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An Atlas of Two-Dimensional Materials

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1. Cartesian coordinates

1.1. Atomically thin 2D materials

Graphene

1.C 0.047580 0.024180 1.675514
2.C 0.047662 1.446213 1.675513

Lattice Vectors

2.464848 -0.000846 0.000000
-1.232661 2.133341 0.000000

Graphane

1.C 0.121438 -0.058360 1.656149
2.C 0.122002 1.403412 1.197834
3.H 0.121114 -0.059441 2.765350
4.H 0.122291 1.404491 0.088555

Lattice Vectors

2.531982 0.000305 0.000000
-1.265401 2.192348 0.000000

Fluorographene

1.C 0.124926 -0.059579 1.672128
2.C 0.123688 1.439380 1.181606
3.F 0.124442 -0.060839 3.043076
4.F 0.122998 1.438768 -0.188923

Lattice Vectors

2.594844 -0.000959 0.000000
-1.299163 2.248298 0.000000

Clorographene

1.C 0.145519 -0.064110 1.680367
2.C 0.137585 1.599909 1.173609
3.Cl 0.163909 -0.056556 3.435946
4.Cl 0.120900 1.590882 -0.582034

Lattice Vectors

2.895004 0.004596 0.000000
-1.437645 2.499267 0.000000

Silicene

1.Si 0.050695 -0.201967 1.104355
2.Si 0.059897 2.012277 1.631313

Lattice Vectors

3.836284 0.005494 0.000000
-1.908837 3.317191 0.000000

Silicane

1.Si 0.212892 -0.104345 1.789106
2.Si 0.210461 2.125208 1.064858
3.H 0.213107 -0.110727 3.290482
4.H 0.211652 2.130402 -0.436559

Lattice Vectors

3.862973 -0.001882 0.000000
-1.935086 3.347903 0.000000

Fluorosilicene

1.Si 0.211732 -0.108592 1.788122
2.Si 0.210933 2.159057 1.063327
3.F 0.213411 -0.112831 3.417406
4.F 0.222091 2.150831 -0.560967

Lattice Vectors

3.926298 -0.000840 0.000000
-1.965273 3.402272 0.000000

Germanene

1.Ge 0.057234 -0.211246 1.002078
2.Ge 0.046614 2.106107 1.733590

Lattice Vectors

4.011935 -0.007766 0.000000
-2.017893 3.479562 0.000000

Germanane

1.Ge 0.220289 -0.105592 1.801220
2.Ge 0.226613 2.219925 1.052720
3.H 0.218657 -0.107220 3.350944
4.H 0.230533 2.217002 -0.496997

Lattice Vectors

4.028878 0.004718 0.000000
-2.008146 3.487648 0.000000

Fluorogermanene

1.Ge 0.222310 -0.121399 1.736070
2.Ge 0.214937 2.315574 1.117871
3.F 0.247217 -0.116401 3.506824
4.F 0.209076 2.308457 -0.652877

Lattice Vectors

4.229179 -0.006277 0.000000
-2.120006 3.659403 0.000000

Clorogermanene

1.Ge 0.155959 -0.463186 1.787282
2.Ge 0.154466 1.914174 1.066656
3.Cl 0.153148 -0.464606 3.967893
4.Cl 0.158336 1.918177 -1.113944

Lattice Vectors

4.121377 -0.003814 0.000000
-2.064130 3.567551 0.000000

Silicon Carbide

1.C 0.062579 0.033329 1.675513
2.Si 0.061221 1.818702 1.675514

Lattice Vectors

3.090619 -0.000546 0.000000
-1.546949 2.678303 0.000000

Boron Nitride

1.N 0.048707 0.036820 1.675509
2.B 0.049682 1.483121 1.675517

Lattice Vectors

2.504855 0.000962 0.000000
-1.251043 2.168793 0.000000

1.2. Atomically thin transition metal chalcogenides

α-ZnO

1.Zn 0.818591 -0.472614 0.000000
2.O -0.818591 0.472614 0.000000
Lattice Vectors
3.274363 0.000000 0.000000
-1.637182 2.835682 0.000000

α-ZnS

1.Zn 0.970521 -0.560331 0.000000
2.S -0.970521 0.560331 0.000000
Lattice Vectors
3.882084 0.000000 0.000000
-1.941042 3.361983 0.000000

α-ZnSe

1.Zn 1.011140 -0.583782 0.000000
2.Se -1.011140 0.583782 0.000000
Lattice Vectors
4.044560 0.000000 0.000000
-2.022280 3.502692 0.000000

α-ZnTe

1.Zn 1.093561 -0.631368 0.000000
2.Te -1.093561 0.631368 0.000000
Lattice Vectors
4.374245 0.000000 0.000000
-2.187123 3.788207 0.000000

α-CdO

1.Cd 0.917024 -0.529444 0.000000
2.O -0.917024 0.529444 0.000000
Lattice Vectors
3.668097 0.000000 0.000000
-1.834049 3.176665 0.000000

α-CdS

1.Cd 1.052635 -0.607739 0.000000
2.S -1.052635 0.607739 0.000000
Lattice Vectors
4.210539 0.000000 0.000000
-2.105270 3.646434 0.000000

α-CdSe

1.Cd 1.100311 -0.635265 0.000000
2.Se -1.100311 0.635265 0.000000
Lattice Vectors
4.401244 0.000000 0.000000
-2.200622 3.811589 0.000000

α-CdTe

1.Cd 1.181986 -0.682420 0.000000
2.Te -1.181986 0.682420 0.000000
Lattice Vectors
4.727942 0.000000 0.000000
-2.363971 4.094518 0.000000

β-ZnO

1.Zn 0.817424 -0.471940 0.000105
2.O -0.817424 0.471940 -0.000105

Lattice Vectors

3.269696 0.000000 0.000000
-1.634848 2.831640 0.000000

β-ZnS

1.Zn 0.971579 -0.560942 -0.005833
2.S -0.971579 0.560942 0.005833

Lattice Vectors

3.886318 0.000000 0.000000
-1.943159 3.365650 0.000000

β-ZnSe

1.Zn 1.005477 -0.580512 0.177037
2.Se -1.005477 0.580512 -0.177037

Lattice Vectors

4.021908 0.000000 0.000000
-2.010954 3.483075 0.000000

β-ZnTe

1.Zn 1.082779 -0.625143 0.261661
2.Te -1.082779 0.625143 -0.261661

Lattice Vectors

4.331117 0.000000 0.000000
-2.165559 3.750857 0.000000

β-CdO

1.Cd 0.915528 -0.528580 -0.008946
2.O -0.915528 0.528580 0.008946

Lattice Vectors

3.662111 0.000000 0.000000
-1.831056 3.171481 0.000000

β-CdS

1.Cd 1.063557 -0.614045 0.025826
2.S -1.063557 0.614045 -0.025826

Lattice Vectors

4.254229 0.000000 0.000000
-2.127114 3.684270 0.000000

β-CdSe

1.Cd 1.099029 -0.634525 0.178634
2.Se -1.099029 0.634525 -0.178634

Lattice Vectors

4.396116 0.000000 0.000000
-2.198058 3.807148 0.000000

β-CdTe

1.Cd 1.156440 -0.667671 0.309381
2.Te -1.156440 0.667671 -0.309381

Lattice Vectors

4.625758 0.000000 0.000000
-2.312879 4.006024 0.000000

1.3. Metalloid chalcogenides

GaS

1.Ga	0.000000	2.068264	5.106493
2.Ga	0.000000	2.068264	2.639507
3.S	1.791169	1.034132	1.533481
4.S	1.791169	1.034132	6.212519

Lattice Vectors

3.582339	0.000000	0.000000
-1.791169	3.102396	0.000000

GaSe

1.Ga	0.000000	2.174878	5.095977
2.Ga	0.000000	2.174878	2.650023
3.Se	1.883500	1.087439	1.469759
4.Se	1.883500	1.087439	6.276241

Lattice Vectors

3.767000	0.000000	0.000000
-1.883500	3.262317	0.000000

InS

1.In	1.911240	-1.103455	1.407533
2.In	1.911240	-1.103455	-1.407533
3.S	-1.911240	1.103455	-2.641715
4.S	-1.911240	1.103455	2.641715

Lattice Vectors

3.822479	0.000000	0.000000
-1.911240	3.310364	0.000000

InSe

1.In	2.004144	-1.157093	1.395717
2.In	2.004144	-1.157093	-1.395717
3.Se	-2.004144	1.157093	-2.698701
4.Se	-2.004144	1.157093	2.698701

Lattice Vectors

4.008288	0.000000	0.000000
-2.004144	3.471279	0.000000

1.4. Transition metal chalcogenides (1T)

HfS_2

1.Hf 0.000000 0.000000 0.000000
2.S -1.783116 1.029482 -1.480402
3.S 0.000000 2.058965 1.480402
Lattice Vectors
3.566232 0.000000 0.000000
-1.783116 3.088447 0.000000

$HfSe_2$

1.Hf 0.000000 0.000000 0.000000
2.Se -1.808001 1.043850 -1.632945
3.Se 0.000000 2.087700 1.632945
Lattice Vectors
3.616002 0.000000 0.000000
-1.808001 3.131550 0.000000

$HfTe_2$

1.Hf -0.008809 0.008120 -0.001474
2.Te -1.946205 1.117713 -1.809504
3.Te -0.037407 2.214500 1.810978
Lattice Vectors
3.907426 -0.055321 0.000000
-1.992422 3.340333 0.000000

MoS_2

1.Mo 0.000000 0.000000 0.000000
2.S -1.542005 0.890277 -1.641947
3.S 0.000000 1.780554 1.641947
Lattice Vectors
3.084010 0.000000 0.000000
-1.542005 2.670831 0.000000

$MoSe_2$

1.Mo 0.000000 0.000000 0.000000
2.Se -1.621542 0.936198 -1.731520
3.Se 0.000000 1.872395 1.731520
Lattice Vectors
3.243083 0.000000 0.000000
-1.621542 2.808593 0.000000

$MoTe_2$

1.Mo 0.000467 -0.001030 -0.000156
2.Te -1.700815 0.981187 -1.905812
3.Te 0.008210 1.978761 1.905968
Lattice Vectors
3.415945 0.014026 0.000000
-1.692137 2.958918 0.000000

NbS_2

1.Nb 0.000000 0.000000 0.000000
2.S -1.655671 0.955902 -1.566507
3.S 0.000000 1.911804 1.566507
Lattice Vectors
3.311342 0.000000 0.000000
-1.655671 2.867707 0.000000

$NbSe_2$

1.Nb 0.000000 0.000000 0.000000
2.Se -1.686869 0.973914 -1.711632
3.Se 0.000000 1.947829 1.711632
Lattice Vectors
3.373739 0.000000 0.000000
-1.686869 2.921743 0.000000

$NbTe_2$

1.Nb	0.000000	0.000000	0.000000
2.Te	-1.737230	1.002990	-1.934905
3.Te	0.000000	2.005981	1.934905

Lattice Vectors

3.474460	0.000000	0.000000
-1.737230	3.008971	0.000000

NiS_2

1.Ni	0.000000	0.000000	0.000000
2.S	-1.653373	0.954575	-1.189242
3.S	0.000000	1.909150	1.189242

Lattice Vectors

3.306745	0.000000	0.000000
-1.653373	2.863725	0.000000

$NiSe_2$

1.Ni	0.000000	0.000000	0.000000
2.Se	-1.750066	1.010401	-1.247763
3.Se	0.000000	2.020803	1.247763

Lattice Vectors

3.500133	0.000000	0.000000
-1.750066	3.031204	0.000000

PdS_2

1.Pd	0.000000	0.000000	0.000000
2.S	-1.744552	1.007218	-1.278202
3.S	0.000000	2.014436	1.278202

Lattice Vectors

3.489105	0.000000	0.000000
-1.744552	3.021654	0.000000

$PdSe_2$

1.Pd	0.000000	0.000000	0.000000
2.Se	-1.832470	1.057977	-1.337368
3.Se	0.000000	2.115954	1.337368

Lattice Vectors

3.664940	0.000000	0.000000
-1.832470	3.173931	0.000000

$PdTe_2$

1.Pd	0.000000	0.000000	0.000000
2.Te	-1.814830	1.047792	-1.710539
3.Te	0.000000	2.095585	1.710539

Lattice Vectors

3.629660	0.000000	0.000000
-1.814830	3.143377	0.000000

PtS_2

1.Pt	0.000000	0.000000	0.000000
2.S	-1.749044	1.009811	-1.274571
3.S	0.000000	2.019622	1.274571

Lattice Vectors

3.498088	0.000000	0.000000
-1.749044	3.029433	0.000000

$PtSe_2$

1.Pt	0.000000	0.000000	0.000000
2.Se	-1.820817	1.051249	-1.358786
3.Se	0.000000	2.102498	1.358786

Lattice Vectors

3.641634	0.000000	0.000000
-1.820817	3.153748	0.000000

$PtTe_2$

1.Pt	-0.000324	0.000561	0.000000
2.Te	-1.983175	1.149100	-1.419718
3.Te	-0.003563	2.292030	1.419718

Lattice Vectors

3.974885	0.000439	0.000000
-1.987062	3.441692	0.000000

ReS_2

1.Re	0.000000	0.000000	0.000000
2.S	-1.521400	0.878381	-1.665736
3.S	0.000000	1.756761	1.665736

Lattice Vectors

3.042799	0.000000	0.000000
-1.521400	2.635142	0.000000

$ReTe_2$

1.Re	0.000000	0.000000	0.000000
2.Te	-1.731553	0.999713	-1.872293
3.Te	0.000000	1.999425	1.872293

Lattice Vectors

3.463106	0.000000	0.000000
-1.731553	2.999138	0.000000

TaS_2

1.Ta	0.000000	0.000000	0.000000
2.S	-1.663325	0.960321	-1.554208
3.S	0.000000	1.920642	1.554208

Lattice Vectors

3.326650	0.000000	0.000000
-1.663325	2.880963	0.000000

$TaSe_2$

1.Ta	0.000000	0.000000	0.000000
2.Se	-1.716333	0.990925	-1.674461
3.Se	0.000000	1.981851	1.674461

Lattice Vectors

3.432666	0.000000	0.000000
-1.716333	2.972776	0.000000

$TaTe_2$

1.Ta	0.000000	0.000000	0.000000
2.Te	-1.765307	1.019200	-1.898608
3.Te	0.000000	2.038401	1.898608

Lattice Vectors

3.530614	0.000000	0.000000
-1.765307	3.057601	0.000000

TiS_2

1.Ti	0.000000	0.000000	0.000000
2.S	-1.681373	0.970741	-1.433759
3.S	0.000000	1.941482	1.433759

Lattice Vectors

3.362746	0.000000	0.000000
-1.681373	2.912224	0.000000

$TiSe_2$

1.Ti	0.000000	0.000000	0.000000
2.Se	-1.733254	1.000695	-1.564081
3.Se	0.000000	2.001390	1.564081

Lattice Vectors

3.466509	0.000000	0.000000
-1.733254	3.002085	0.000000

$TiTe_2$

1.Ti	0.000000	0.000000	0.000000
2.Te	-1.884326	1.087916	-1.719543
3.Te	0.000000	2.175832	1.719543

Lattice Vectors

3.768651	0.000000	0.000000
-1.884326	3.263748	0.000000

WS_2

1.W	0.000000	0.000000	0.000000
2.S	-1.584224	0.914652	-1.596010
3.S	0.000000	1.829304	1.596010

Lattice Vectors

3.168447	0.000000	0.000000
-1.584224	2.743956	0.000000

WSe_2

1.W	0.000000	0.000000	0.000000
2.Se	-1.624559	0.937940	-1.736760
3.Se	0.000000	1.875879	1.736760

Lattice Vectors

3.249118	0.000000	0.000000
-1.624559	2.813819	0.000000

WTe_2

1.W	0.010364	-0.017950	0.000000
2.Te	-1.779942	0.945459	-1.898163
3.Te	0.071179	2.014204	1.898163

Lattice Vectors

3.467896	0.041049	0.000000
-1.698398	2.941712	0.000000

ZrS_2

1.Zr	0.000000	0.000000	0.000000
2.S	-1.823430	1.052758	-1.459307
3.S	0.000000	2.105515	1.459307

Lattice Vectors

3.646859	0.000000	0.000000
-1.823430	3.158273	0.000000

$ZrSe_2$

1.Zr	0.000000	0.000000	0.000000
2.Se	-1.873840	1.081862	-1.596466
3.Se	0.000000	2.163724	1.596466

Lattice Vectors

3.747679	0.000000	0.000000
-1.873840	3.245586	0.000000

$ZrTe_2$

1.Zr	0.000161	-0.000278	0.000000
2.Te	-1.934649	1.115137	-1.840312
3.Te	0.001588	2.233024	1.840312

Lattice Vectors

3.874501	0.005023	0.000000
-1.932900	3.347881	0.000000

1.5. Transition metal chalcogenides (2H)

HfS_2

1.Hf	0.578654	1.670430	0.000000
2.S	2.314615	0.668172	-1.582780
3.S	2.314615	0.668172	1.582780

Lattice Vectors

3.471923	0.000000	0.000000
-1.735962	3.006774	0.000000

$HfSe_2$

1.Hf	0.598785	1.728544	0.000000
2.Se	2.395141	0.691418	-1.697171
3.Se	2.395141	0.691418	1.697171

Lattice Vectors

3.592712	0.000000	0.000000
-1.796356	3.111380	0.000000

$HfTe_2$

1.Hf	0.654157	1.888387	0.000000
2.Te	2.616627	0.755355	-1.842768
3.Te	2.616627	0.755355	1.842768

