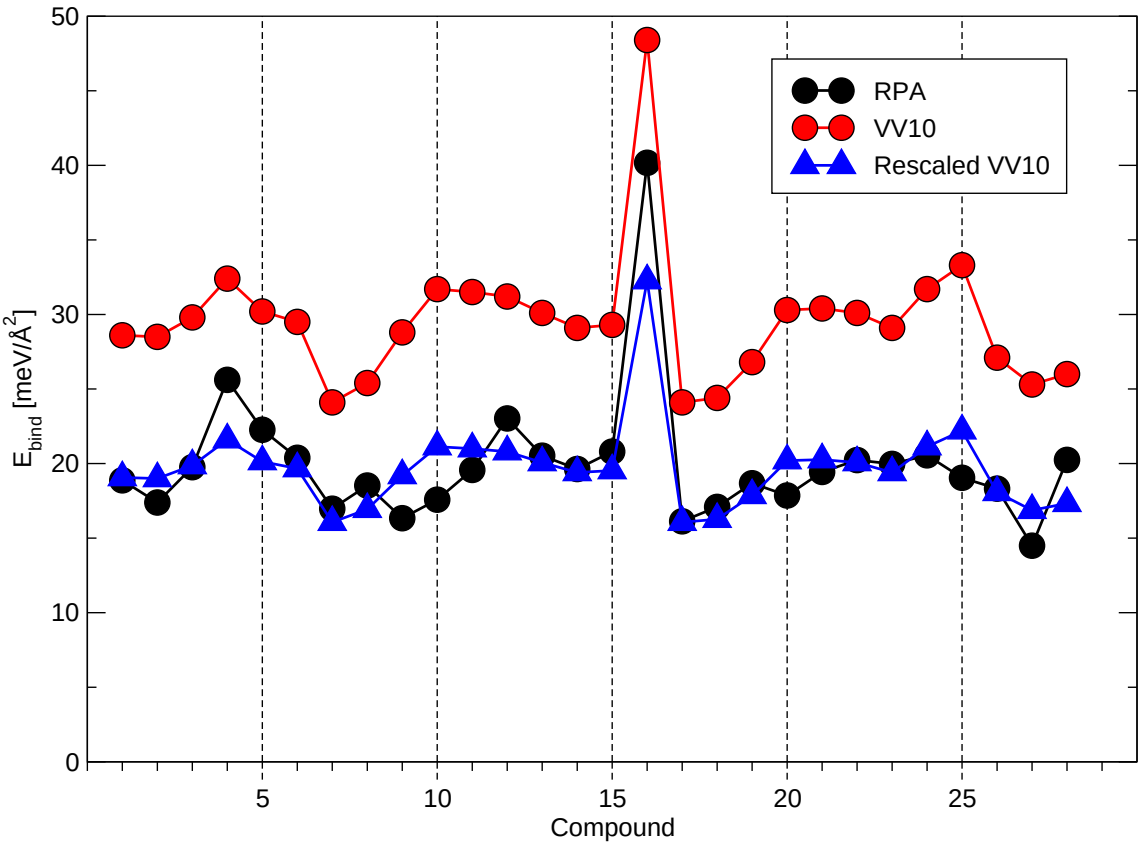

FIG. 2. Interlayer binding energies for a set of compounds calculated with RPA and VV10. Also shown is the result of rescaling the VV10 binding energies by a factor of 0.66. The numbering of the compounds can be found in Table IV.

functionals are in fact closer to the RPA results. However, the failure of these functionals to produce the correct van der Waals bond lengths produces anomalies for the outliers of the interlayer binding energy distribution, the Co family ditellurides and $NiTe_2$ and $PdTe_2$, as discussed in the main paper. For this reason, we prefer to use the VV10 functional to estimate the interlayer binding energies.

III. CRYSTAL STRUCTURES OF HYPOTHETICAL COMPOUNDS

We performed relaxations of the crystal structures of layered MX_2 compounds not found in the literature. To more completely investigate the trends in binding energies, we also included NiS_2 and $NiSe_2$, which experimentally are found in the pyrite structure, but which where found to be electronically stable in the layered $P\bar{3}m1$ structure, which indicates that they might also be possible to synthesize in layered structures. The relaxed cell parameters are given below in Table II.

TABLE II: Crystallographic parameters of hypothetical layered compounds calculated using the VV10 functional. M refers to the transition metal and X to the chalcogenide and units for a, b and c are Å, angles are in degrees and the wyckoff positions are given.

	$TcSe_2$ ($P\bar{1}$)	$TcTe_2$ ($P\bar{1}$)	$ReTe_2$ ($P\bar{1}$)	$CrTe_2$ ($P\bar{3}m1$)	NiS_2 ($P\bar{3}m1$)	$NiSe_2$ ($P\bar{3}m1$)
a	6.77	7.17	7.18	3.59	3.42	3.65
b	6.89	7.33	7.32	3.59	3.42	3.65
c	6.97	7.18	7.27	6.74	4.68	5.00
α	63.85	92.10	92.01	90	90	90
β	103.87	105.05	104.95	90	90	90
γ	118.91	118.96	118.99	120	120	120
M1 x	0.067	0.069	0.072	0	0	0
y	0.313	0.321	0.322	0	0	0
z	0.511	0.492	0.491	0	0	0
M2 x	0.488	0.487	0.486	–	–	–
y	0.290	0.297	0.298	–	–	–
z	0.504	0.496	0.495	–	–	–
X1 x	0.365	0.245	0.245	1/3	1/3	1/3
y	0.307	0.380	0.382	2/3	2/3	2/3
z	0.803	0.197	0.195	0.250	0.249	0.248
X2 x	0.824	0.717	0.717	–	–	–

TABLE II – continued from previous page

		$TcSe_2$ ($P\bar{1}$)	$TcTe_2$ ($P\bar{1}$)	$ReTe_2$ ($P\bar{1}$)	$CrTe_2$ ($P\bar{3}m1$)	NiS_2 ($P\bar{3}m1$)	$NiSe_2$ ($P\bar{3}m1$)
	y	0.276	0.333	0.333	–	–	–
	z	0.772	0.233	0.235	–	–	–
X3	x	0.140	0.225	0.224	–	–	–
	y	0.170	0.107	0.107	–	–	–
	z	0.269	0.723	0.723	–	–	–
X4	x	0.679	0.753	0.755	–	–	–
	y	0.188	0.136	0.138	–	–	–
	z	0.296	0.698	0.695	–	–	–

IV. BINDING AND EXFOLIATION ENERGIES

Here a brief explanation of the different energies discussed in the text, we tabulate the dichalcogenide binding energies shown in Figure 3 of the main paper, as well as all energies calculated using RPA. Last, we list the results of all the different functionals investigated, giving E_B, the C_{33} lattice constant and the c axis lengths and their deviation from experimental values. The c axis deviations are given as an interval calculated from the range of different values found in the ICSD database.

A. Relations between different energies discussed in the paper

In the literature, four different energies are used more or less interchangeably when discussing the interlayer binding strength in layered solids. These are the interlayer binding energy, E_B, the exfoliation energy, E_{XF}, the surface energy E_{surf} and the cleavage energy, E_{cleav}. If we, instead of doing full calculations as in the main paper, assume only pairwise interactions between the planes, we get simple expressions that can be compared to see the relations between them. The relation between the two last quantities is simple. The cleavage energy is the energy required to cleave the material in two halves, and the surface energy is the energy required to create one unit of surface by cleavage, and so $E_{surf} = \frac{1}{2}E_{cleav}$. To see

how the other quantities are related, we consider the three systems in Figure 3 and assume that we only have pairwise interactions between the planes and ignore all relaxation effects. The interaction energies between pairs of layers are labelled ε_1, ε_2 and ε_3, for adjacent lay-