Lattice Vectors

3.924940	0.000000	0.000000
-1.962470	3.399098	0.000000

MoS_2

1.Mo	0.524650	1.514534	0.000000
2.S	2.098600	0.605814	-1.574987
3.S	2.098600	0.605814	1.574987

Lattice Vectors

3.147900	0.000000	0.000000
-1.573950	2.726161	0.000000

$MoSe_2$

1.Mo	0.546952	1.578915	0.000000
2.Se	2.187809	0.631566	-1.671118
3.Se	2.187809	0.631566	1.671118

Lattice Vectors

3.281713	0.000000	0.000000
-1.640857	2.842047	0.000000

$MoTe_2$

1.Mo	0.586790	1.693916	0.000000
2.Te	2.347159	0.677566	-1.820893
3.Te	2.347159	0.677566	1.820893

Lattice Vectors

3.520739	0.000000	0.000000
-1.760369	3.049049	0.000000

NbS_2

1.Nb	0.549710	1.586877	0.000000
2.S	2.198842	0.634751	-1.576772
3.S	2.198842	0.634751	1.576772

Lattice Vectors

3.298262	0.000000	0.000000
-1.649131	2.856379	0.000000

$NbSe_2$

1.Nb	0.565463	1.632352	0.000000
2.Se	2.261854	0.652941	-1.699301
3.Se	2.261854	0.652941	1.699301

Lattice Vectors

3.392781	0.000000	0.000000
-1.696390	2.938234	0.000000

$NbTe_2$

1.Nb	0.579560	1.673045	0.000000
2.Te	2.318239	0.669218	-1.936231
3.Te	2.318239	0.669218	1.936231

Lattice Vectors

3.477358	0.000000	0.000000
-1.738679	3.011480	0.000000

NiS_2

1.Ni	0.580406	1.675488	0.000000
2.S	2.321624	0.670195	-1.077778
3.S	2.321624	0.670195	1.077778

Lattice Vectors

3.482436	0.000000	0.000000
-1.741218	3.015878	0.000000

$NiSe_2$

1.Ni	0.537065	1.550374	0.000000
2.Se	2.148261	0.620150	-1.514619
3.Se	2.148261	0.620150	1.514619

Lattice Vectors

3.222391	0.000000	0.000000
-1.611196	2.790673	0.000000

$NiTe_2$

1.Ni	0.579193	1.671986	0.000000
2.Te	2.316772	0.668795	-1.635301
3.Te	2.316772	0.668795	1.635301

Lattice Vectors

3.475159	0.000000	0.000000
-1.737579	3.009576	0.000000

PdS_2

1.Pd	0.573914	1.656746	0.000000
2.S	2.295654	0.662698	-1.385747
3.S	2.295654	0.662698	1.385747

Lattice Vectors

3.443482	0.000000	0.000000
-1.721741	2.982143	0.000000

$PdSe_2$

1.Pd	0.561075	1.619685	0.000000
2.Se	2.244301	0.647874	-1.663915
3.Se	2.244301	0.647874	1.663915

Lattice Vectors

3.366452	0.000000	0.000000
-1.683226	2.915433	0.000000

$PdTe_2$

1.Pd	0.578918	1.671191	0.000000
2.Te	2.315670	0.668476	-1.863312
3.Te	2.315670	0.668476	1.863312

Lattice Vectors

3.473506	0.000000	0.000000
-1.736753	3.008144	0.000000

PtS_2

1.Pt	0.562431	1.623600	0.000000
2.S	2.249726	0.649440	-1.463641
3.S	2.249726	0.649440	1.463641

Lattice Vectors

3.374588	0.000000	0.000000
-1.687294	2.922479	0.000000

$PtSe_2$

1.Pt	0.594172	1.715226	0.000000
2.Se	2.376687	0.686091	-1.507407
3.Se	2.376687	0.686091	1.507407

Lattice Vectors

3.565031	0.000000	0.000000
-1.782516	3.087407	0.000000

$PtTe_2$

1.Pt	0.597783	1.719035	0.000000
2.Te	2.424228	0.712676	-1.764886
3.Te	2.424228	0.712676	1.764886

Lattice Vectors

3.615497	0.026550	0.000000
-1.784755	3.091287	0.000000

ReS_2

1.Re	0.546579	1.577837	0.000000
2.S	2.186315	0.631135	-1.460249
3.S	2.186315	0.631135	1.460249

Lattice Vectors

3.279473	0.000000	0.000000
-1.639736	2.840107	0.000000

$ReSe_2$

1.Re	0.512599	1.479746	0.000000
2.Se	2.050396	0.591898	-1.810483
3.Se	2.050396	0.591898	1.810483

Lattice Vectors

3.075595	0.000000	0.000000
-1.537797	2.663543	0.000000

$ReTe_2$

1.Re	0.565269	1.631790	0.000000
2.Te	2.261074	0.652716	-1.891942
3.Te	2.261074	0.652716	1.891942

Lattice Vectors

3.391611	0.000000	0.000000
-1.695806	2.937221	0.000000

TaS_2

1.Ta	0.550720	1.589790	0.000000
2.S	2.202878	0.635916	-1.572800
3.S	2.202878	0.635916	1.572800

Lattice Vectors

3.304317	0.000000	0.000000
-1.652159	2.861623	0.000000

$TaSe_2$

1.Ta	0.571535	1.649878	0.000000
2.Se	2.286139	0.659951	-1.682312
3.Se	2.286139	0.659951	1.682312

Lattice Vectors

3.429208	0.000000	0.000000
-1.714604	2.969781	0.000000

$TaTe_2$

1.Ta	0.593307	1.716866	0.000000
2.Te	2.373230	0.681378	-1.893133
3.Te	2.373230	0.681378	1.893133

Lattice Vectors

3.559846	0.000000	0.000000
-1.779923	3.079623	0.000000

TiS_2

1.Ti	0.548832	1.584341	0.000000
2.S	2.195327	0.633736	-1.517545
3.S	2.195327	0.633736	1.517545

Lattice Vectors

3.292991	0.000000	0.000000
-1.646495	2.851814	0.000000

$TiSe_2$

1.Ti	0.574923	1.659660	0.000000
2.Se	2.299692	0.663864	-1.622582
3.Se	2.299692	0.663864	1.622582

Lattice Vectors

3.449538	0.000000	0.000000
-1.724769	2.987388	0.000000

$TiTe_2$

1.Ti	0.614634	1.774296	0.000000
2.Te	2.458537	0.709719	-1.793266
3.Te	2.458537	0.709719	1.793266

Lattice Vectors

3.687806	0.000000	0.000000
-1.843903	3.193734	0.000000

WS_2

1.W	0.524862	1.515147	0.000000
2.S	2.099449	0.606059	-1.584501
3.S	2.099449	0.606059	1.584501

Lattice Vectors

3.149174	0.000000	0.000000
-1.574587	2.727264	0.000000

WSe_2

1.W	0.549512	1.586305	0.000000
2.Se	2.198048	0.634522	-1.680527
3.Se	2.198048	0.634522	1.680527

Lattice Vectors

3.297072	0.000000	0.000000
-1.648536	2.855348	0.000000

WTe_2

1.W	0.583768	1.705994	0.000000
2.Te	2.335072	0.676496	-1.831461
3.Te	2.335072	0.676496	1.831461

Lattice Vectors

3.502608	0.000000	0.000000
-1.751304	3.058984	0.000000

ZrS_2

1.Zr	0.585721	1.690831	0.000000
2.S	2.342884	0.676332	-1.587825
3.S	2.342884	0.676332	1.587825

Lattice Vectors

3.514326	0.000000	0.000000
-1.757163	3.043496	0.000000

$ZrSe_2$

1.Zr	0.607816	1.754614	0.000000
2.Se	2.431264	0.701846	-1.695388
3.Se	2.431264	0.701846	1.695388

Lattice Vectors

3.646897	0.000000	0.000000
-1.823448	3.158305	0.000000

$ZrTe_2$

1.Zr 0.621699 1.849558 0.000000
2.Te 2.512269 0.743779 -1.900907
3.Te 2.512269 0.743779 1.900907

Lattice Vectors

3.768926 0.015185 0.000000
-1.891615 3.306744 0.000000

1.6. Transition metal halides (MY_2)

$CoCl_2$

1.Co	0.000000	0.000000	0.000000
2.Cl	-1.673607	0.966257	-1.282705
3.Cl	1.673607	-0.966257	1.282705

Lattice Vectors

3.347213	0.000000	0.000000
-1.673607	2.898772	0.000000

$CoBr_2$

1.Co	0.000000	0.000000	0.000000
2.Br	-1.763531	1.018175	-1.372883
3.Br	1.763531	-1.018175	1.372883

Lattice Vectors

3.527063	0.000000	0.000000
-1.763531	3.054526	0.000000

CoI_2

1.Co	0.000000	0.000000	2.200000
2.Cl	1.674170	0.966583	0.915499
3.Cl	0.000000	1.933165	3.484501

Lattice Vectors

3.348341	0.000000	0.000000
-1.674170	2.899748	0.000000

$FeCl_2$

1.Fe	0.000000	0.000000	0.000000
2.Cl	-1.673600	0.966254	-1.235545
3.Cl	1.673600	-0.966254	1.235545

Lattice Vectors

3.347201	0.000000	0.000000
-1.673600	2.898761	0.000000

$FeBr_2$

1.Fe	0.000000	0.000000	0.000000
2.Br	-1.776648	1.025748	-1.315674
3.Br	1.776648	-1.025748	1.315674

Lattice Vectors

3.553296	0.000000	0.000000
-1.776648	3.077244	0.000000

$HfCl_2$

1.Hf	0.000000	0.000000	0.000000
2.Cl	-1.611003	0.930113	-1.836024
3.Cl	1.611003	-0.930113	1.836024

Lattice Vectors

3.222006	0.000000	0.000000
-1.611003	2.790339	0.000000

$HfBr_2$

1.Hf	0.000000	0.000000	0.000000
2.Br	-1.685077	0.972880	-1.946205
3.Br	1.685077	-0.972880	1.946205

Lattice Vectors

3.370154	0.000000	0.000000
-1.685077	2.918639	0.000000

HfI_2

1.Hf	0.000000	0.000000	0.000000
2.I	-1.814698	1.047716	-2.040344
3.I	1.814698	-1.047716	2.040344

Lattice Vectors

3.629396	0.000000	0.000000
-1.814698	3.143149	0.000000

$MnCl_2$

1.Mn	0.000000	0.000000	0.000000
2.Cl	-1.649224	0.952180	-1.347183
3.Cl	1.649224	-0.952180	1.347183

Lattice Vectors

3.298448	0.000000	0.000000
-1.649224	2.856540	0.000000

$MnBr_2$

1.Mn	0.000000	0.000000	0.000000
2.Br	-1.737699	1.003261	-1.437535
3.Br	1.737699	-1.003261	1.437535

Lattice Vectors

3.475397	0.000000	0.000000
-1.737699	3.009782	0.000000

$MoCl_2$

1.Mo	0.000000	0.000000	0.000000
2.Cl	-1.565343	0.903751	-1.704542
3.Cl	1.565343	-0.903751	1.704542

Lattice Vectors

3.130686	0.000000	0.000000
-1.565343	2.711253	0.000000

$MoBr_2$

1.Mo	0.000000	0.000000	0.000000
2.Br	-1.639730	0.946699	-1.805457
3.Br	1.639730	-0.946699	1.805457

Lattice Vectors

3.279460	0.000000	0.000000
-1.639730	2.840096	0.000000

MoI_2

1.Mo	0.000000	0.000000	0.000000
2.I	-1.840920	1.062855	-1.828657
3.I	1.840920	-1.062855	1.828657

Lattice Vectors

3.681839	0.000000	0.000000
-1.840920	3.188566	0.000000

$NbCl_2$

1.Nb	0.000000	0.000000	0.000000
2.Cl	-1.572528	0.907899	-1.773088
3.Cl	1.572528	-0.907899	1.773088

Lattice Vectors

3.145056	0.000000	0.000000
-1.572528	2.723698	0.000000

$NbBr_2$

1.Nb	0.000000	0.000000	0.000000
2.Br	-1.671041	0.964776	-1.859596
3.Br	1.671041	-0.964776	1.859596

Lattice Vectors

3.342083	0.000000	0.000000
-1.671041	2.894329	0.000000

NbI_2

1.Nb	0.000000	0.000000	0.000000
2.I	-1.836228	1.060147	-1.908515
3.I	1.836228	-1.060147	1.908515

Lattice Vectors

3.672457	0.000000	0.000000
-1.836228	3.180441	0.000000

$NiCl_2$

1.Ni	0.000000	0.000000	0.000000
2.Cl	-1.679402	0.969603	-1.343256
3.Cl	1.679402	-0.969603	1.343256

Lattice Vectors

3.358804	0.000000	0.000000
-1.679402	2.908810	0.000000

$NiBr_2$

1.Ni	0.000000	0.000000	0.000000
2.Br	-1.773579	1.023977	-1.426976
3.Br	1.773579	-1.023977	1.426976

Lattice Vectors

3.547159	0.000000	0.000000
-1.773579	3.071930	0.000000

$TaCl_2$

1.Ta	0.000000	0.000000	0.000000
2.Cl	-1.544227	0.891560	-1.818564
3.Cl	1.544227	-0.891560	1.818564

Lattice Vectors

3.088453	0.000000	0.000000
-1.544227	2.674679	0.000000

$TaBr_2$

1.Ta	0.000000	0.000000	0.000000
2.Br	-1.660412	0.958639	-1.887493
3.Br	1.660412	-0.958639	1.887493

Lattice Vectors

3.320824	0.000000	0.000000
-1.660412	2.875918	0.000000

TaI_2

1.Ta	0.000000	0.000000	2.200000
2.I	1.784406	1.030227	0.234244
3.I	0.000000	2.060454	4.165756

Lattice Vectors

3.568812	0.000000	0.000000
-1.784406	3.090681	0.000000

$TiCl_2$

1.Ti	0.000000	0.000000	0.000000
2.Cl	-1.596393	0.921678	-1.644786
3.Cl	1.596393	-0.921678	1.644786

Lattice Vectors

3.192786	0.000000	0.000000
-1.596393	2.765034	0.000000

$TiBr_2$

1.Ti	0.000000	0.000000	0.000000
2.Br	-1.721803	0.994083	-1.716200
3.Br	1.721803	-0.994083	1.716200

Lattice Vectors

3.443605	0.000000	0.000000
-1.721803	2.982249	0.000000

TiI_2

1.Ti	0.000000	0.000000	0.000000
2.I	-1.860133	1.073948	-1.816868
3.I	1.860133	-1.073948	1.816868

Lattice Vectors

3.720266	0.000000	0.000000
-1.860133	3.221845	0.000000

VCl_2

1.V	0.000000	0.000000	0.000000
2.Cl	-1.572566	0.907922	-1.571698
3.Cl	1.572566	-0.907922	1.571698

Lattice Vectors

3.145133	0.000000	0.000000
-1.572566	2.723765	0.000000

VBr_2

1.V	0.000000	0.000000	0.000000
2.Br	-1.685177	0.972937	-1.648327
3.Br	1.685177	-0.972937	1.648327

Lattice Vectors

3.370353	0.000000	0.000000
-1.685177	2.918811	0.000000

VI_2

1.V	0.000000	0.000000	0.000000
2.I	-1.838362	1.061379	-1.730941
3.I	1.838362	-1.061379	1.730941

Lattice Vectors

3.676723	0.000000	0.000000
-1.838362	3.184136	0.000000

WCl_2

1.W	0.000000	0.000000	0.000000
2.Cl	-1.537813	0.887857	-1.763151
3.Cl	1.537813	-0.887857	1.763151

Lattice Vectors

3.075626	0.000000	0.000000
-1.537813	2.663571	0.000000

WBr_2

1.W	0.000000	0.000000	2.200000
2.Br	1.627184	0.939455	0.359569
3.Br	0.000000	1.878910	4.040431

Lattice Vectors

3.254367	0.000000	0.000000
-1.627184	2.818365	0.000000

WI_2

1.W	0.000000	0.000000	0.000000
2.I	-1.836400	1.060246	-1.825083
3.I	1.836400	-1.060246	1.825083

Lattice Vectors

3.672800	0.000000	0.000000
-1.836400	3.180738	0.000000

$ZrCl_2$

1.Zr	0.000000	0.000000	0.000000
2.Cl	-1.626512	0.939067	-1.823804
3.Cl	1.626512	-0.939067	1.823804

Lattice Vectors

3.253024	0.000000	0.000000
-1.626512	2.817201	0.000000

$ZrBr_2$

1.Zr	0.000000	0.000000	0.000000
2.Br	-1.701446	0.982330	-1.936820
3.Br	1.701446	-0.982330	1.936820

Lattice Vectors

3.402891	0.000000	0.000000
-1.701446	2.946990	0.000000

ZrI_2

1.Zr	0.000000	0.000000	2.200000
2.I	1.830742	1.056980	0.150089
3.I	0.000000	2.113959	4.249911

Lattice Vectors

3.661485	0.000000	0.000000
-1.830742	3.170939	0.000000

1.7. Transition metal halides (MY_3)

$AsCl_3$

1.Cl	4.250441	3.728769	4.366675
2.Cl	5.354429	1.818708	7.299992
3.Cl	4.252262	-0.092405	4.366675
4.Cl	0.942117	1.816605	4.366675
5.Cl	2.046106	-0.093457	7.299992
6.Cl	2.044285	3.727718	7.299992
7.As	0.000000	3.635313	5.837184
8.As	0.000000	0.000000	5.829483

Lattice Vectors

6.296546	0.000000	0.000000
-3.148273	5.452969	0.000000

$CrCl_3$

1.Cl	3.982394	3.510973	4.501929
2.Cl	5.031789	1.693453	7.164737
3.Cl	3.982468	-0.124110	4.501929
4.Cl	0.834357	1.693367	4.501929
5.Cl	1.883752	-0.124153	7.164737
6.Cl	1.883677	3.510930	7.164737
7.Cr	0.000000	3.386821	5.833404
8.Cr	0.000000	0.000000	5.833262

Lattice Vectors

5.866145	0.000000	0.000000
-2.933073	5.080231	0.000000

$CrBr_3$

1.Br	3.955353	3.421254	4.365255
2.Br	4.940570	1.713248	7.301411
3.Br	3.954001	0.006022	4.365255
4.Br	0.997000	1.714809	4.365255
5.Br	1.982216	0.006803	7.301411
6.Br	1.983568	3.422035	7.301411
7.Cr	0.000000	3.428057	5.832772
8.Cr	0.000000	0.000000	5.833895

Lattice Vectors

5.937569	0.000000	0.000000
-2.968785	5.142086	0.000000

CrI_3

1.I	4.409274	3.850990	4.264617
2.I	5.539692	1.897332	7.402049
3.I	4.412984	-0.058469	4.264617
4.I	1.025438	1.893048	4.264617
5.I	2.155857	-0.060610	7.402049
6.I	2.152147	3.848848	7.402049
7.Cr	0.000000	3.790380	5.831194
8.Cr	0.000000	0.000000	5.835473

Lattice Vectors

6.565131	0.000000	0.000000
-3.282565	5.685570	0.000000

$FeCl_3$

1.Cl	3.883190	3.421725	4.540492
2.Cl	4.904896	1.652337	7.126174
3.Cl	3.883414	-0.117180	4.540492
4.Cl	0.818521	1.652079	4.540492
5.Cl	1.840226	-0.117309	7.126174
6.Cl	1.840003	3.421596	7.126174
7.Fe	0.000000	3.304416	5.832697
8.Fe	0.000000	0.000000	5.833969

Lattice Vectors

5.723417	0.000000	0.000000
-2.861708	4.956624	0.000000

$FeBr_3$

1.Br	4.105105	3.613121	4.448535
2.Br	5.181607	1.749796	7.218131
3.Br	4.106172	-0.114144	4.448535
4.Br	0.877732	1.748565	4.448535
5.Br	1.954234	-0.114760	7.218131
6.Br	1.953168	3.612505	7.218131
7.Fe	0.000000	3.498361	5.835343
8.Fe	0.000000	0.000000	5.831324

Lattice Vectors

6.059339	0.000000	0.000000
-3.029670	5.247542	0.000000

$MoCl_3$

1.Cl	3.646172	3.122998	4.316124
2.Cl	4.527682	1.595926	7.350543
3.Cl	3.645953	0.068980	4.316124
4.Cl	1.001206	1.596179	4.316124
5.Cl	1.882715	0.069107	7.350543
6.Cl	1.882934	3.123124	7.350543
7.Mo	0.000000	3.192105	5.834825
8.Mo	0.000000	0.000000	5.831841

Lattice Vectors

5.528887	0.000000	0.000000
-2.764444	4.788157	0.000000

$MoBr_3$

1.Br	3.881856	3.324580	4.232746
2.Br	4.820099	1.697828	7.433921
3.Br	3.880412	0.071910	4.232746
4.Br	1.064238	1.699496	4.232746
5.Br	2.002481	0.072744	7.433921
6.Br	2.003926	3.325414	7.433921
7.Mo	0.000000	3.397324	5.834321
8.Mo	0.000000	0.000000	5.832346

Lattice Vectors

5.884338	0.000000	0.000000
-2.942169	5.095986	0.000000

$SbCl_3$

1.Cl	4.419159	3.848365	4.261722
2.Cl	5.542361	1.901615	7.404945
3.Cl	4.418027	-0.044482	4.261722
4.Cl	1.047289	1.902921	4.261722
5.Cl	2.170491	-0.043829	7.404945
6.Cl	2.171623	3.849018	7.404945
7.Sb	0.000000	3.804536	5.830698
8.Sb	0.000000	0.000000	5.835969

Lattice Vectors

6.589650	0.000000	0.000000
-3.294825	5.706804	0.000000

$ScCl_3$

1.Cl	4.300590	3.788445	4.404725
2.Cl	5.431184	1.829550	7.261942
3.Cl	4.300029	-0.129020	4.404725
4.Cl	0.907686	1.830198	4.404725
5.Cl	2.038280	-0.128696	7.261942
6.Cl	2.038841	3.788768	7.261942
7.Sc	0.000000	3.659748	5.834037
8.Sc	0.000000	0.000000	5.832629

Lattice Vectors

6.338870	0.000000	0.000000
-3.169435	5.489623	0.000000

$ScBr_3$

1.Br	4.367750	3.808786	4.276102
2.Br	5.482381	1.874928	7.390565
3.Br	4.364925	-0.057300	4.276102
4.Br	1.018209	1.878189	4.276102
5.Br	2.132839	-0.055669	7.390565
6.Br	2.135664	3.810417	7.390565
7.Sc	0.000000	3.753117	5.835252
8.Sc	0.000000	0.000000	5.831415

Lattice Vectors

6.500589	0.000000	0.000000
-3.250295	5.629676	0.000000

$TiCl_3$

1.Cl	3.979699	3.468896	4.409707
2.Cl	4.994001	1.711560	7.256960
3.Cl	3.979255	-0.045520	4.409707
4.Cl	0.935903	1.712072	4.409707
5.Cl	1.950206	-0.045264	7.256960
6.Cl	1.950649	3.469152	7.256960
7.Ti	0.000000	3.423632	5.832393
8.Ti	0.000000	0.000000	5.834273

Lattice Vectors

5.929904	0.000000	0.000000
-2.964952	5.135448	0.000000

$TiBr_3$

1.Br	4.253156	3.710569	4.312751
2.Br	5.340025	1.830392	7.353915
3.Br	4.255178	-0.050954	4.312751
4.Br	0.996593	1.828056	4.312751
5.Br	2.083462	-0.052121	7.353915
6.Br	2.081439	3.709402	7.353915
7.Ti	0.000000	3.658448	5.833283
8.Ti	0.000000	0.000000	5.833384

Lattice Vectors

6.336618	0.000000	0.000000
-3.168309	5.487672	0.000000

VCl_3

1.Cl	3.765153	3.261780	4.426612
2.Cl	4.707361	1.630947	7.240055
3.Cl	3.766122	-0.000446	4.426612
4.Cl	0.940467	1.629828	4.426612
5.Cl	1.882675	-0.001005	7.240055
6.Cl	1.881706	3.261221	7.240055
7.V	0.000000	3.260775	5.832974
8.V	0.000000	0.000000	5.833693

Lattice Vectors

5.647828	0.000000	0.000000
-2.823914	4.891162	0.00000

VBr_3

1.Br	4.011011	3.473776	4.333158
2.Br	5.013884	1.737635	7.333509
3.Br	4.011777	0.001050	4.333158
4.Br	1.003926	1.736749	4.333158
5.Br	2.006798	0.000608	7.333509
6.Br	2.006032	3.473333	7.333509
7.V	0.000000	3.474384	5.833447
8.V	0.000000	0.000000	5.833220

Lattice Vectors

6.017809	0.000000	0.000000
-3.008905	5.211576	0.000000

YCl_3

1.Cl	4.620727	4.083922	4.339139
2.Cl	5.847144	1.960476	7.327528
3.Cl	4.621394	-0.163355	4.339139
4.Cl	0.942811	1.959706	4.339139
5.Cl	2.169228	-0.163740	7.327528
6.Cl	2.168561	4.083537	7.327528
7.Y	0.000000	3.920182	5.835577
8.Y	0.000000	0.000000	5.831090

Lattice Vectors

6.789955	0.000000	0.000000
-3.394977	5.880273	0.000000

$ZrCl_3$

1.Cl	3.998311	3.440777	4.307599
2.Cl	4.978956	1.734184	7.359068
3.Cl	3.991326	0.031624	4.307599
4.Cl	1.042405	1.742250	4.307599
5.Cl	2.023050	0.035657	7.359068
6.Cl	2.030035	3.444810	7.359068
7.Zr	0.000000	3.476434	5.839532
8.Zr	0.000000	0.000000	5.827135

Lattice Vectors

6.021361	0.000000	0.000000
-3.010681	5.214652	0.000000

2. Band Gaps (in eV)

2.1. Atomically thin 2D materials[a]

		GGA			metaGGA	Model	
Material	**Unit Cell Formula**	**PBE (scalar)**	**PBE (SO)**	**SO splitting**	**M06-L**	**GLLB-SC (quasiparticle)**	**GLLB-SC (no quasiparticle)**
Graphene	C	Dirac Point	Dirac Point	-	Dirac Point	Dirac Point	Dirac Point
Graphane	CH	3.56	3.55	0.01	4.31	7.00	5.05
Fluorographene	CF	3.29	3.28	0.01	3.25	5.16	3.91
Clorographene	CCl	1.50	1.46	0.04	2.00	2.45	1.85
Silicene	Si	Dirac Point	Dirac Point	-	Dirac Point	Dirac Point	Dirac Point
Silicane	SiH	2.26	2.25	0.01	2.80	3.56	2.47
Fluorosilicene	SiF	0.66	0.65	0.01	-c	1.66	1.15
Germanene	Ge	Dirac Point	Dirac Point	-	Dirac Point	Dirac Point	Dirac Point
Germanane	GeH	1.16	1.08	0.08	1.61	1.84	1.32
Fluorogermanene	GeF	-	0.05	>0.05	0.32	0.39	0.28
Clorogermanene	GeCl	0.30	0.22	0.08	0.72	0.74	0.53
Silicon Carbide	SiC	2.55	2.55	0.00	2.89	3.63	2.55
Boron Nitride	BN	4.69	4.69	0.00	5.34	7.92	5.81

[a] All low spin.

2.2. Atomically thin transition metal chalcogenides

			GGA		metaGGA	Model	
Material	**Spin**	**Δh[a]**	**PBE (scalar)**	**PBE (SO)**	**M06-L**	**GLLB-SC (quasiparticle)**	**GLLB-SC (no quasiparticle)**
α-ZnO	Low Spin	0.00	1.71	1.67	2.08	4.12	2.85
α-ZnS	Low Spin	0.00	2.58	2.57	3.27	4.50	3.12
α-ZnSe	Low Spin	0.00	1.91	1.83	2.52	3.37	2.33
α-ZnTe	Low Spin	0.00	1.44	1.33	1.92	2.58	1.78
α-CdO	Low Spin	0.00	0.82	0.77	1.10	2.49	1.69
α-CdS	Low Spin	0.00	1.72	1.71	2.40	3.23	2.22
α-CdSe	Low Spin	0.00	1.20	1.10	1.70	2.34	1.59
α-CdTe	Low Spin	0.00	0.90	0.80	1.26	1.89	1.28
β-ZnS	Low Spin	0.01	2.57	2.56	3.26	4.48	3.11
β-ZnSe	Low Spin	0.36	2.01	1.90	2.64	3.48	2.41
β-ZnTe	Low Spin	0.52	1.79	1.53	2.29	2.87	1.99
β-CdO	Low Spin	0.02	0.82	0.77	1.10	2.49	1.69
β-CdS	Low Spin	0.06	1.65	1.64	2.32	3.14	2.15
β-CdSe	Low Spin	0.36	1.30	1.20	1.75	2.47	1.68
β-CdTe	Low Spin	0.62	1.42	1.18	1.76	2.41	1.65

[a] Height difference between the two atoms.

2.3. Metalloid chalcogenides

			GGA		metaGGA	Model	
Material	**Spin**	**Unit Cell Formula**	**PBE (scalar)**	**PBE (SO)**	**M06-L**	**GLLB-SC (quasiparticle)**	**GLLB-SC (no quasiparticle)**
GaS	Low Spin	Ga_2S_2	2.57	2.56	2.60	4.12	2.83
GaSe	Low Spin	Ga_2Se_2	2.05	2.02	2.87	3.38	2.39
InS	Low Spin	In_2S_2	2.09	2.09	-	3.58	2.48
InSe	Low Spin	In_2Se_2	1.70	1.66	2.21	2.93	2.02

5

2.4. Transition metal chalcogenides (1T)

		GGA		metaGGA	Model	
Material	**Spin**	**PBE (scalar)**	**PBE (SO)**	**M06-L**	**GLLB-SC (quasiparticle)**	**GLLB-SC (no quasiparticle)**
HfS_2	Low Spin	1.02	0.96	1.47	2.10	1.49
$HfSe_2$	Low Spin	0.06	Metallic	0.30	0.59	0.42
$HfTe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
MoS_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$MoSe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$MoTe_2$	Low Spin	Metallic	0.05	-	Metallic	Metallic
NbS_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$NbSe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$NbTe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
NiS_2	Low Spin	0.49		0.65	0.56	0.39
$NiSe_2$	Low Spin	0.14	Metallic	0.25	0.04	0.03
PdS_2	Low Spin	1.17	1.15	1.39	1.73	1.20
$PdSe_2$	Low Spin	0.67	0.51	-	0.97	0.67
$PdTe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
PtS_2	Low Spin	1.83	1.78	2.19	2.85	1.99
$PtSe_2$	Low Spin	0.62	1.12	1.56	1.82	1.27
$PtTe_2$	Low Spin	1.10	0.24	0.68	0.75	0.52
ReS_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$ReTe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
TaS_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$TaSe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$TaTe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
TiS_2	Low Spin	Metallic	Metallic	-	0.34	0.25
$TiSe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$TiTe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
WS_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
WSe_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
WTe_2	Low Spin	Metallic	0.04	-	Metallic	Metallic
ZrS_2	Low Spin	1.10	1.06	-	2.30	1.64
$ZrSe_2$	Low Spin	0.36	0.20	-	1.10	0.78
$ZrTe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic

5

2.5. Transition metal chalcogenides (2H)

		GGA		metaGGA	Model	
Material	**Spin**	**PBE (scalar)**	**PBE (SO)**	**M06-L**	**GLLB-SC (quasiparticle)**	**GLLB-SC (no quasiparticle)**
HfS_2	Low Spin	1.02	1.01	1.09	2.25	1.51
$HfSe_2$	Low Spin	0.73	0.61	0.68	1.54	1.02
$HfTe_2$	Low Spin	0.38	0.17	0.20	0.83	0.54
MoS_2	Low Spin	1.82	1.74	1.78	2.51	1.84
$MoSe_2$	Low Spin	1.56	1.45	1.56	2.17	1.58
$MoTe_2$	Low Spin	1.15	1.01	1.16	1.66	1.16
NbS_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$NbSe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$NbTe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
NiS_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$NiSe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$NiTe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
PdS_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$PdSe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$PdTe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
PtS_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$PtSe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$PtTe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
ReS_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$ReSe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$ReTe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
TaS_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$TaSe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$TaTe_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
TiS_2	Low Spin	0.69	0.68	0.54	1.57	1.09
$TiSe_2$	Low Spin	0.48	0.40	0.42	1.11	0.76
$TiTe_2$	Low Spin	0.05	Metallic	-	0.36	0.24
WS_2	Low Spin	1.98	1.64	2.01	2.66	1.97
WSe_2	Low Spin	1.63	1.33	1.68	2.21	1.61
WTe_2	Low Spin	1.18	0.87	1.21	1.63	1.15
ZrS_2	Low Spin	0.92	0.90	-	2.03	1.38
$ZrSe_2$	Low Spin	0.73	0.67	0.70	1.64	1.10
$ZrTe_2$	Low Spin	0.07	Metallic	-	0.25	0.17

5

2.6. Transition metal halides (MY_2). Most stable in bold.

		GGA		metaGGA	Model	
Material	**Spin**	**PBE (scalar)**	**PBE (SO)**	**M06-L**	**GLLB-SC (quasiparticle)**	**GLLB-SC (no quasiparticle)**
$CoCl_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
	High Spin	0.08	-	-	-	-
$CoBr_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
	High Spin	Metallic	-	-	-	-
$FeCl_2$	Low Spin	0.893	0.892	1.635	2.617	1.888
	High Spin	Metallic	Metallic	-	Metallic	Metallic
$FeBr_2$	Low Spin	0.785	0.778	1.690	2.412	1.716
	High Spin	Metallic	Metallic	-	Metallic	Metallic
FeI_2	Low Spin	0.438	0.409	1.163	0.466	0.319
	High Spin	Metallic	Metallic	-	Metallic	Metallic
$HfCl_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$HfBr_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
HfI_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$MnCl_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
	High Spin	0.37	-	-	-	-
$MnBr_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
	High Spin	0.18		-	-	-
MnI_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
	High Spin	Metallic	-	-	-	-
$MoCl_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$MoBr_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
MoI_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$NbCl_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$NbBr_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
NbI_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$NiCl_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
	High Spin	1.06	-	-	-	-
$NiBr_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
	High Spin	0.64	-	-	-	-
$TaCl_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$TaBr_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
TaI_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$TiCl_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$TiBr_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
TiI_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
VCl_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
	High Spin	Metallic	-	-	-	-
VBr_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
	High Spin	Metallic	-	-	-	-
VI_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
	High Spin	Metallic	-	-	-	-
WCl_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
WBr_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
WI_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$ZrCl_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$ZrBr_2$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
ZrI_2	Low Spin	Metallic	Metallic	-	Metallic	Metallic