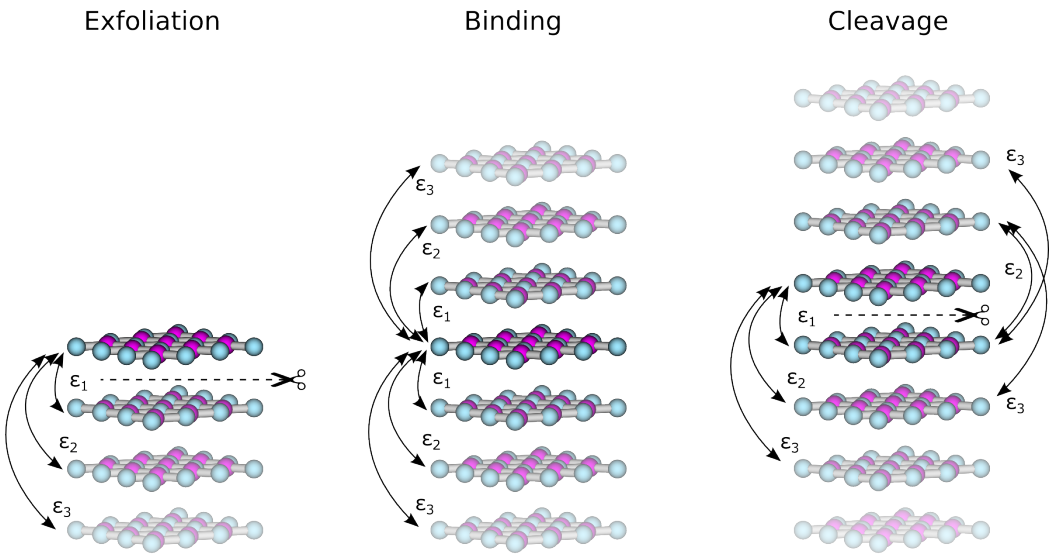

FIG. 3. The bonds involved in the binding of layers in the solid. The layer under consideration is solid, and layers get more transparent as we move away from this layer, to illustrate that each layer only are affected by its nearest neighbours. The dashed line and scissors for the exfoliation and cleavage cases illustrate how we cut the crystal.

ers, second nearest layers, third nearest layers, and so on. Ignoring all effects of relaxing the layer positions, which are expected to be small, we see that the exfoliation energy is just the sum, $E_{XF} = \varepsilon_1 + \varepsilon_2 + \ldots = \sum_{n=1}^{\infty} \varepsilon_n$. When stretching the crystal to determine the binding energy we break two of each bonds, but since the bonds are shared we need to divide by two to get, $E_B = \frac{1}{2}\sum_{n=1}^{\infty} 2\varepsilon_n = E_{XF}$. The expression for the cleavage energy is $E_{cleav} = \varepsilon_1 + 2\cdot\varepsilon_2 + 3\cdot\varepsilon_3 + \ldots = \sum_{n=1}^{\infty} n\cdot\varepsilon_n$. The ε interaction energies in a solid will decay more rapidly than the factor n in front of the terms, and if we account for only the first term, all three quantities are equal, and in general we have $E_B = E_{XF} \approx E_{cleav} = 2\cdot E_{surf}$.

B. Dichalcogenide binding energies and exfoliation energies

We here tabulate the binding energies using RPA (Table IV) as well as the full set of binding energies for the MX_2 compounds calculated with the VV10 functional (Table III). Note that the estimate used for the binding energies in the main paper is 0.66 times the binding energies as calculated with VV10. In Subsections A-G we tabulate all data calculated for the comparison of van der Waals functionals. These are the range of experimentally reported values of the c axis lengths, the calculated c axis lengths and the range of their deviations from experiments. We also give the C_{33} lattice constants, the interlayer binding energies, E_B and the bandgap, E_g (the letter "M" marks metals).

TABLE III. Interlayer binding energies (E_B), calculated using RPA and NLCF . The NLCF estimates, denoted by an asterisk (*) after the number, were obtained by a VV10 calculation rescaled by a factor 0.66. Two asterisks (**) after the compound name denotes structures not previously reported experimentally.

$3d$		$4d$		$5d$	
Compound	E_B [meV/Å^2]	Compound	E_B [meV/Å^2]	Compound	E_B [meV/Å^2]
TiS_2	18.9	ZrS_2	17.0	HfS_2	16.1
$TiSe_2$	17.4	$ZrSe_2$	18.5	$HfSe_2$	17.1
$TiTe_2$	19.7	$ZrTe_2$	16.3	$HfTe_2$	18.7
VS_2	25.6	NbS_2	17.6	TaS_2	17.9
VSe_2	22.3	$NbSe_2$	19.6	$TaSe_2$	19.4
VTe_2	20.4	$NbTe_2$	23.0	$TaTe_2$	23.2*
CrS_2	19.5*	MoS_2	20.5	WS_2	20.2
$CrSe_2$	23.9*	$MoSe_2$	19.6	WSe_2	20.0
$CrTe_2$**	29.9*	$MoTe_2$	20.8	WTe_2	18.5*
		TcS_2	19.7*	ReS_2	19.9*
		$TcSe_2$**	18.8*	$ReSe_2$	18.2*
		$TcTe_2$**	18.8*	$ReTe_2$**	18.5*
$CoTe_2$	32.9*	$RhTe_2$	36.5*	$IrTe_2$	36.3*
NiS_2**	24.9*	PdS_2	21.4*	PtS_2	20.6
$NiSe_2$**	29.2*	$PdSe_2$	27.8*	$PtSe_2$	19.1
$NiTe_2$	30.2*	$PdTe_2$	40.2	$PtTe_2$	25.1*

C. RPA binding energies

TABLE IV. Binding energies calculated with RPA. The numbering of the compounds in the table is the same as in Figure 2.

No.	Compound	E_B [meV/Å^2]	No.	Compound	E_B [meV/Å^2]
1	TiS_2	18.88	16	$PdTe_2$	40.17
2	$TiSe_2$	17.39	17	HfS_2	16.13
3	$TiTe_2$	19.76	18	$HfSe_2$	17.09
4	VS_2	25.61	19	$HfTe_2$	18.68
5	VSe_2	22.26	20	TaS_2	17.86
6	VTe_2	20.39	21	$TaSe_2$	19.44
7	ZrS_2	16.98	22	WS_2	20.24
8	$ZrSe_2$	18.53	23	WSe_2	19.98
9	$ZrTe_2$	16.34	24	PtS_2	20.55
10	NbS_2	17.58	25	$PtSe_2$	19.05
11	$NbSe_2$	19.57	26	Graphite[5]	18.32
12	$NbTe_2$	23.03	27	BN	14.49
13	MoS_2	20.53	28	PbO	20.25
14	$MoSe_2$	19.63			
15	$MoTe_2$	20.80			

D. VV10

Name	c_{exp} [Å]	c_{calc}	c dev. [%]	C_{33} [GPa]	E_B [meV/Å^2]	E_g [eV]
$AgBiP_2Se_6$	39.615	39.402	-0.5	35.6	23.396	1.027
BBr_3	6.847 – 6.864	6.754	-1.4 – -1.6	18.1	12.314	3.470
BI_3	7.261 – 7.460	7.202	-0.8 – -3.5	17.9	13.956	2.471
BN	6.661 – 6.690	6.679	-0.2 – 0.3	41.2	25.336	4.233
BaFI	7.962 – 8.102	8.053	-0.6 – 1.1	35.8	26.387	3.843
Bi_2Se_3	28.615 – 28.636	29.014	1.3 – 1.4	45.9	25.596	0.249
Bi_2Te_3	30.440 – 30.497	31.061	1.9 – 2.0	39.8	26.193	0.734
BiIO	9.128 – 9.151	9.449	3.3 – 3.5	36.9	21.164	1.985
C	6.704 – 6.930	6.777	-0.3 – -2.2	46.1	27.073	M
CdI_2	6.835 – 6.864	6.932	1.0 – 1.4	28.2	16.711	2.004
$CoTe_2$	5.405	5.672	4.9	55.4	49.269	M
$CrSe_2$	5.915	6.054	2.4	38.0	30.627	M
$CrSiTe_3$	20.528 – 20.582	20.692	0.5 – 0.8	34.7	24.158	0.382
Cu_2S	6.670 – 6.680	6.755	1.1 – 1.3	31.9	32.111	M
GaS	14.230 – 15.530	15.658	0.8 – 10.0	45.6	20.144	1.800
GaSe	15.919 – 15.995	16.111	0.7 – 1.2	40.2	20.073	1.406
$Ge_2Sb_2Te_5$	16.960 – 17.239	18.452	7.0 – 8.8	38.6	25.880	M
HfS_2	5.837 – 5.856	5.856	-0.0 – 0.3	46.4	24.172	0.951
$HfSe_2$	6.143 – 6.159	6.241	1.3 – 1.6	47.1	25.091	0.432
$HfTe_2$	6.650 – 6.670	6.816	2.2 – 2.5	41.0	27.162	M
HgI_2	12.088 – 12.450	12.512	0.5 – 3.5	22.5	17.815	0.866
$In_2Zn_2S_5$	46.270	46.554	0.6	93.6	47.137	0.311
$Mg_2(P_2Se_6)$	20.194	20.286	0.5	36.0	21.074	1.904
$MgBr_2$	6.260 – 6.269	6.290	0.3 – 0.5	29.5	15.322	4.236
MgI_2	6.862 – 6.895	6.875	0.2 – -0.3	27.7	15.816	3.303
MoS_2	12.290 – 12.530	12.387	0.5 – -1.1	61.3	30.820	0.881
MoS_2	18.330 – 18.450	18.267	-0.3 – -1.0	55.2	30.514	1.182
$MoSe_2$	12.900 – 12.930	13.186	2.0 – 2.2	57.5	30.062	0.938

$MoTe_2$	13.964 – 13.974	14.240	1.9 – 2.0	50.9	30.408	0.857
NbS_2	17.800 – 17.918	18.031	0.6 – 1.3	65.9	30.036	M
$NbSe_2$	12.482 – 12.550	12.743	1.5 – 2.1	55.0	32.888	M
$NbSe_2$	25.230 – 25.450	25.590	0.6 – 1.4	57.1	33.878	M
$NbTe_2$	6.610	7.040	6.5	44.0	30.074	M
Ni_2SbTe_2	15.634 – 15.682	16.177	3.2 – 3.5	48.8	34.636	M
NiSbSi	8.179	8.224	0.6	62.4	66.807	M
$NiTe_2$	5.251 – 5.308	5.556	4.7 – 5.8	50.4	42.807	M
$PbBi_4Te_7$	23.600 – 23.892	24.355	1.9 – 3.2	10.8	13.096	0.764
PbFI	8.770 – 8.800	9.120	3.6 – 4.0	26.5	19.606	1.748
PbO	4.988 – 5.071	5.213	2.8 – 4.5	25.9	26.033	1.335
$PbSb_2Te_4$	41.712	41.545	-0.4	5.2	9.108	0.331
$PdTe_2$	5.113 – 5.270	5.469	3.8 – 7.0	72.3	46.510	M
PtS_2	5.019 – 5.043	5.232	3.8 – 4.2	33.2	29.384	0.721
$PtSe_2$	5.031 – 5.082	5.418	6.6 – 7.7	33.5	29.920	M
$PtTe_2$	5.201 – 5.224	5.603	7.3 – 7.7	49.6	33.945	M
$Re(AgCl_3)_2$	16.731 – 16.731	16.633	-0.6 – -0.6	39.3	23.063	M
$RhTe_2$	5.410 – 5.442	5.688	4.5 – 5.1	59.7	51.159	M
SnS_2	5.460 – 5.960	5.962	0.0 – 9.2	37.1	22.438	1.263
$SnSe_2$	6.128 – 6.141	6.298	2.6 – 2.8	37.1	23.413	0.264
SrFI	8.888 – 8.916	8.715	-2.0 – -2.3	23.8	18.975	4.117
TaS_2	5.853 – 5.900	5.993	1.6 – 2.4	57.3	30.792	M
TaS_2	12.097 – 12.100	12.184	0.7 – 0.7	57.4	31.466	M
$TaSe_2$	6.203 – 6.272	6.364	1.5 – 2.6	56.5	31.489	M
$TaSe_2$	12.696 – 12.720	12.828	0.8 – 1.0	58.3	31.999	M
$TaSe_2$	25.143 – 25.500	25.511	0.0 – 1.5	59.1	33.783	M
Ti_2PTe_2	28.486	28.764	1.0	49.1	29.746	M
TiS_2	5.680 – 5.716	5.752	0.6 – 1.3	50.6	28.618	M
$TiSe_2$	5.981 – 6.011	6.112	1.7 – 2.2	44.2	28.223	M
$TiTe_2$	6.459 – 6.539	6.712	2.6 – 3.9	44.9	29.462	M

VBr_2	6.206	6.087	-1.9	34.6	19.955	M
VCl_2	5.798 – 5.835	5.640	-2.7 – -3.3	34.8	19.334	M
VI_2	6.714	6.582	-2.0	32.0	20.622	M
VS_2	5.755 – 5.755	5.839	1.5 – 1.5	55.6	31.573	M
VSe_2	6.048 – 6.150	6.296	2.4 – 4.1	49.0	30.349	M
WS_2	12.323 – 12.500	12.360	-0.0 – -1.1	62.1	31.020	1.134
WS_2	18.490	18.409	-0.4	56.7	30.492	1.172
WSe_2	12.960 – 12.980	13.152	1.3 – 1.5	58.3	30.598	1.148
$Y_2I_2Ga_2$	11.434	11.495	0.5	44.7	19.058	M
YI_3	20.880	20.901	0.1	25.2	15.495	2.407
ZrNCl	27.178 – 27.672	27.472	0.2 – 1.1	66.5	25.191	1.800
ZrS_2	5.810 – 5.850	5.855	0.1 – 0.8	47.6	24.467	0.656
$ZrSe_2$	6.125 – 6.192	6.229	0.6 – 1.7	47.7	25.644	0.214
$ZrTe_2$	6.630 – 6.660	6.805	2.2 – 2.6	49.9	28.983	M

E. vdW-DF1

Name	c_{exp} [Å]	c_{calc}	c dev. [%]	C_{33} [GPa]	E_B [meV/Å^2]	E_g [eV]
$AgBiP_2Se_6$	39.615	40.069	1.1	13.8	13.192	1.306
BBr_3	6.847 – 6.864	7.247	5.6 – 5.8	8.8	11.046	3.744
BI_3	7.261 – 7.460	7.671	2.8 – 5.6	8.1	10.619	2.636
BN	6.661 – 6.690	6.926	3.5 – 4.0	20.2	18.093	4.649
BaFI	7.962 – 8.102	8.986	10.9 – 12.9	10.4	13.801	4.317
Bi_2Se_3	28.615 – 28.636	29.741	3.9 – 3.9	17.2	12.914	0.988
Bi_2Te_3	30.440 – 30.497	31.907	4.6 – 4.8	14.5	12.159	1.150
BiIO	9.128 – 9.151	10.202	11.5 – 11.8	19.4	12.800	2.115
C	6.704 – 6.930	7.199	3.9 – 7.4	23.0	18.900	M
CdI_2	6.835 – 6.864	7.572	10.3 – 10.8	15.0	11.418	2.145
$CoTe_2$	5.405	6.043	11.8	27.1	25.531	M
$CrSe_2$	5.915	6.697	13.2	18.4	15.704	M
$CrSiTe_3$	20.528 – 20.582	21.193	3.0 – 3.2	14.8	13.101	0.366
Cu_2S	6.670 – 6.680	7.250	8.5 – 8.7	11.0	16.494	M
GaS	14.230 – 15.530	16.152	4.0 – 13.5	23.8	14.063	2.339
GaSe	15.919 – 15.995	16.759	4.8 – 5.3	19.7	12.731	1.929
$Ge_2Sb_2Te_5$	16.960 – 17.239	20.898	21.2 – 23.2	24.2	14.745	0.314
HfS_2	5.837 – 5.856	6.354	8.5 – 8.9	21.8	15.686	1.318
$HfSe_2$	6.143 – 6.159	6.777	10.0 – 10.3	19.4	14.739	0.598
$HfTe_2$	6.650 – 6.670	7.439	11.5 – 11.9	16.9	14.293	M
HgI_2	12.088 – 12.450	13.357	7.3 – 10.5	10.5	11.229	1.207
$In_2Zn_2S_5$	46.270	47.102	1.8	53.3	31.454	0.321
$Mg_2(P_2Se_6)$	20.194	20.882	3.4	18.2	13.381	2.031
$MgBr_2$	6.260 – 6.269	6.719	7.2 – 7.3	18.9	13.045	4.811
MgI_2	6.862 – 6.895	7.399	7.3 – 7.8	15.7	11.746	3.631
MoS_2	12.290 – 12.530	12.812	2.2 – 4.2	24.4	16.707	1.396
$MoSe_2$	12.900 – 12.930	13.662	5.7 – 5.9	20.4	15.329	1.252
$MoTe_2$	13.964 – 13.974	14.683	5.1 – 5.2	17.6	14.368	0.958