5

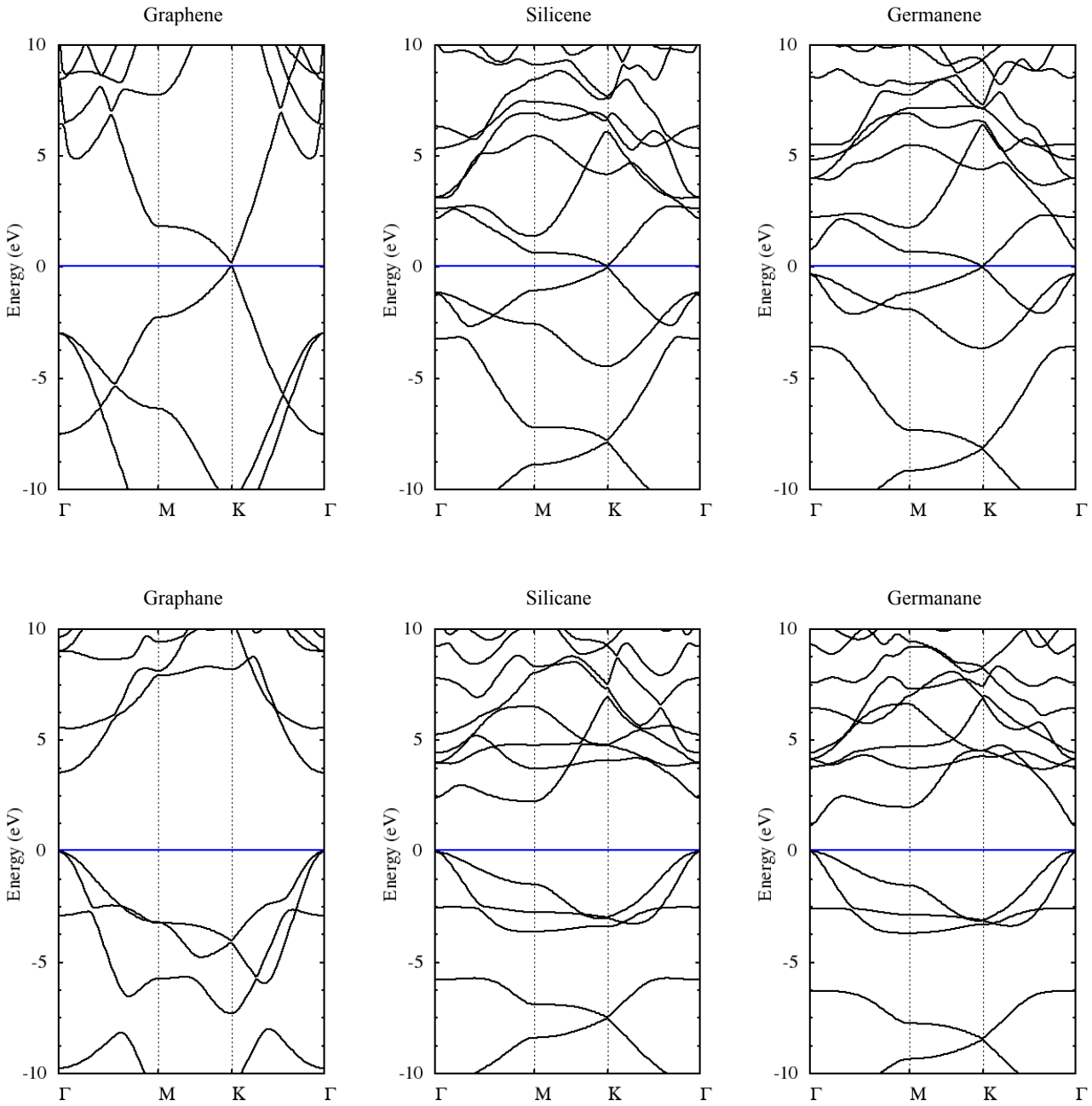
2.7. Transition metal halides (MY_3). Most stable in bold.

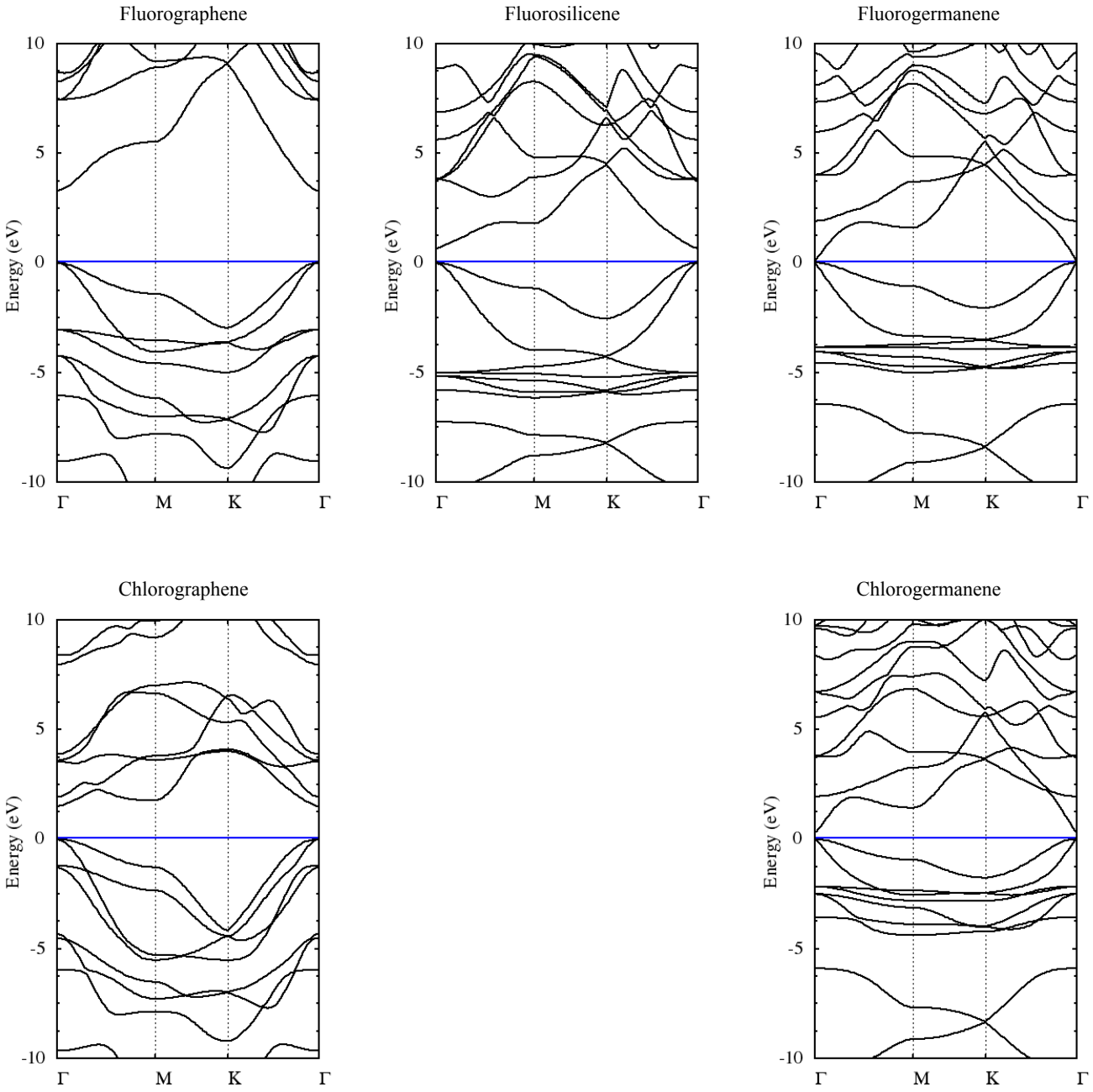
		GGA		metaGGA	Model	
Material	**Spin**	**PBE (scalar)**	**PBE (SO)**	**M06-L**	**GLLB-SC (quasiparticle)**	**GLLB-SC (no quasiparticle)**
$AsCl_3$	Low Spin	3.02	2.98	3.54	4.76	3.40
$CrCl_3$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
	High Spin	1.93	-	-	-	-
$CrBr_3$	Low Spin	Metallic	Metallic	-	0.10	0.06
	High Spin	1.49	-	-	-	-
CrI_3	Low Spin	Metallic	Metallic	-	0.13	0.08
	High Spin	1.14	-	-	-	-
$FeCl_3$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$FeBr_3$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
$MoCl_3$	Low Spin	0.80	0.71	-	1.20	0.82
$MoBr_3$	Low Spin	0.56	0.49	0.57	0.87	0.59
$SbCl_3$	Low Spin	2.90	2.76	3.42	4.68	3.36
$ScCl_3$	Low Spin	3.78	3.73	3.05	6.56	4.99
$ScBr_3$	Low Spin	2.75	-	4.20	4.89	3.68
$TiCl_3$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
	High Spin	Metallic	-	-	-	-
$TiBr_3$	Low Spin	Metallic	Metallic	-	Metallic	Metallic
	High Spin	Metallic	-	-	-	-
VCl_3	Low Spin	Metallic	Metallic	-	Metallic	Metallic
	High Spin	Metallic	-	-	-	-
VBr_3	Low Spin	Metallic	Metallic	-	Metallic	Metallic
	High Spin	Metallic	-	-	-	-
YCl_3	Low Spin	4.92	4.91	5.50	8.52	6.21
$ZrCl_3$	Low Spin	Metallic	Metallic	-	Metallic	Metallic

5

3. Band Structures

3.1. Atomically thin 2D materials

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Fluorosilicene
Fluorogermanene
Chlorographene
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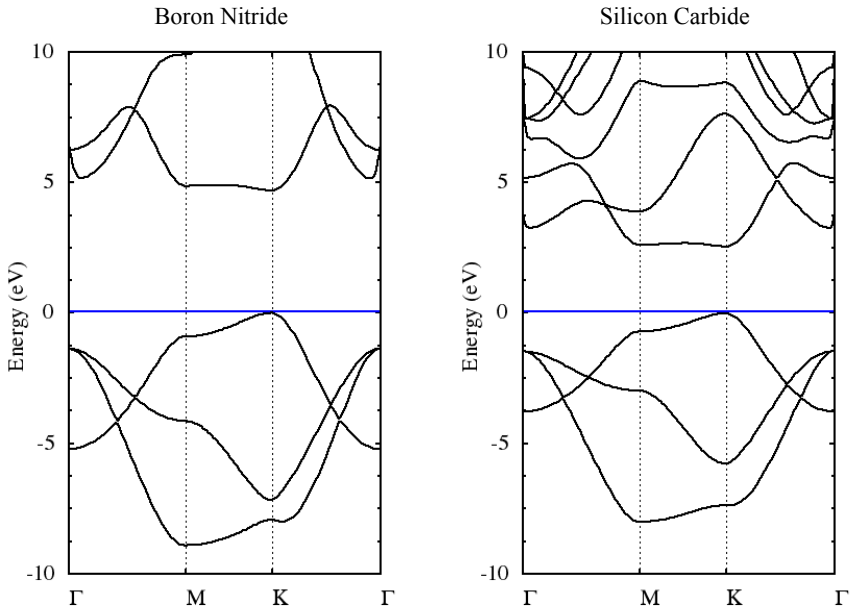
K
Γ

5

10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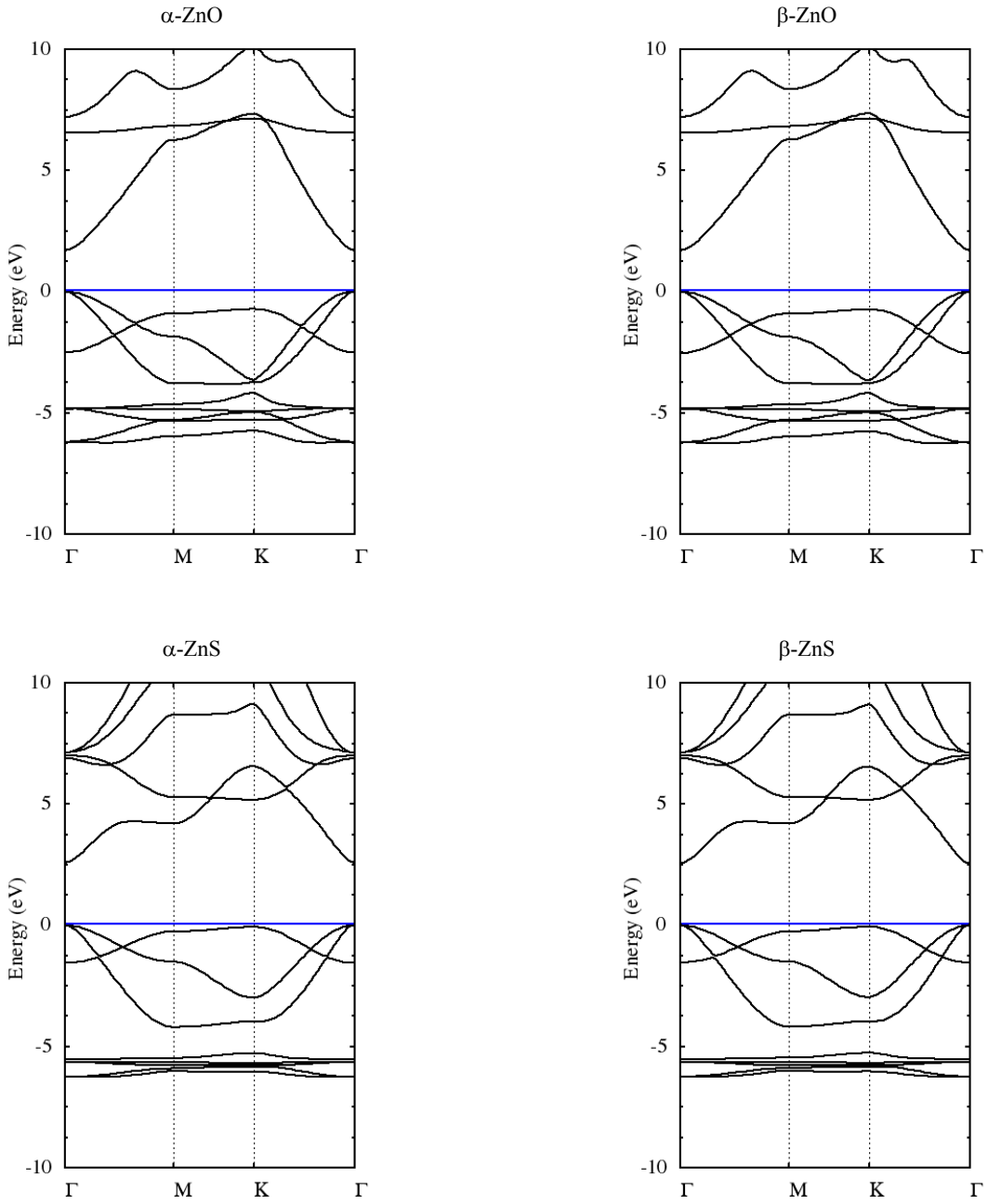
3.2. Atomically thin transition metal chalcogenides



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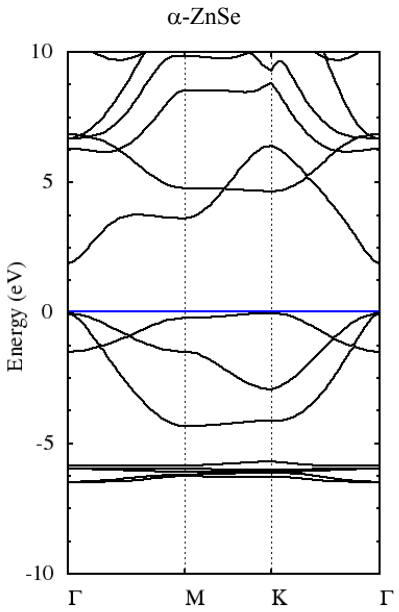
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Energy (eV)
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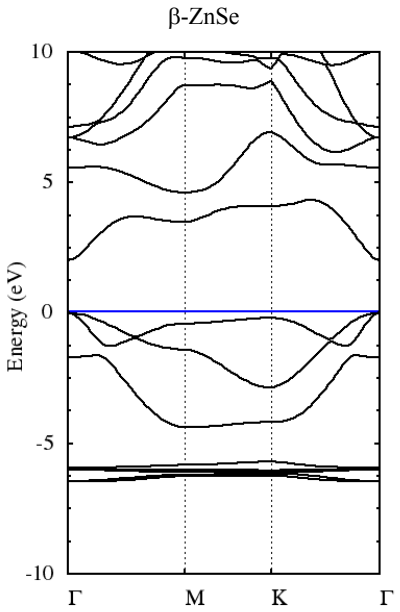
-10
Γ
M
K
Γ