NbS_2	17.800 – 17.918	18.346	2.4 – 3.1	26.8	16.662	M
$NbSe_2$	12.482 – 12.550	13.278	5.8 – 6.4	21.8	16.750	M
$NbSe_2$	25.230 – 25.450	26.127	2.7 – 3.6	22.0	17.523	M
$NbTe_2$	6.610	7.710	16.6	15.8	14.637	M
Ni_2SbTe_2	15.634 – 15.682	16.978	8.3 – 8.6	16.1	15.047	M
NiSbSi	8.179	8.578	4.9	53.6	38.880	M
$NiTe_2$	5.251 – 5.308	5.973	12.5 – 13.8	19.1	19.249	M
$PbBi_4Te_7$	23.600 – 23.892	25.437	6.5 – 7.8	4.0	5.939	1.143
PbFI	8.770 – 8.800	10.115	14.9 – 15.3	15.6	12.056	2.381
PbO	4.988 – 5.071	6.084	20.0 – 22.0	7.8	9.923	2.215
$PbSb_2Te_4$	41.712	42.920	2.9	2.3	4.072	0.821
$PdTe_2$	5.113 – 5.270	5.699	8.1 – 11.5	35.6	19.653	M
PtS_2	5.019 – 5.043	6.013	19.2 – 19.8	16.3	14.851	1.264
$PtSe_2$	5.031 – 5.082	6.312	24.2 – 25.5	12.6	13.449	0.831
$PtTe_2$	5.201 – 5.224	6.782	29.8 – 30.4	5.9	12.019	0.199
$Re(AgCl_3)_2$	16.731 – 16.731	17.198	2.8 – 2.8	31.9	18.445	M
$RhTe_2$	5.410 – 5.442	6.013	10.5 – 11.1	29.5	25.776	M
SnS_2	5.460 – 5.960	6.524	9.5 – 19.5	19.2	14.396	1.445
$SnSe_2$	6.128 – 6.141	6.930	12.8 – 13.1	16.0	13.348	0.505
SrFI	8.888 – 8.916	9.766	9.5 – 9.9	13.9	11.802	4.379
TaS_2	5.853 – 5.900	6.512	10.4 – 11.3	25.4	17.714	M
TaS_2	12.097 – 12.100	12.732	5.2 – 5.3	24.4	17.532	M
$TaSe_2$	6.203 – 6.272	6.880	9.7 – 10.9	22.8	16.798	M
$TaSe_2$	12.696 – 12.720	13.331	4.8 – 5.0	21.1	16.339	M
$TaSe_2$	25.143 – 25.500	25.786	1.1 – 2.6	22.5	17.380	M
Ti_2PTe_2	28.486	29.620	4.0	23.0	14.255	M
TiS_2	5.680 – 5.716	6.301	10.2 – 10.9	22.6	17.093	M
$TiSe_2$	5.981 – 6.011	6.723	11.8 – 12.4	19.7	15.715	M
$TiTe_2$	6.459 – 6.539	7.429	13.6 – 15.0	16.9	14.876	M
$TlCrTe_2$	7.839 – 7.935	8.345	5.2 – 6.5	42.7	48.379	M

VBr_2	6.206	6.612	6.5	20.1	14.183	M
VCl_2	5.798 – 5.835	6.137	5.2 – 5.9	22.3	15.206	M
VI_2	6.714	7.202	7.3	16.4	12.861	M
VS_2	5.755 – 5.755	6.392	11.1 – 11.1	24.8	18.121	M
VSe_2	6.048 – 6.150	6.861	11.6 – 13.4	21.4	16.334	M
WS_2	12.323 – 12.500	12.874	3.0 – 4.5	24.3	16.575	1.572
WS_2	18.490	18.983	2.7	23.5	16.399	1.582
WSe_2	12.960 – 12.980	13.707	5.6 – 5.8	21.0	15.203	1.342
$Y_2I_2Ga_2$	11.434	12.196	6.7	23.8	12.040	M
YI_3	20.880	21.511	3.0	13.3	9.864*	2.736
ZrNCl	27.178 – 27.672	28.067	1.4 – 3.3	38.1	16.087	1.907
ZrS_2	5.810 – 5.850	6.358	8.7 – 9.4	21.4	15.775	1.050
$ZrSe_2$	6.125 – 6.192	6.771	9.3 – 10.5	19.2	15.017	0.363
$ZrTe_2$	6.630 – 6.660	7.446	11.8 – 12.3	17.2	14.856	M

F. vdW-DF2

Name	c_{exp} [Å]	c_{calc}	c dev. [%]	C_{33} [GPa]	E_B [meV/Å^2]	E_g [eV]
$AgBiP_2Se_6$	39.615	40.016	1.0	23.0	14.220	0.987
BBr_3	6.847 – 6.864	7.011	2.1 – 2.4	13.1	10.020	3.653
BI_3	7.261 – 7.460	7.445	-0.2 – 2.5	11.7	10.244	2.569
BN	6.661 – 6.690	6.878	2.8 – 3.3	29.7	17.677	4.567
BaFI	7.962 – 8.102	8.705	7.4 – 9.3	19.0	15.047	4.078
Bi_2Se_3	28.615 – 28.636	29.750	3.9 – 4.0	27.2	14.245	0.695
Bi_2Te_3	30.440 – 30.497	31.750	4.1 – 4.3	22.8	13.570	0.873
BiIO	9.128 – 9.151	10.124	10.6 – 10.9	27.5	12.775	1.968
C	6.704 – 6.930	6.944	0.2 – 3.6	33.5	18.630	M
CdI_2	6.835 – 6.864	7.411	8.0 – 8.4	21.3	11.056	1.877
$CoTe_2$	5.405	6.249	15.6	31.8	24.201	M
$CrSe_2$	5.915	6.554	10.8	31.8	17.177	M
$CrSiTe_3$	20.528 – 20.582	21.282	3.4 – 3.7	22.7	13.863	0.323
Cu_2S	6.670 – 6.680	7.156	7.1 – 7.3	16.9	17.571	M
$Fe(PSe_3)$	19.800 – 19.812	20.105	1.5 – 1.5	25.0	14.449	M
GaS	14.230 – 15.530	15.838	2.0 – 11.3	33.6	13.645	2.163
GaSe	15.919 – 15.995	16.463	2.9 – 3.4	26.7	12.674	1.691
$Ge_2Sb_2Te_5$	16.960 – 17.239	20.771	20.5 – 22.5	17.8	12.524	0.105
HfS_2	5.837 – 5.856	6.162	5.2 – 5.6	32.7	16.097	1.245
$HfSe_2$	6.143 – 6.159	6.604	7.2 – 7.5	30.7	15.717	0.486
$HfTe_2$	6.650 – 6.670	7.320	9.7 – 10.1	27.6	15.682	M
HgI_2	12.088 – 12.450	13.145	5.6 – 8.8	15.4	11.594	0.867
$In_2Zn_2S_5$	46.270	47.249	2.1	65.3	31.457	0.315
$Mg_2(P_2Se_6)$	20.194	20.386	1.0	25.7	13.675	1.801
$MgBr_2$	6.260 – 6.269	6.532	4.2 – 4.3	24.8	11.814	4.481
MgI_2	6.862 – 6.895	7.226	4.8 – 5.3	22.1	11.314	3.347
MoS_2	12.290 – 12.530	12.682	1.2 – 3.2	38.6	17.870	1.193
MoS_2	18.330 – 18.450	18.798	1.9 – 2.6	39.1	17.641	1.384