β-ZnSe
Energy (eV)
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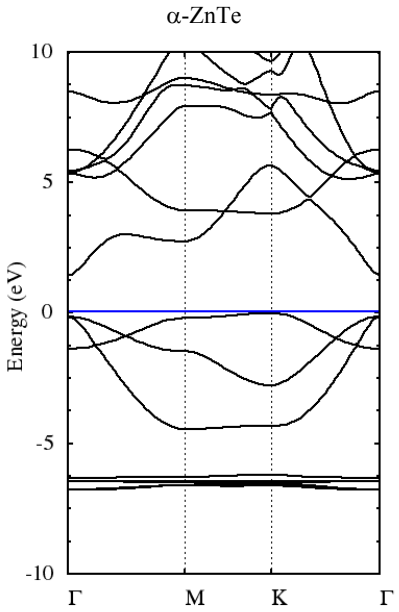
5
0
-5
-10
Γ
M
K
Γ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Energy (eV)
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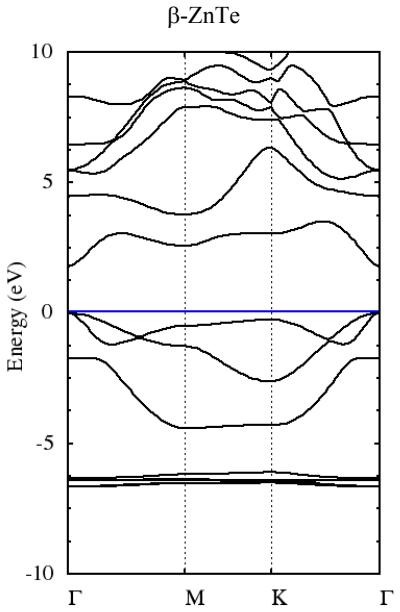
Γ
M
K
Γ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Energy (eV)
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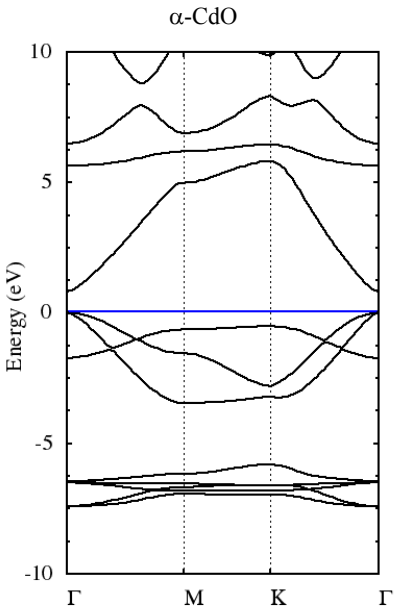
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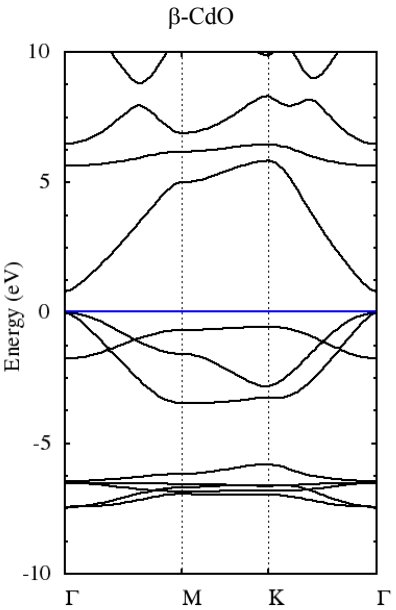
M
K
Γ


β-CdO
Energy (eV)
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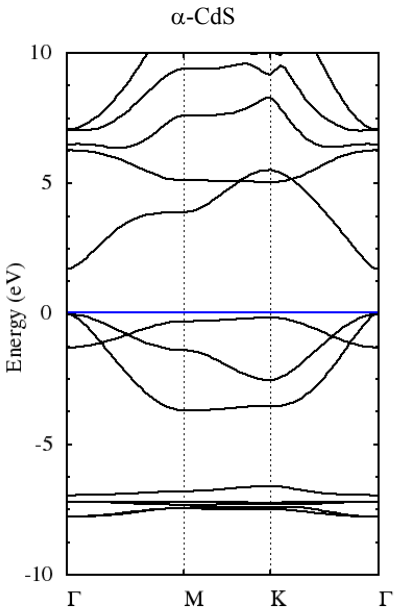
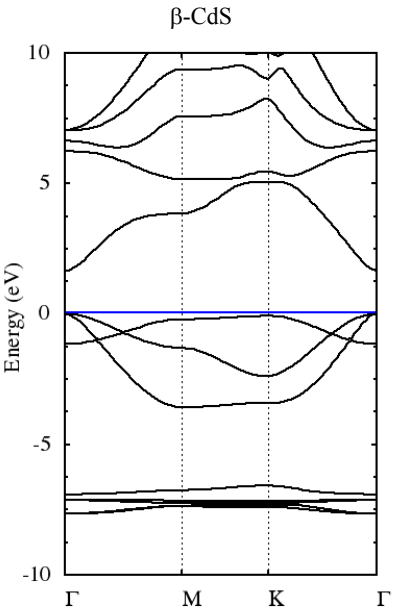
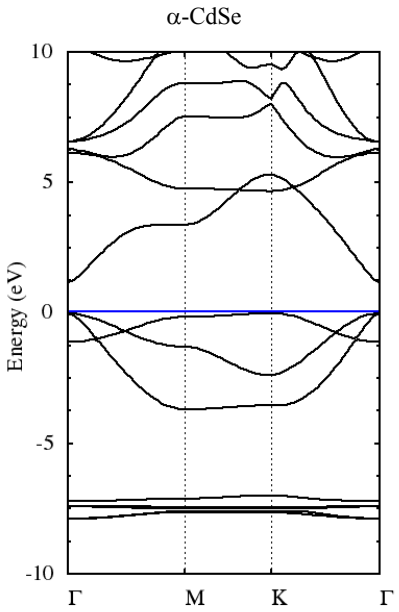
Γ
M
K
Γ