$MoSe_2$	12.900 – 12.930	13.401	3.6 – 3.9	34.3	16.637	1.098
$MoTe_2$	13.964 – 13.974	14.762	5.6 – 5.7	28.6	16.027	0.830
NbS_2	17.800 – 17.918	18.324	2.3 – 2.9	45.4	20.100	M
$NbSe_2$	12.482 – 12.550	13.218	5.3 – 5.9	37.2	18.768	M
$NbSe_2$	25.230 – 25.450	25.680	0.9 – 1.8	36.8	19.623	M
$NbTe_2$	6.610	7.643	15.6	25.8	15.819	M
Ni_2SbTe_2	15.634 – 15.682	16.923	7.9 – 8.2	26.0	17.182	M
$NiTe_2$	5.251 – 5.308	6.226	17.3 – 18.6	25.7	19.479	M
$PbBi_4Te_7$	23.600 – 23.892	25.971	8.7 – 10.0	6.8	6.612	0.901
PbFI	8.770 – 8.800	9.938	12.9 – 13.3	21.4	11.807	2.094
PbO	4.988 – 5.071	5.904	16.4 – 18.4	12.7	11.012	1.910
$PbSb_2Te_4$	41.712	43.940	5.3	2.9	4.565	0.499
$PdTe_2$	5.113 – 5.270	6.045	14.7 – 18.2	23.7	20.815	M
PtS_2	5.019 – 5.043	5.826	15.5 – 16.1	23.7	15.883	1.027
$PtSe_2$	5.031 – 5.082	6.146	20.9 – 22.2	20.2	15.055	0.563
$PtTe_2$	5.201 – 5.224	6.523	24.9 – 25.4	10.1	13.479	M
$RhTe_2$	5.410 – 5.442	6.287	15.5 – 16.2	29.5	24.516	M
SnS_2	5.460 – 5.960	6.326	6.1 – 15.9	27.2	14.528	1.220
$SnSe_2$	6.128 – 6.141	6.752	10.0 – 10.2	24.4	14.192	0.220
SrFI	8.888 – 8.916	9.484	6.4 – 6.7	18.8	11.620	4.029
TaS_2	5.853 – 5.900	6.333	7.3 – 8.2	39.6	19.324	M
TaS_2	12.097 – 12.100	12.567	3.9 – 3.9	39.0	18.879	M
$TaSe_2$	6.203 – 6.272	6.752	7.7 – 8.9	36.7	18.874	M
$TaSe_2$	12.696 – 12.720	13.238	4.1 – 4.3	35.3	18.289	M
$TaSe_2$	25.143 – 25.500	25.899	1.6 – 3.0	36.9	19.645	M
Ti_2PTe_2	28.486	29.477	3.5	35.0	15.690	M
TiS_2	5.680 – 5.716	6.099	6.7 – 7.4	35.7	18.170	M
$TiSe_2$	5.981 – 6.011	6.559	9.1 – 9.7	31.8	17.106	M
$TiTe_2$	6.459 – 6.539	7.334	12.2 – 13.5	26.1	16.115	M
VBr_2	6.206	6.458	4.1	27.1	13.669	M

VCl_2	5.798 – 5.835	5.953	2.0 – 2.7	30.1	13.961	M
VI_2	6.714	7.079	5.4	22.9	13.022	M
VS_2	5.755 – 5.755	6.214	8.0 – 8.0	38.1	19.617	M
VSe_2	6.048 – 6.150	6.731	9.5 – 11.3	32.7	17.862	M
WS_2	12.323 – 12.500	12.742	1.9 – 3.4	38.8	17.901	1.367
WS_2	18.490	18.883	2.1	36.1	17.552	1.391
WSe_2	12.960 – 12.980	13.452	3.6 – 3.8	34.3	16.601	1.189
$Y_2I_2Ga_2$	11.434	12.105	5.9	32.1	11.944	0.202
YI_3	20.880	21.316	2.1	18.3	10.795	2.540
ZrNCl	27.178 – 27.672	27.712	0.1 – 2.0	51.2	15.125	1.894
ZrS_2	5.810 – 5.850	6.165	5.4 – 6.1	32.8	16.316	0.948
$ZrSe_2$	6.125 – 6.192	6.602	6.6 – 7.8	31.1	16.194	0.276
$ZrTe_2$	6.630 – 6.660	7.350	10.4 – 10.9	28.0	16.391	M

G. vdW-DF1 (PBE)

Name	c_{exp} [Å]	c_{calc}	c dev. [%]	C_{33} [GPa]	E_B [meV/Å^2]	E_g [eV]
$AgBiP_2Se_6$	39.615	40.444	2.1	24.7	19.024	1.194
BBr_3	6.847 – 6.864	6.915	0.7 – 1.0	14.6	15.120	3.689
BI_3	7.261 – 7.460	7.396	0.4 – 1.9	12.7	14.808	2.615
BN	6.661 – 6.690	6.696	0.1 – 0.5	32.4	24.689	4.481
BaFI	7.962 – 8.102	8.262	2.0 – 3.8	27.9	22.804	4.089
Bi_2Se_3	28.615 – 28.636	29.325	2.4 – 2.5	28.7	19.311	0.596
Bi_2Te_3	30.440 – 30.497	31.290	2.6 – 2.8	24.0	18.530	0.978
BiIO	9.128 – 9.151	9.722	6.2 – 6.5	30.0	17.876	2.086
C	6.704 – 6.930	6.892	-0.6 – 2.8	35.6	25.671	M
CdI_2	6.835 – 6.864	7.170	4.5 – 4.9	22.1	15.682	2.124
$CoTe_2$	5.405	5.790	7.1	41.0	37.809	M
$CrSe_2$	5.915	6.277	6.1	32.9	23.394	M
Cu_2S	6.670 – 6.680	6.804	1.9 – 2.0	20.6	24.635	M
$Fe(PSe_3)$	19.800 – 19.812	19.983	0.9 – 0.9	27.1	19.611	M
GaS	14.230 – 15.530	15.688	1.0 – 10.2	35.4	19.190	2.139
GaSe	15.919 – 15.995	16.403	2.6 – 3.0	29.2	17.673	1.617
$Ge_2Sb_2Te_5$	16.960 – 17.239	19.099	10.8 – 12.6	26.6	18.182	0.114
HfS_2	5.837 – 5.856	6.039	3.1 – 3.5	33.9	21.470	1.250
$HfSe_2$	6.143 – 6.159	6.431	4.4 – 4.7	31.8	20.930	0.554
$HfTe_2$	6.650 – 6.670	7.062	5.9 – 6.2	28.3	20.740	M
HgI_2	12.088 – 12.450	12.914	3.7 – 6.8	16.5	16.443	1.033
$In_2Zn_2S_5$	46.270	46.604	0.7	76.9	41.288	0.151
$Mg_2(P_2Se_6)$	20.194	20.456	1.3	27.2	18.637	1.994
$MgBr_2$	6.260 – 6.269	6.397	2.0 – 2.2	27.0	17.262	4.667
MgI_2	6.862 – 6.895	7.049	2.2 – 2.7	23.1	15.808	3.544
MoS_2	12.290 – 12.530	12.586	0.4 – 2.4	39.3	23.612	1.105
MoS_2	18.330 – 18.450	18.716	1.4 – 2.1	36.4	23.272	1.309
$MoSe_2$	12.900 – 12.930	13.385	3.5 – 3.8	35.6	21.895	1.137