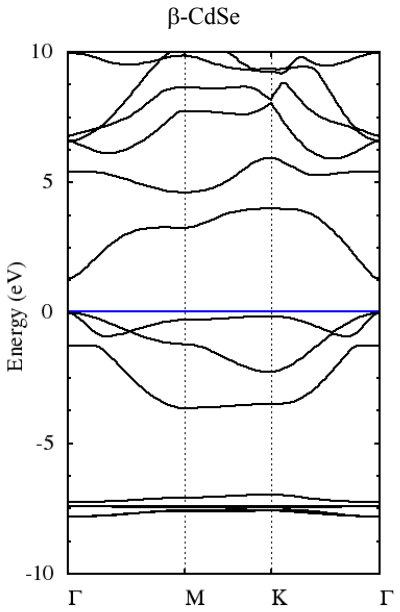

α-CdS
Energy (eV)
10
5
0
-5
-10
Γ
M
K
Γ

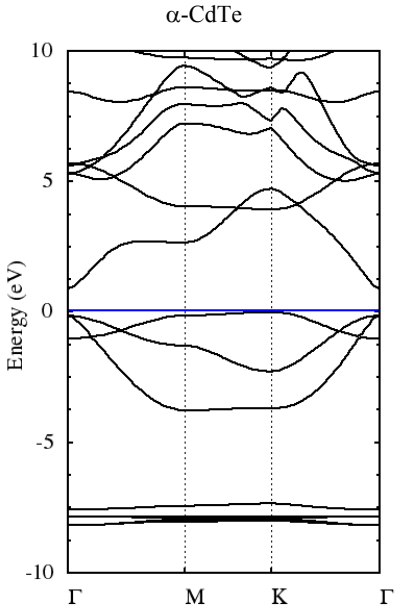

β-CdS
Energy (eV)
10
5
0
-5
-10
Γ
M
K
Γ

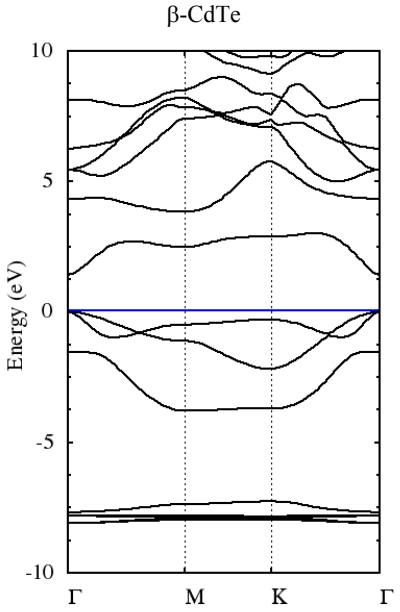
5

10

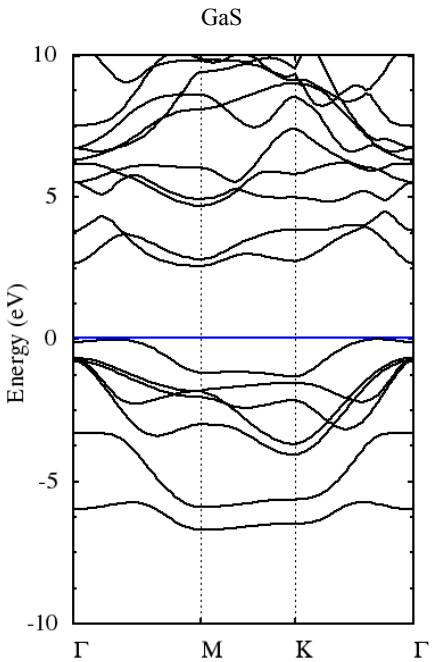

α-CdSe
10
5
0
-5
-10
Energy (eV)
Γ
M
K
Γ

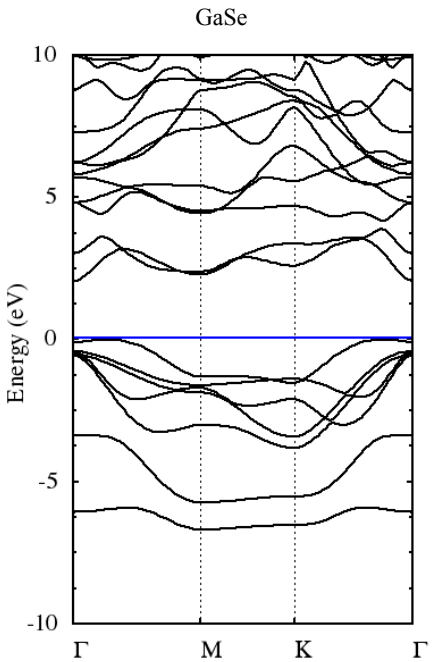

β-CdSe
10
5
0
-5
-10
Energy (eV)
Γ
M
K
Γ

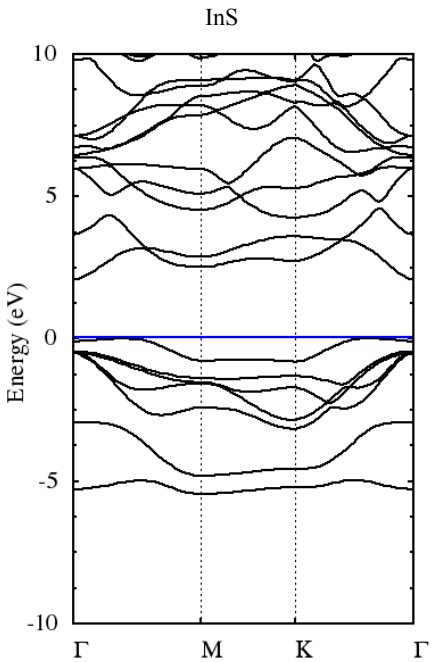

α-CdTe
10
5
0
-5
-10
Energy (eV)
Γ
M
K
Γ

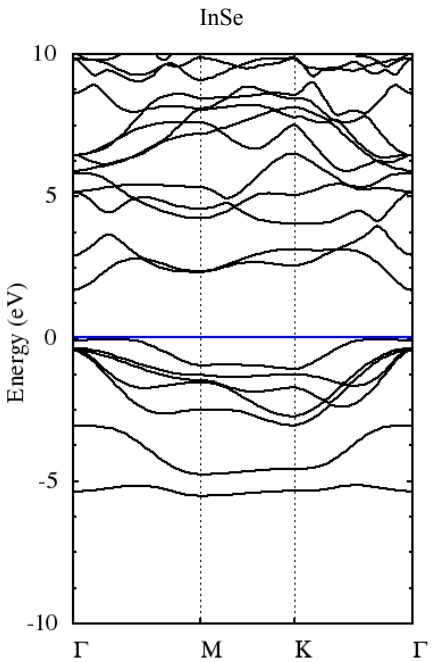

β-CdTe
10
5
0
-5
-10
Energy (eV)
Γ
M
K
Γ

3.3. Metalloid chalcogenides

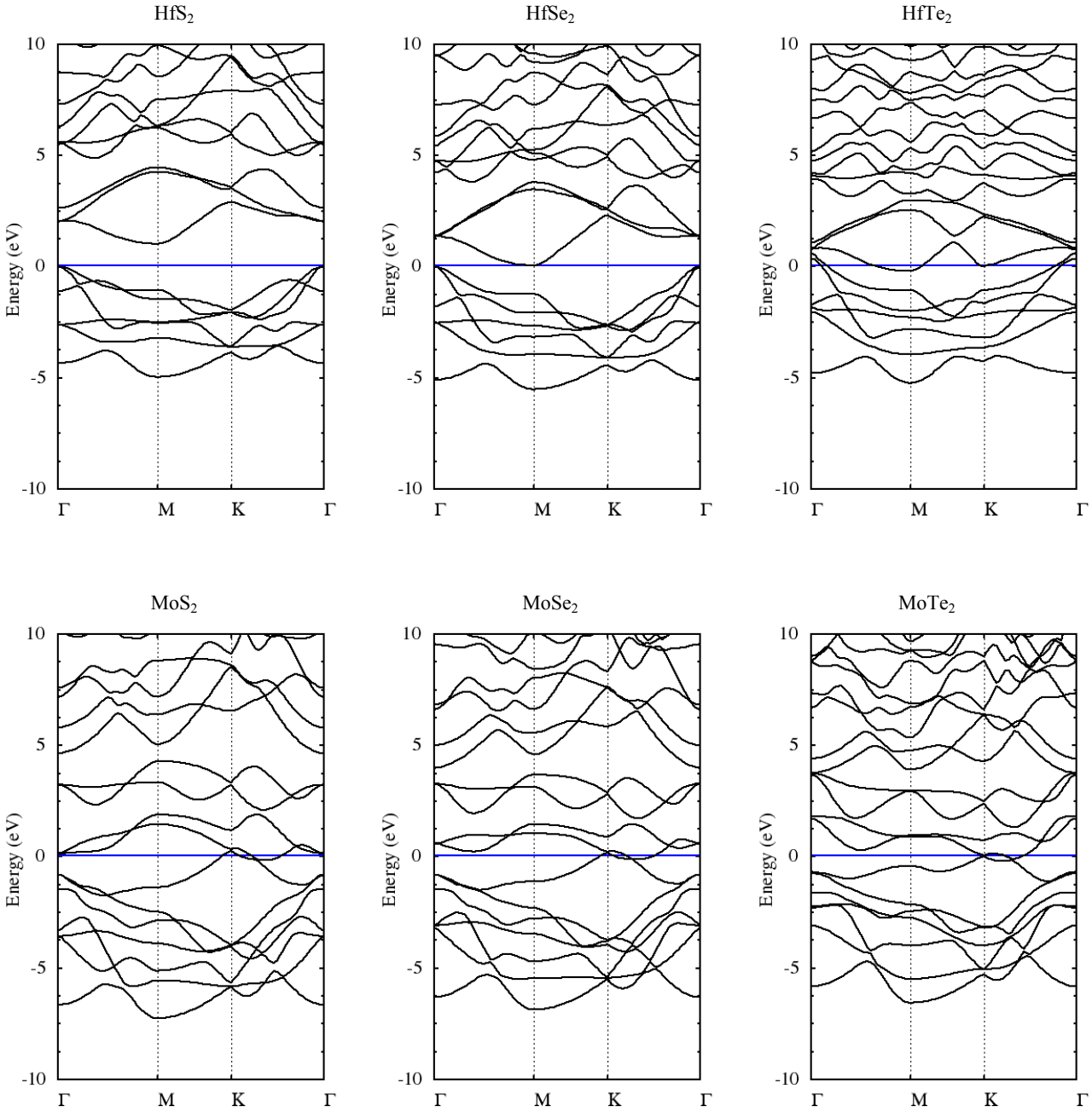


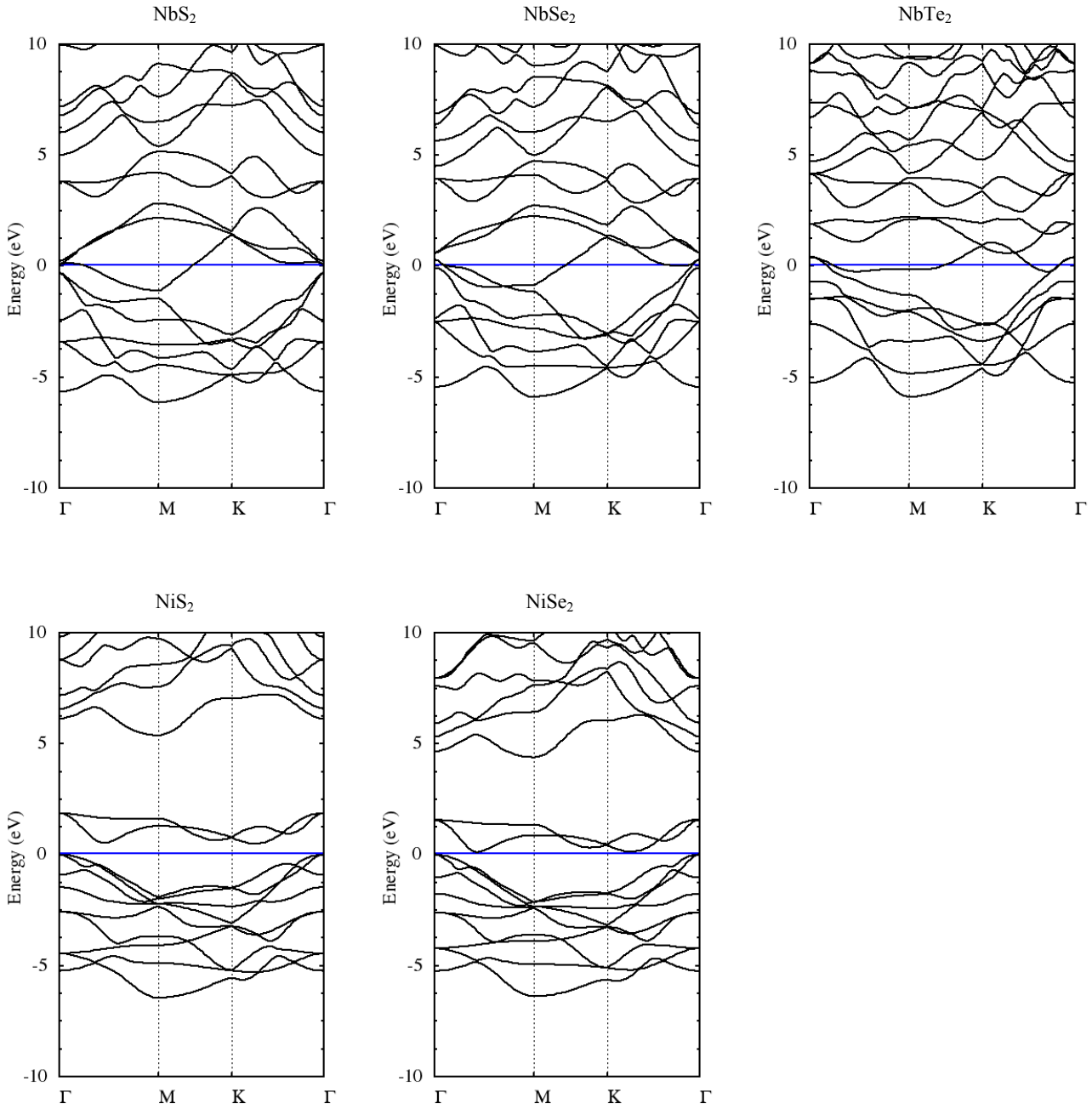


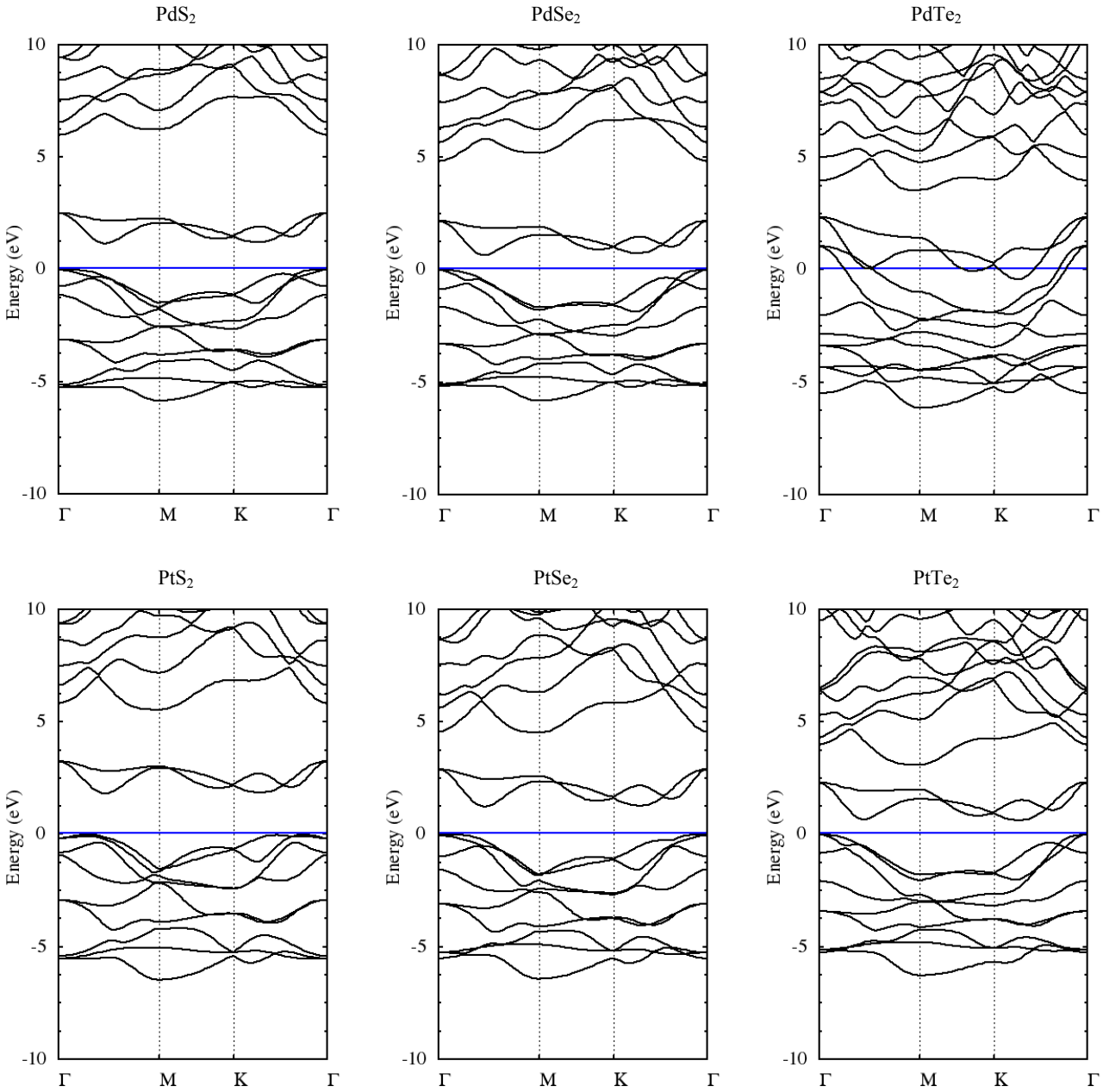


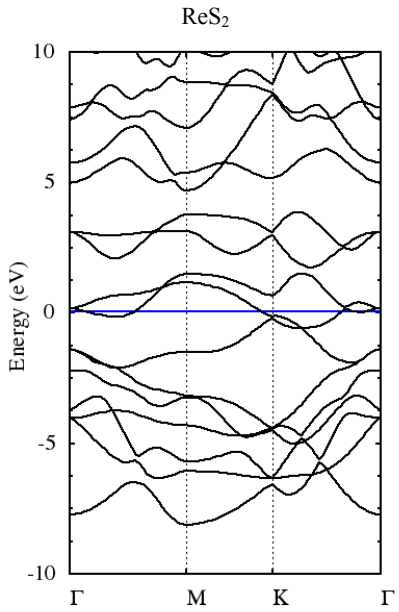


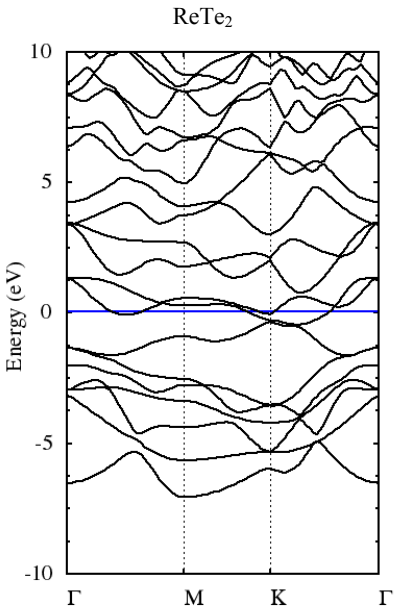
3.4. Transition metal chalcogenides (1T)