$MoTe_2$	13.964 – 13.974	14.372	2.9 – 2.9	31.0	20.880	0.932
NbS_2	17.800 – 17.918	18.315	2.2 – 2.9	45.3	23.840	M
$NbSe_2$	12.482 – 12.550	12.979	3.4 – 4.0	34.6	24.501	M
$NbSe_2$	25.230 – 25.450	25.390	-0.2 – 0.6	39.2	25.553	M
$NbTe_2$	6.610	7.278	10.1	26.6	21.807	M
Ni_2SbTe_2	15.634 – 15.682	16.241	3.6 – 3.9	29.6	23.715	M
NiSbSi	8.179	8.368	2.3	57.2	52.245	M
$NiTe_2$	5.251 – 5.308	5.659	6.6 – 7.8	35.6	31.309	M
$PbBi_4Te_7$	23.600 – 23.892	24.683	3.3 – 4.6	6.7	9.324	0.972
PbFI	8.770 – 8.800	9.491	7.9 – 8.2	20.9	17.151	2.099
PbO	4.988 – 5.071	5.546	9.4 – 11.2	15.4	17.128	1.763
$PbSb_2Te_4$	41.712	43.166	3.5	3.3	6.300	0.576
$PdTe_2$	5.113 – 5.270	5.522	4.8 – 8.0	55.7	33.171	M
PtS_2	5.019 – 5.043	5.562	10.3 – 10.8	23.0	22.131	1.004
$PtSe_2$	5.031 – 5.082	5.786	13.9 – 15.0	18.3	20.978	0.364
$PtTe_2$	5.201 – 5.224	5.744	10.0 – 10.4	28.3	22.009	M
$Re(AgCl_3)_2$	16.731 – 16.731	16.767	0.2 – 0.2	34.6	23.806	M
$RhTe_2$	5.410 – 5.442	5.781	6.2 – 6.9	45.5	39.102	M
SnS_2	5.460 – 5.960	6.180	3.7 – 13.2	27.9	20.046	1.368
$SnSe_2$	6.128 – 6.141	6.538	6.5 – 6.7	25.0	19.214	0.431
SrFI	8.888 – 8.916	9.103	2.1 – 2.4	17.1	17.039	4.340
TaS_2	5.853 – 5.900	6.188	4.9 – 5.7	39.5	25.120	M
TaS_2	12.097 – 12.100	12.285	1.5 – 1.6	39.1	24.730	M
$TaSe_2$	6.203 – 6.272	6.546	4.4 – 5.5	38.0	24.250	M
$TaSe_2$	12.696 – 12.720	13.034	2.5 – 2.7	36.4	23.756	M
$TaSe_2$	25.143 – 25.500	25.664	0.6 – 2.1	38.2	25.247	M
Ti_2PTe_2	28.486	29.157	2.4	36.1	20.769	M
TiS_2	5.680 – 5.716	5.950	4.1 – 4.8	36.1	24.552	M
$TiSe_2$	5.981 – 6.011	6.339	5.5 – 6.0	29.6	22.952	M
$TiTe_2$	6.459 – 6.539	6.984	6.8 – 8.1	21.2	22.016	M

$TlCrTe_2$	7.839 – 7.935	8.062	1.6 – 2.8	52.3	59.521	M
VBr_2	6.206	6.252	0.7	28.7	19.446	M
VCl_2	5.798 – 5.835	5.795	-0.0 – -0.7	31.2	20.499	M
VI_2	6.714	6.809	1.4	23.9	18.024	M
VS_2	5.755 – 5.755	6.048	5.1 – 5.1	38.3	26.047	M
VSe_2	6.048 – 6.150	6.496	5.6 – 7.4	33.9	23.787	M
WS_2	12.323 – 12.500	12.652	1.2 – 2.7	39.9	23.341	1.282
WS_2	18.490	18.833	1.9	37.2	23.001	1.310
WSe_2	12.960 – 12.980	13.442	3.6 – 3.7	36.5	21.704	1.279
$Y_2I_2Ga_2$	11.434	11.743	2.7	33.6	16.632	M
YI_3	20.880	20.944	0.3	21.3	15.188	2.697
ZrNCl	27.178 – 27.672	27.466	0.2 – 1.1	55.2	21.413	1.876
ZrS_2	5.810 – 5.850	6.038	3.2 – 3.9	34.0	21.840	0.966
$ZrSe_2$	6.125 – 6.192	6.421	3.7 – 4.8	32.5	21.522	0.325
$ZrTe_2$	6.630 – 6.660	7.045	5.8 – 6.3	24.3	21.868	M

H. LDA

Name	c_{exp} [Å]	c_{calc}	c dev. [%]	C_{33} [GPa]	E_B [meV/Å^2]	E_g [eV]
$AgBiP_2Se_6$	39.615	39.390	-0.6	33.0	11.962	1.050
BBr_3	6.847 – 6.864	6.508	-4.9 – -5.2	21.1	8.090	3.597
BI_3	7.261 – 7.460	6.977	-3.9 – -6.5	15.3	8.810	2.453
BN	6.661 – 6.690	6.579	-1.2 – -1.7	28.5	10.191	4.038
BaFI	7.962 – 8.102	7.470	-6.2 – -7.8	53.3	22.712	3.865
BiIO	9.128 – 9.151	8.873	-2.8 – -3.0	31.5	10.163	1.830
C	6.704 – 6.930	6.750	0.7 – -2.6	29.9	9.432	M
CdI_2	6.835 – 6.864	6.551	-4.1 – -4.6	23.5	7.926	2.171
$CoTe_2$	5.405	5.172	-4.3	72.6	43.277	M
$CrSe_2$	5.915	5.476	-7.4	72.4	24.679	M
$CrSiTe_3$	20.528 – 20.582	20.135	-1.9 – -2.2	26.5	13.402	M
Cu_2S	6.670 – 6.680	6.275	-5.9 – -6.1	40.9	23.929	M
$Fe(PSe_3)$	19.800 – 19.812	18.548	-6.3 – -6.4	72.2	25.699	0.184
GaS	14.230 – 15.530	15.201	-0.4 – 6.8	36.7	8.807	1.624
GaSe	15.919 – 15.995	15.636	-1.8 – -2.2	36.9	9.120	1.253
$Ge_2Sb_2Te_5$	16.960 – 17.239	16.797	-1.0 – -2.6	70.5	20.529	M
HfS_2	5.837 – 5.856	5.630	-3.5 – -3.9	39.7	11.684	0.797
$HfSe_2$	6.143 – 6.159	5.939	-3.3 – -3.6	42.2	13.024	0.210
$HfTe_2$	6.650 – 6.670	6.397	-3.8 – -4.1	53.2	17.611	M
HgI_2	12.088 – 12.450	12.084	-0.0 – -2.9	21.0	11.588	0.918
$In_2Zn_2S_5$	46.270	45.702	-1.2	103.4	41.971	0.295
$Mg_2(P_2Se_6)$	20.194	19.992	-1.0	30.9	9.809	1.956
$MgBr_2$	6.260 – 6.269	6.061	-3.2 – -3.3	21.9	7.004	4.151
MgI_2	6.862 – 6.895	6.596	-3.9 – -4.3	22.9	7.188	3.144
MoS_2	12.290 – 12.530	12.135	-1.3 – -3.2	53.0	13.412	0.727
MoS_2	18.330 – 18.450	18.295	-0.2 – -0.8	47.8	13.506	0.891
$MoSe_2$	12.900 – 12.930	12.781	-0.9 – -1.2	53.8	13.924	0.832
$MoTe_2$	13.964 – 13.974	13.777	-1.3 – -1.4	55.0	15.468	0.796

NbS_2	17.800 – 17.918	17.898	-0.1 – 0.6	57.4	14.623	M
$NbSe_2$	12.482 – 12.550	12.312	-1.4 – -1.9	74.4	22.091	M
$NbSe_2$	25.230 – 25.450	25.117	-0.4 – -1.3	74.6	22.524	M
$NbTe_2$	6.610	6.475	-2.0	61.6	22.503	M
Ni_2SbTe_2	15.634 – 15.682	15.316	-2.0 – -2.3	86.2	30.896	M
NiSbSi	8.179	7.266	-11.2	107.2	41.165	M
$NiTe_2$	5.251 – 5.308	5.038	-4.1 – -5.1	86.6	44.862	M
$PbBi_4Te_7$	23.600 – 23.892	23.740	0.6 – -0.6	14.0	9.721	0.506
PbFI	8.770 – 8.800	8.196	-6.5 – -6.9	21.9	12.007	1.434
PbO	4.988 – 5.071	4.847	-2.8 – -4.4	24.9	19.082	1.405
$PbSb_2Te_4$	41.712	41.354	-0.9	7.6	7.056	0.414
$PdTe_2$	5.113 – 5.270	5.018	-1.9 – -4.8	94.4	45.843	M
PtS_2	5.019 – 5.043	4.575	-8.9 – -9.3	49.0	21.599	0.112
$PtSe_2$	5.031 – 5.082	4.797	-4.6 – -5.6	67.3	25.136	M
$PtTe_2$	5.201 – 5.224	5.086	-2.2 – -2.6	80.5	32.849	M
$RhTe_2$	5.410 – 5.442	5.197	-3.9 – -4.5	86.5	51.709	M
SnS_2	5.460 – 5.960	5.690	0.2 – -4.5	30.0	11.235	1.113
$SnSe_2$	6.128 – 6.141	5.910	-3.6 – -3.8	30.6	13.477	0.275
SrFI	8.888 – 8.916	7.859	-11.6 – -11.9	22.5	13.449	4.161
TaS_2	5.853 – 5.900	5.691	-2.8 – -3.5	50.9	16.563	M
TaS_2	12.097 – 12.100	11.804	-2.4 – -2.4	56.1	16.897	M
$TaSe_2$	6.203 – 6.272	5.998	-3.3 – -4.4	53.3	18.043	M
$TaSe_2$	12.696 – 12.720	12.495	-1.6 – -1.8	60.7	18.396	M
$TaSe_2$	25.143 – 25.500	25.147	-0.0 – -1.4	49.5	20.085	M
TiS_2	5.680 – 5.716	5.386	-5.2 – -5.8	63.9	18.651	M
$TiSe_2$	5.981 – 6.011	5.698	-4.7 – -5.2	69.0	20.279	M
$TiTe_2$	6.459 – 6.539	6.225	-3.6 – -4.8	67.1	24.132	M
$TlCrTe_2$	7.839 – 7.935	7.712	-1.6 – -2.8	77.6	70.366	M
VBr_2	6.206	5.715	-7.9	29.1	9.775	M
VCl_2	5.798 – 5.835	5.330	-8.1 – -8.6	30.2	9.181	M