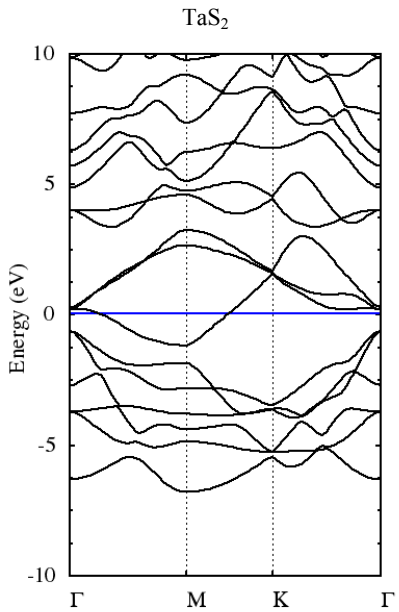


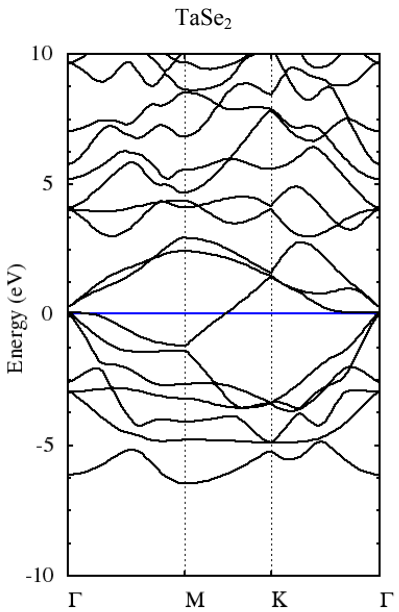

NbS2
NbSe2
NbTe2
NiS2
NiSe2
Energy (eV)
10
5
0
-5
-10
Γ
M
K
Γ

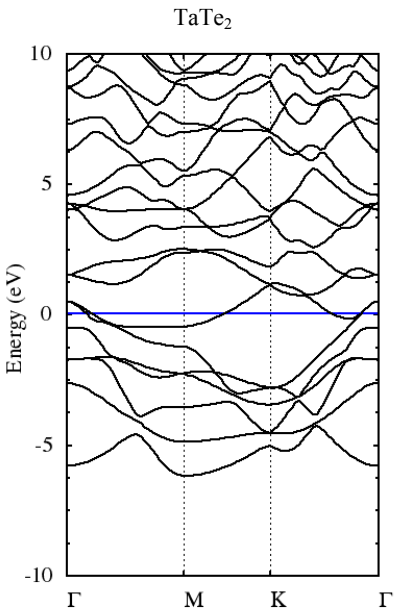

PdS2
PdSe2
PdTe2
PtS2
PtSe2
PtTe2
Energy (eV)
10
5
0
-5
-10
Γ
M
K
Γ

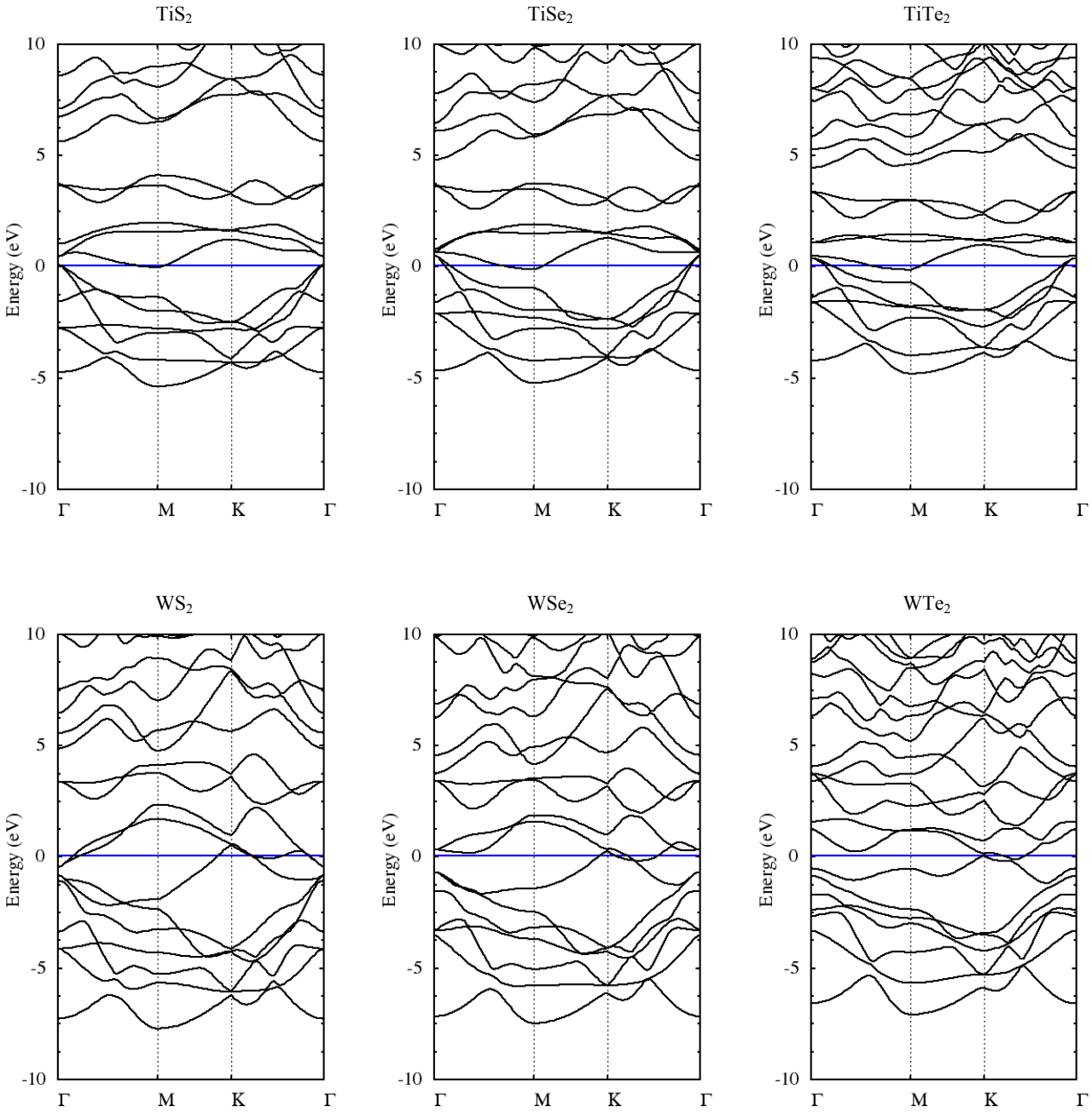

ReS2
10
5
0
-5
-10
Energy (eV)
Γ
M
K
Γ


ReTe2
10
5
0
-5
-10
Energy (eV)
Γ
M
K
Γ


TaS2
10
5
0
-5
-10
Energy (eV)
Γ
M
K
Γ

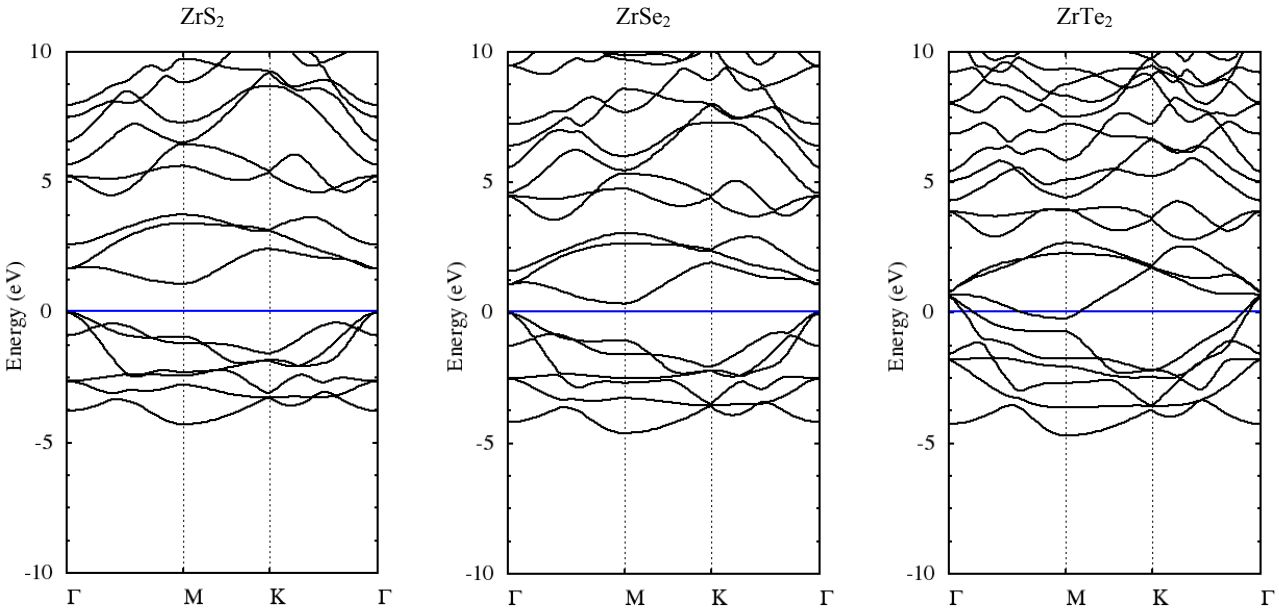

TaSe2
10
5
0
-5
-10
Energy (eV)
Γ
M
K
Γ


TaTe2
10
5
0
-5
-10
Energy (eV)
Γ
M
K
Γ

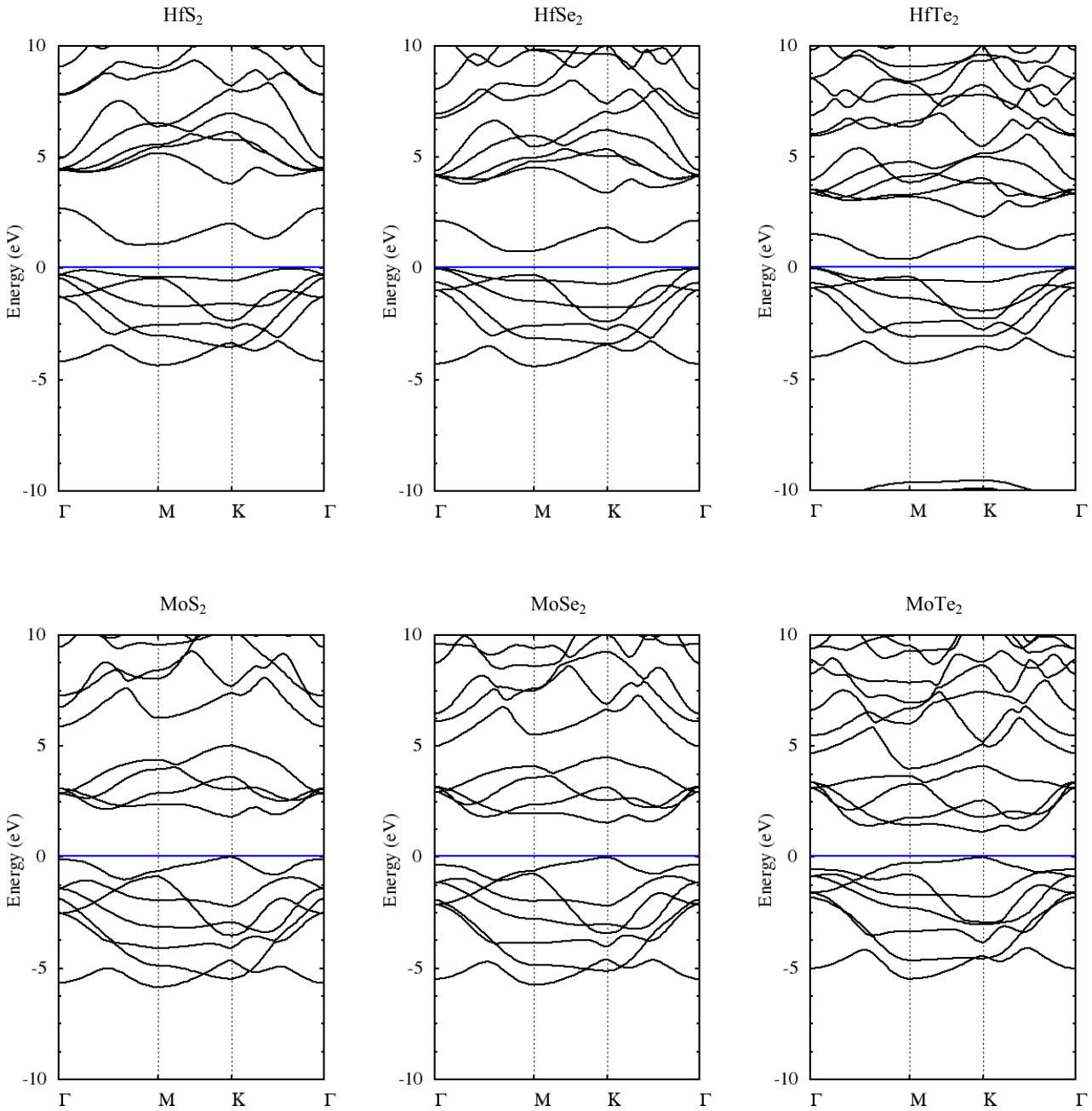


5

10


ZrS2
ZrSe2
ZrTe2
Energy (eV)
10
5
0
-5
-10
Γ
M
K
Γ

3.5. Transition metal chalcogenides (2H)



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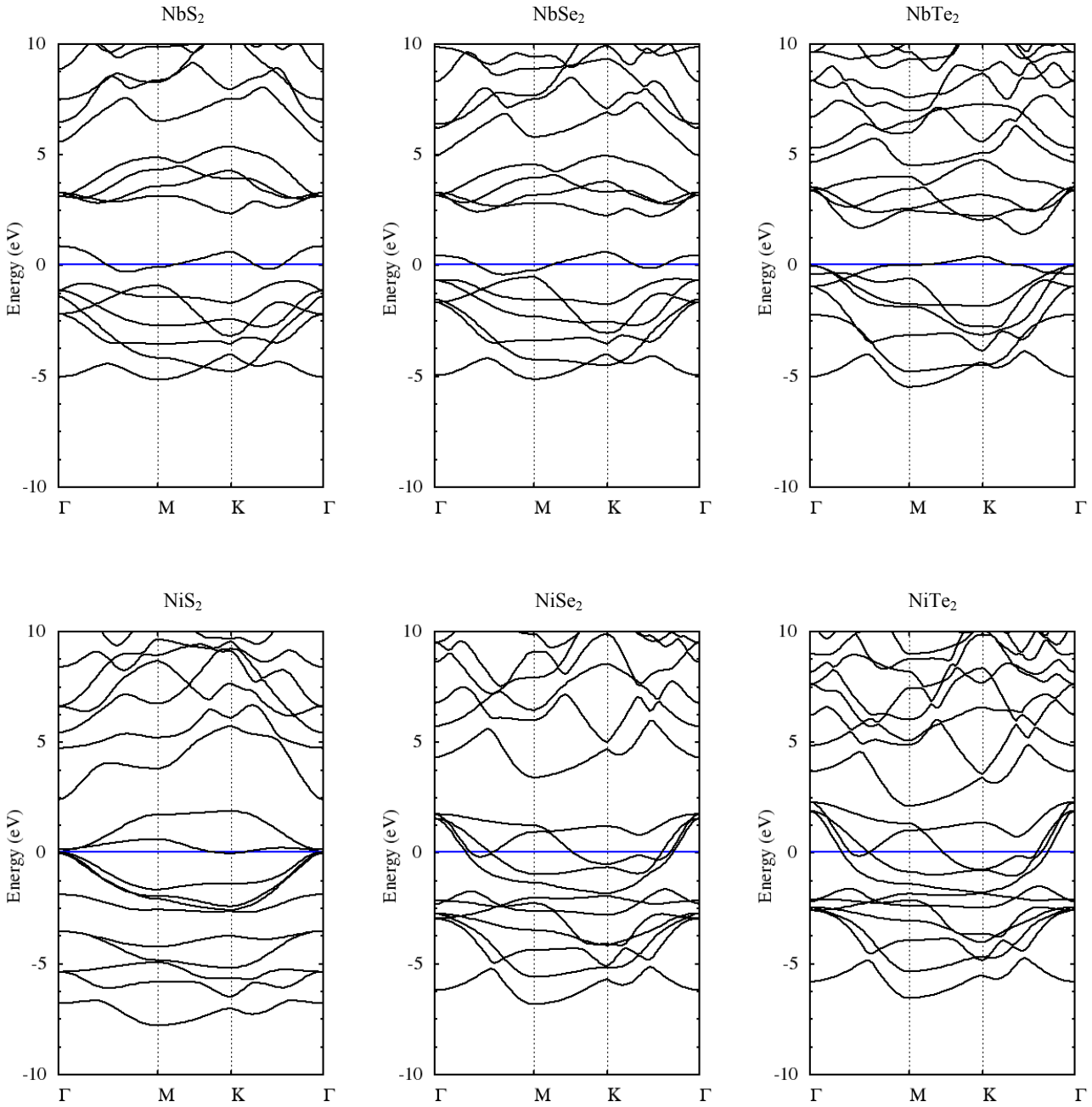
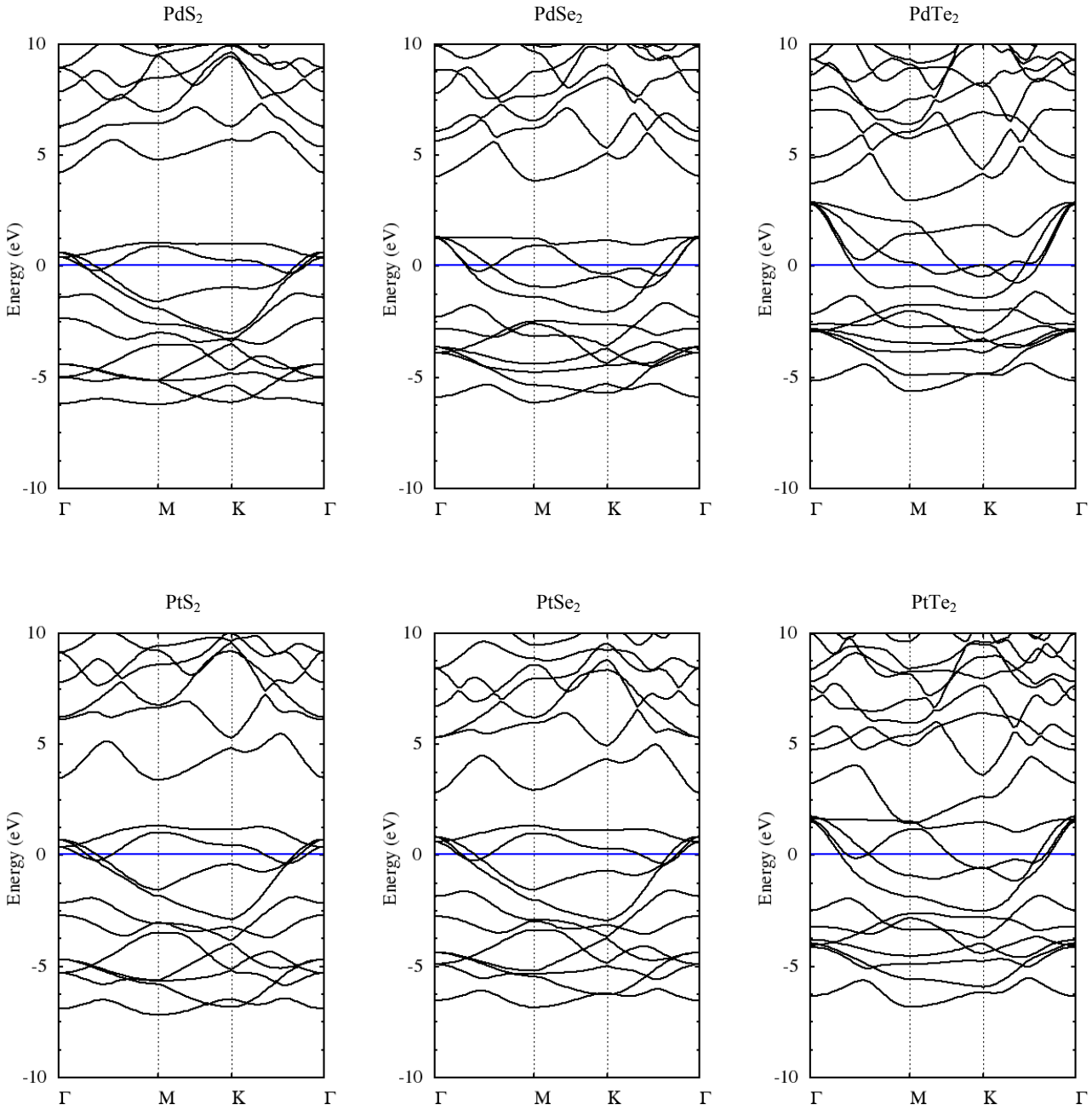


5

10



5

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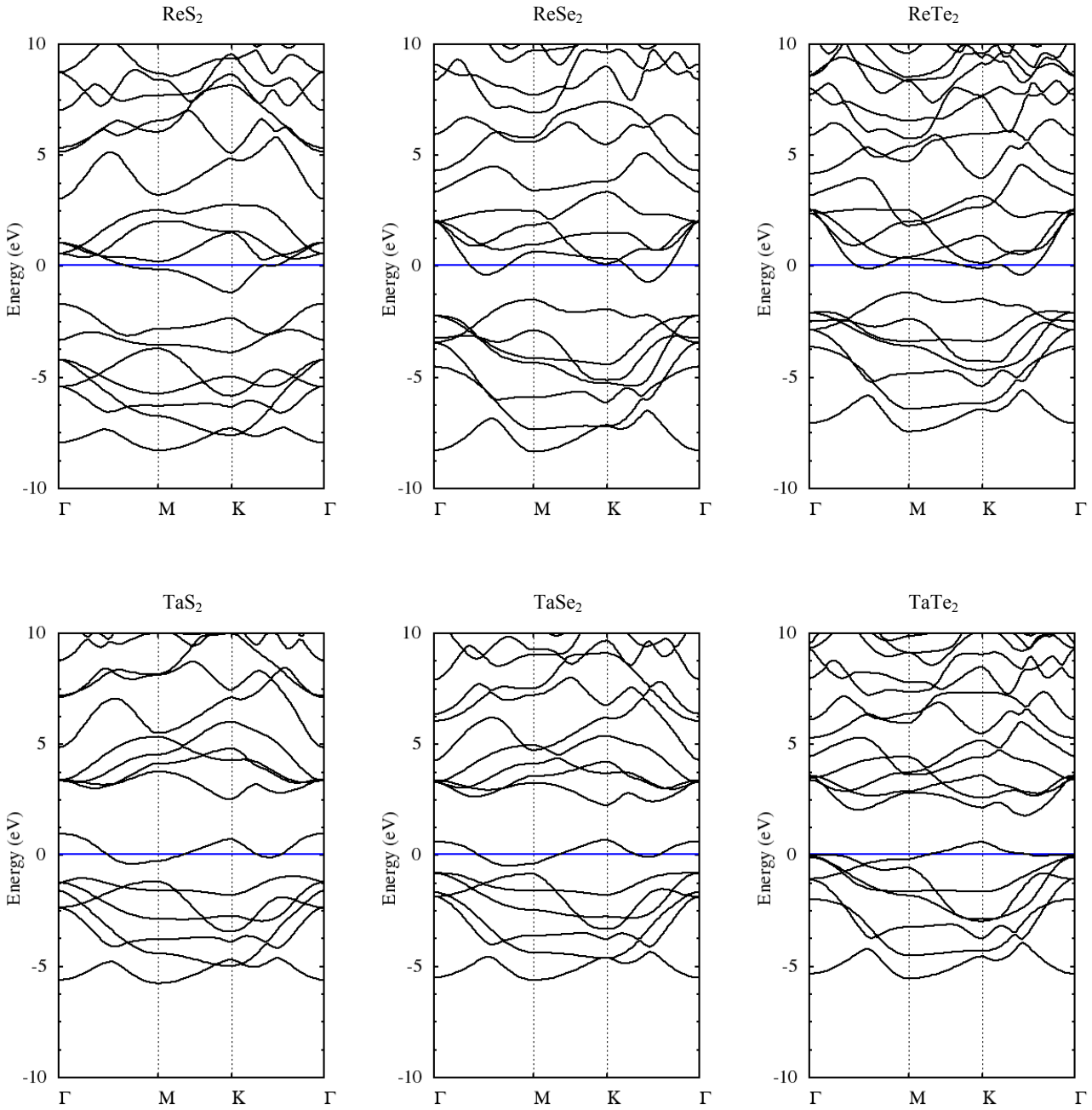

5

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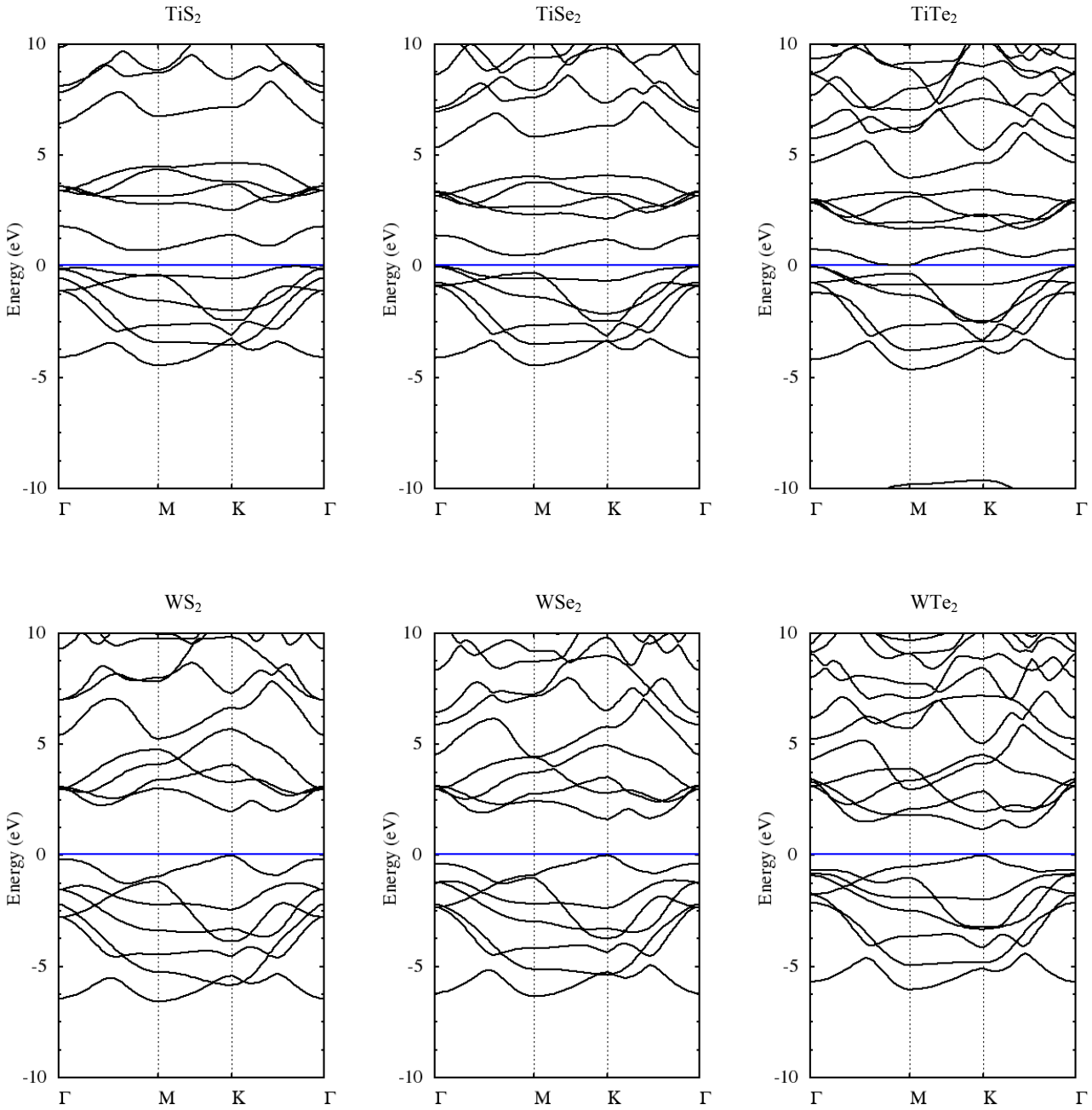