VI_2	6.714	6.148	-8.4	27.9	10.462	M
VS_2	5.755 – 5.755	5.390	-6.3 – -6.3	55.4	21.171	M
VSe_2	6.048 – 6.150	5.770	-4.6 – -6.2	62.0	20.504	M
WS_2	12.323 – 12.500	12.230	-0.8 – -2.2	51.3	12.898	0.924
WS_2	18.490	18.288	-1.1	45.1	12.549	0.759
WSe_2	12.960 – 12.980	12.871	-0.7 – -0.8	52.5	13.355	0.996
$Y_2I_2Ga_2$	11.434	10.968	-4.1	30.9	8.443	M
YI_3	20.880	20.528	-1.7	20.0	7.868	2.450
ZrNCl	27.178 – 27.672	27.148	-0.1 – -1.9	41.6	6.975	1.801
ZrS_2	5.810 – 5.850	5.626	-3.2 – -3.8	42.7	12.681	0.536
$ZrSe_2$	6.125 – 6.192	5.912	-3.5 – -4.5	46.7	14.678	M
$ZrTe_2$	6.630 – 6.660	6.403	-3.4 – -3.9	62.9	20.929	M

I. PBE-D

Name	c_{exp} [Å]	c_{calc}	c dev. [%]	C_{33} [GPa]	E_B [meV/Å^2]	E_g [eV]
$AgBiP_2Se_6$	39.615	40.029	1.0	23.0	8.630	1.246
BBr_3	6.847 – 6.864	6.757	-1.3 – -1.6	13.9	8.768	3.563
BI_3	7.261 – 7.460	7.015	-3.4 – -6.0	21.9	12.027	2.545
BN	6.661 – 6.690	6.477	-2.8 – -3.2	69.1	28.057	4.146
BaFI	7.962 – 8.102	8.059	-0.5 – 1.2	103.4	44.343	3.869
Bi_2Te_3	30.440 – 30.497	30.785	0.9 – 1.1	48.3	25.628	0.783
C	6.704 – 6.930	6.740	0.5 – -2.7	44.0	21.148	M
CdI_2	6.835 – 6.864	6.808	-0.4 – -0.8	33.2	14.652	2.268
$CoTe_2$	5.405	5.447	0.8	40.8	53.724	M
$CrSe_2$	5.915	6.022	1.8	40.8	22.541	M
Cu_2S	6.670 – 6.680	6.175	-7.4 – -7.6	54.6	52.033	M
FeLiAs	6.349	5.782	-8.9	209.2	80.748	M
FeS	5.039	4.443	-11.8	35.4	24.178	M
GaS	14.230 – 15.530	15.632	0.7 – 9.9	31.4	12.967	1.853
GaSe	15.919 – 15.995	15.881	-0.2 – -0.7	51.5	15.768	1.465
$Ge_2Sb_2Te_5$	16.960 – 17.239	17.472	1.4 – 3.0	43.2	24.107	0.119
HfS_2	5.837 – 5.856	6.043	3.2 – 3.5	21.6	7.657	1.223
$HfSe_2$	6.143 – 6.159	6.029	-1.9 – -2.1	54.6	30.752	0.337
$HfTe_2$	6.650 – 6.670	6.678	0.1 – 0.4	56.3	25.983	M
HgI_2	12.088 – 12.450	12.366	-0.6 – 2.3	25.7	16.524	1.108
$In_2Zn_2S_5$	46.270	45.957	-0.7	100.8	45.257	0.361
$Mg_2(P_2Se_6)$	20.194	20.173	-0.1	34.9	12.561	2.025
$MgBr_2$	6.260 – 6.269	6.343	1.2 – 1.3	24.6	9.801	4.563
MgI_2	6.862 – 6.895	6.822	-0.6 – -1.1	30.2	12.222	3.482
MoS_2	12.290 – 12.530	12.389	0.5 – -1.1	51.2	18.211	0.970
MoS_2	18.330 – 18.450	18.469	0.1 – 0.8	53.0	19.032	1.187
$MoSe_2$	12.900 – 12.930	13.012	0.6 – 0.9	69.1	24.158	1.024
$MoTe_2$	13.964 – 13.974	14.025	0.4 – 0.4	85.6	31.969	0.885

NbS_2	17.800 – 17.918	17.859	0.3 – 0.3	51.2	18.050	M
$NbSe_2$	12.482 – 12.550	12.691	1.1 – 1.7	50.9	25.222	M
$NbTe_2$	6.610	6.877	4.0	61.3	31.169	M
Ni_2SbTe_2	15.634 – 15.682	15.673	-0.1 – 0.3	33.3	40.323	M
NiSbSi	8.179	7.813	-4.5	57.4	75.287	M
$NiTe_2$	5.251 – 5.308	5.216	-0.7 – -1.7	50.1	48.955	M
$PdTe_2$	5.113 – 5.270	5.114	0.0 – -3.0	84.2	54.430	M
PtS_2	5.019 – 5.043	5.457	8.2 – 8.7	21.3	10.301	1.043
$PtSe_2$	5.031 – 5.082	5.471	7.7 – 8.7	13.4	19.306	M
$PtTe_2$	5.201 – 5.224	5.190	-0.2 – -0.7	62.2	41.530	M
$RhTe_2$	5.410 – 5.442	5.348	-1.2 – -1.7	55.4	59.688	M
SnS_2	5.460 – 5.960	5.962	0.0 – 9.2	30.2	14.109	1.472
$SnSe_2$	6.128 – 6.141	6.221	1.3 – 1.5	42.0	18.703	0.535
SrFI	8.888 – 8.916	8.473	-4.7 – -5.0	22.0	17.121	4.337
TaS_2	5.853 – 5.900	6.164	4.5 – 5.3	33.8	11.188	M
TaS_2	12.097 – 12.100	12.209	0.9 – 0.9	33.8	11.080	M
$TaSe_2$	6.203 – 6.272	6.385	1.8 – 2.9	55.3	19.641	M
$TaSe_2$	12.696 – 12.720	12.889	1.3 – 1.5	57.7	20.057	M
$TaSe_2$	25.143 – 25.500	25.483	-0.1 – 1.4	86.4	22.251	M
Ti_2PTe_2	28.486	28.375	-0.4	96.1	27.842	M
TiS_2	5.680 – 5.716	5.832	2.0 – 2.7	40.7	14.371	M
$TiSe_2$	5.981 – 6.011	6.120	1.8 – 2.3	42.8	19.553	M
$TiTe_2$	6.459 – 6.539	6.609	1.1 – 2.3	59.7	28.211	M
VBr_2	6.206	6.095	-1.8	34.0	13.654	M
VCl_2	5.798 – 5.835	5.777	-0.4 – -1.0	22.8	14.091	M
VI_2	6.714	6.488	-3.4	41.1	17.363	M
VS_2	5.755 – 5.755	5.905	2.6 – 2.6	44.5	17.071	M
VSe_2	6.048 – 6.150	6.266	1.9 – 3.6	55.1	22.468	M
WS_2	12.323 – 12.500	12.523	0.2 – 1.6	34.0	11.042	1.307
WS_2	18.490	18.656	0.9	30.6	10.698	1.333

WSe_2	12.960 – 12.980	13.176	1.5 – 1.7	65.2	19.936	1.173
$Y_2I_2Ga_2$	11.434	11.358	-0.7	47.9	15.947	M
YS_2	7.846	7.952	1.4	172.4	80.072	0.404
ZrNCl	27.178 – 27.672	27.629	-0.2 – 1.7	54.8	12.785	1.818
ZrS_2	5.810 – 5.850	5.907	1.0 – 1.7	33.5	12.739	0.817
$ZrSe_2$	6.125 – 6.192	6.215	0.4 – 1.5	47.1	17.909	0.246
$ZrTe_2$	6.630 – 6.660	6.714	0.8 – 1.3	60.1	26.737	M

J. PBE

Name	c_{exp} [Å]	c_{calc}	c dev. [%]	C_{33} [GPa]	E_B [meV/Å^2]	E_g [eV]
$AgBiP_2Se_6$	39.615	40.427	2.0	1.9	0.568	1.377
BBr_3	6.847 – 6.864	7.728	12.6 – 12.9	0.9	0.616	3.641
BI_3	7.261 – 7.460	8.062	8.1 – 11.0	1.0	0.556	2.542
BN	6.661 – 6.690	7.686	14.9 – 15.4	1.1	0.571	4.409
BaFI	7.962 – 8.102	8.331	2.8 – 4.6	16.0	4.326	4.078
BiIO	9.128 – 9.151	10.509	14.8 – 15.1	2.1	0.569	2.067
C	6.704 – 6.930	7.809	12.7 – 16.5	1.2	0.399	M
CdI_2	6.835 – 6.864	7.937	15.6 – 16.1	1.5	0.448	2.366
$CoTe_2$	5.405	5.560	2.9	42.2	21.750	M
$CrSe_2$	5.915	6.699	13.3	3.2	0.619	M
$CrSiTe_3$	20.528 – 20.582	21.448	4.2 – 4.5	2.4	0.914	0.427
Cu_2S	6.670 – 6.680	7.091	6.2 – 6.3	4.6	2.165	M
$Fe(PSe_3)$	19.800 – 19.812	20.890	5.4 – 5.5	2.0	0.544	M
GaS	14.230 – 15.530	16.721	7.7 – 17.5	2.1	0.747	2.377
GaSe	15.919 – 15.995	17.261	7.9 – 8.4	1.8	0.442	2.161
$Ge_2Sb_2Te_5$	16.960 – 17.239	18.665	8.3 – 10.1	3.6	1.475	0.177
HfS_2	5.837 – 5.856	6.855	17.1 – 17.4	2.1	0.760	1.317
$HfSe_2$	6.143 – 6.159	7.086	15.0 – 15.3	1.9	0.706	0.599
$HfTe_2$	6.650 – 6.670	7.210	8.1 – 8.4	8.0	1.989	M
HgI_2	12.088 – 12.450	13.550	8.8 – 12.1	2.0	0.784	1.391
$Mg_2(P_2Se_6)$	20.194	21.178	4.9	1.6	0.481	2.035
$MgBr_2$	6.260 – 6.269	7.329	16.9 – 17.1	1.7	0.598	4.655
MgI_2	6.862 – 6.895	7.927	15.0 – 15.5	1.7	0.415	3.617
MoS_2	12.290 – 12.530	13.521	7.9 – 10.0	1.5	0.714	1.673
MoS_2	18.330 – 18.450	19.723	6.9 – 7.6	1.5	0.598	1.745
$MoSe_2$	12.900 – 12.930	14.099	9.0 – 9.3	1.1	0.397	1.468
$MoTe_2$	13.964 – 13.974	14.671	5.0 – 5.1	4.0	1.248	1.044
NbS_2	17.800 – 17.918	18.418	2.8 – 3.5	6.8	1.664	M

$NbSe_2$	12.482 – 12.550	13.172	5.0 – 5.5	6.9	1.522	M
$NbSe_2$	25.230 – 25.450	25.511	0.2 – 1.1	10.5	2.643	M
$NbTe_2$	6.610	7.330	10.9	7.5	2.349	M
Ni_2SbTe_2	15.634 – 15.682	15.971	1.8 – 2.2	27.7	5.857	M
NiSbSi	8.179	7.760	-5.1	48.5	26.875	M
$NiTe_2$	5.251 – 5.308	5.393	1.6 – 2.7	45.7	17.068	M
$PbBi_4Te_7$	23.600 – 23.892	24.785	3.7 – 5.0	2.8	1.088	0.937
PbFI	8.770 – 8.800	10.347	17.6 – 18.0	1.7	0.461	2.324
PbO	4.988 – 5.071	5.779	14.0 – 15.9	6.9	2.983	1.945
$PbSb_2Te_4$	41.712	42.434	1.7	1.3	0.724	0.580
$PdTe_2$	5.113 – 5.270	5.298	0.5 – 3.6	69.9	18.314	M
PtS_2	5.019 – 5.043	6.581	30.5 – 31.1	1.6	0.741	1.509
$PtSe_2$	5.031 – 5.082	6.651	30.9 – 32.2	1.5	0.626	0.921
$PtTe_2$	5.201 – 5.224	5.473	4.8 – 5.2	33.1	5.416	M
$Re(AgCl_3)_2$	16.731 – 16.731	17.109	2.3 – 2.3	8.9	1.297	M
$RhTe_2$	5.410 – 5.442	5.544	1.9 – 2.5	48.6	25.649	M
SnS_2	5.460 – 5.960	7.068	18.6 – 29.4	1.9	0.808	1.551
$SnSe_2$	6.128 – 6.141	7.209	17.4 – 17.6	2.1	0.734	0.668
SrFI	8.888 – 8.916	9.876	10.8 – 11.1	2.5	0.708	4.323
TaS_2	5.853 – 5.900	6.894	16.8 – 17.8	3.0	1.126	M
TaS_2	12.097 – 12.100	13.139	8.6 – 8.6	2.3	1.029	M
$TaSe_2$	6.203 – 6.272	6.904	10.1 – 11.3	6.0	1.519	M
$TaSe_2$	12.696 – 12.720	13.534	6.4 – 6.6	3.5	1.065	M
$TaSe_2$	25.143 – 25.500	26.317	3.2 – 4.7	6.9	2.133	M
Ti_2PTe_2	28.486	28.702	0.8	13.9	4.008	M
TiS_2	5.680 – 5.716	6.589	15.3 – 16.0	2.3	1.075	M
$TiSe_2$	5.981 – 6.011	6.728	11.9 – 12.5	4.6	1.067	M
$TiTe_2$	6.459 – 6.539	6.856	4.8 – 6.1	9.7	2.799	M
$TlCrTe_2$	7.839 – 7.935	8.036	1.3 – 2.5	60.6	48.774	M
VBr_2	6.206	7.077	14.0	2.0	0.815	M

VCl_2	5.798 – 5.835	6.674	14.4 – 15.1	2.3	0.753	M
VI_2	6.714	7.482	11.4	2.2	0.644	M
VS_2	5.755 – 5.755	6.636	15.3 – 15.3	3.4	1.310	M
VSe_2	6.048 – 6.150	6.899	12.2 – 14.1	4.7	1.237	M
WS_2	12.323 – 12.500	13.657	9.3 – 10.8	1.3	0.626	1.845
WS_2	18.490	19.956	7.9	1.4	0.608	1.838
WSe_2	12.960 – 12.980	14.203	9.4 – 9.6	1.4	0.431	1.550
$Y_2I_2Ga_2$	11.434	12.444	8.8	3.5	0.531	M
YI_3	20.880	21.476	2.9	2.0	0.524	2.804
ZrNCl	27.178 – 27.672	28.534	3.1 – 5.0	3.5	0.539	1.931
ZrS_2	5.810 – 5.850	6.779	15.9 – 16.7	2.1	0.877	1.061
$ZrSe_2$	6.125 – 6.192	6.917	11.7 – 12.9	2.7	0.883	0.362
$ZrTe_2$	6.630 – 6.660	7.005	5.2 – 5.7	8.4	2.950	M

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