5

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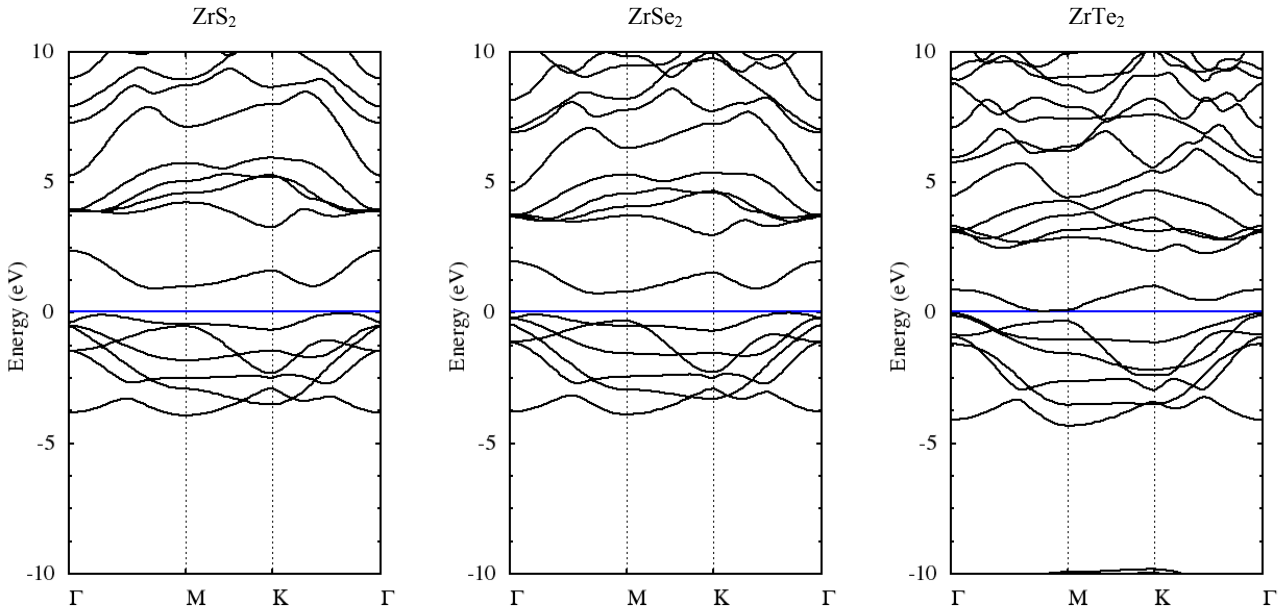
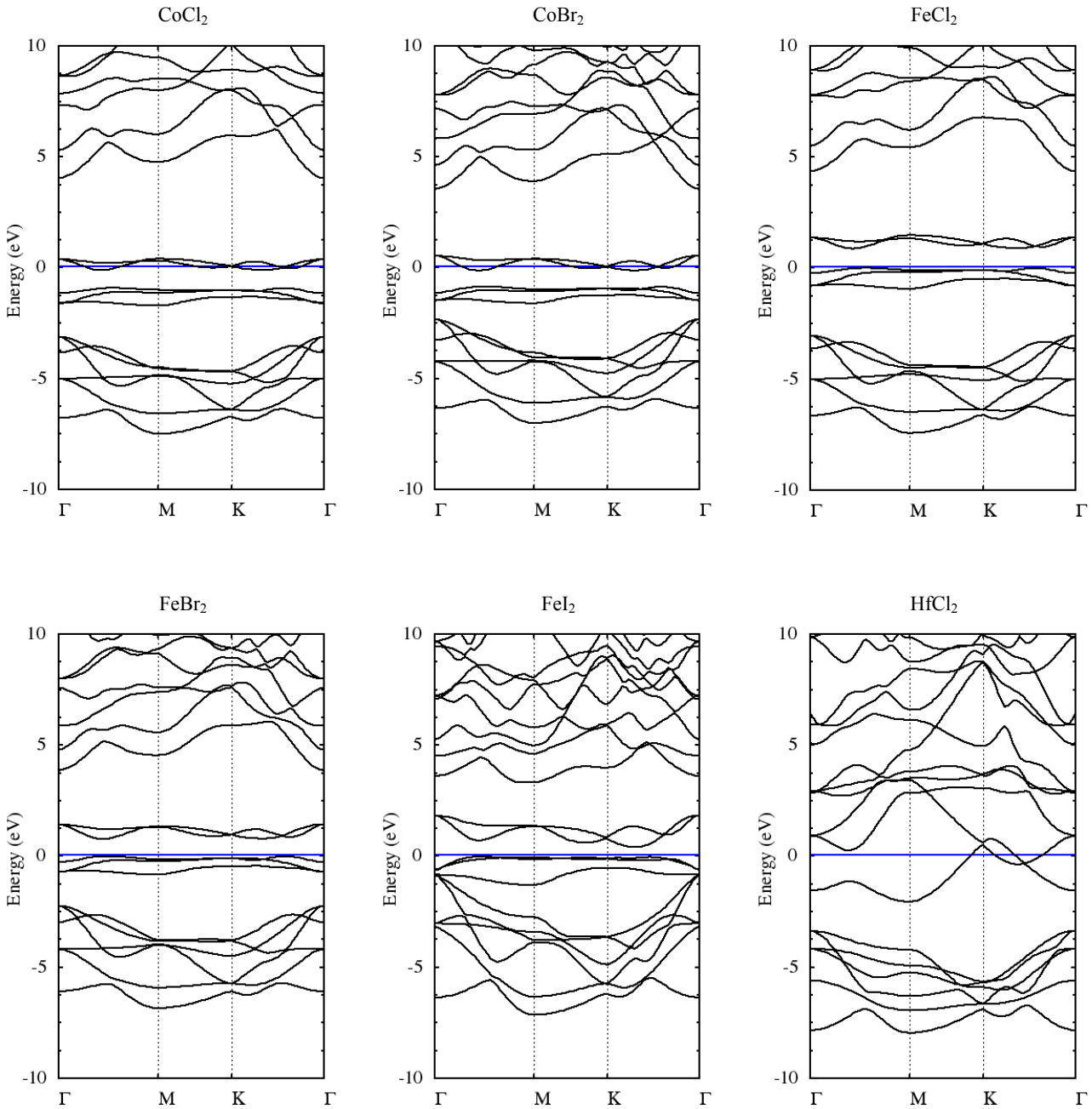
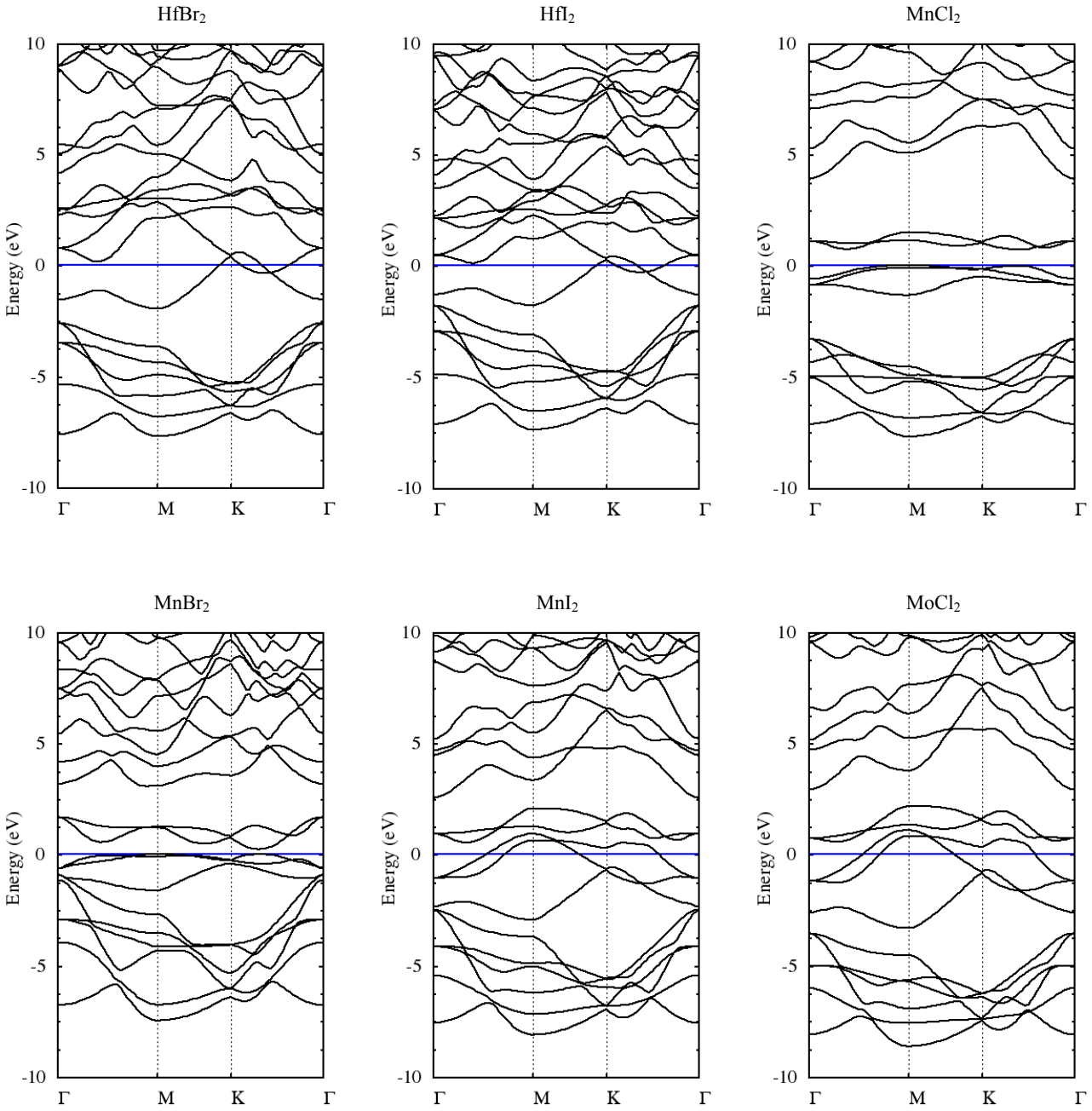


5

3.6. Transition metal halides (MY_2)

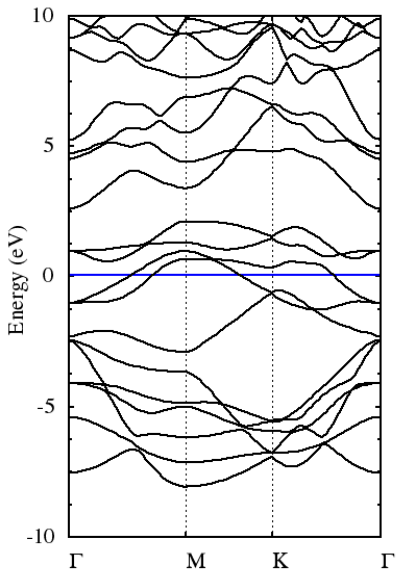




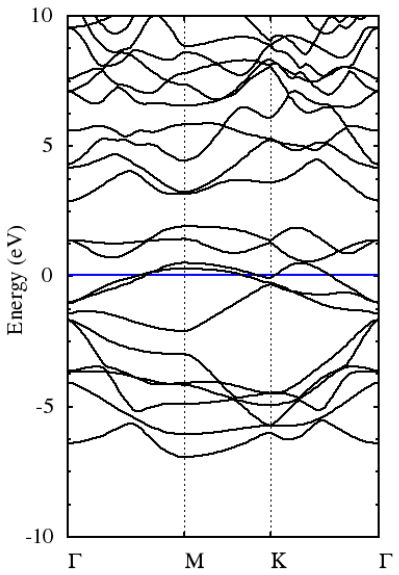
5

10

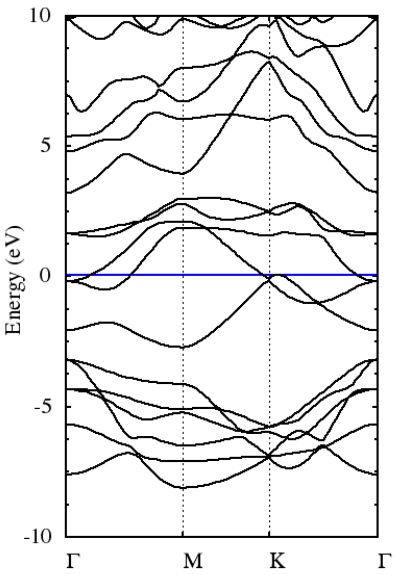
MoBr2 MoI2 NbCl2



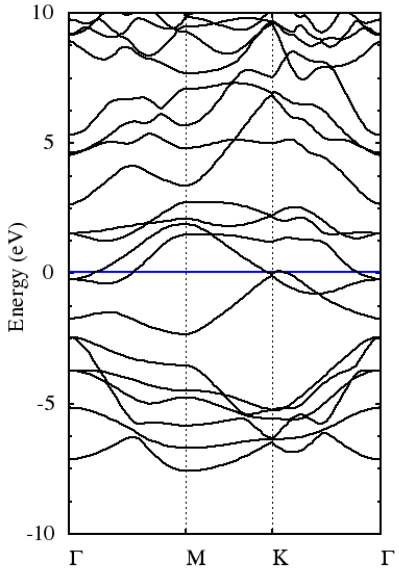
$NbBr_2$



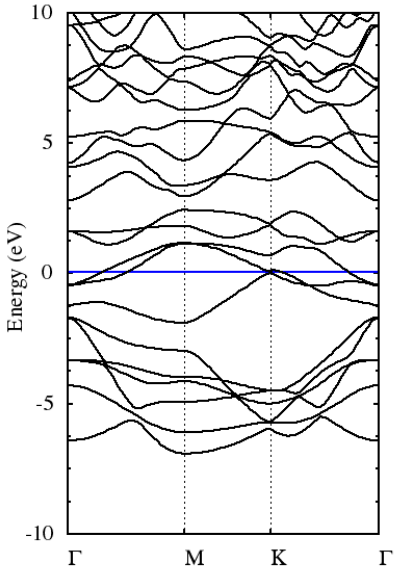
NbI_2



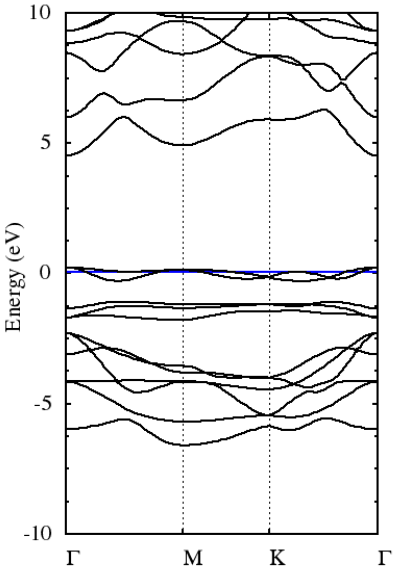
$NiCl_2$



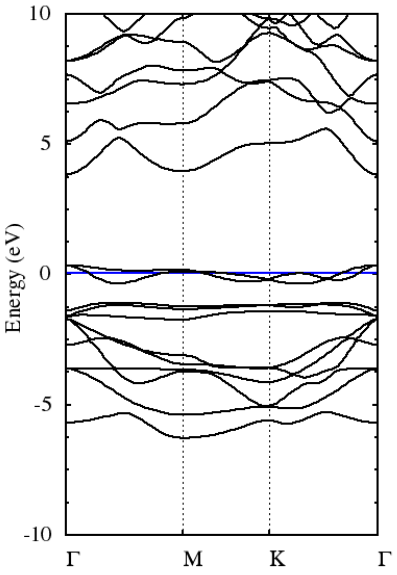
$NiBr_2$



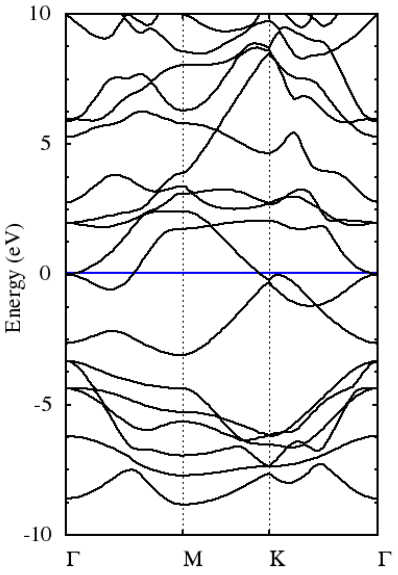
$TaCl_2$



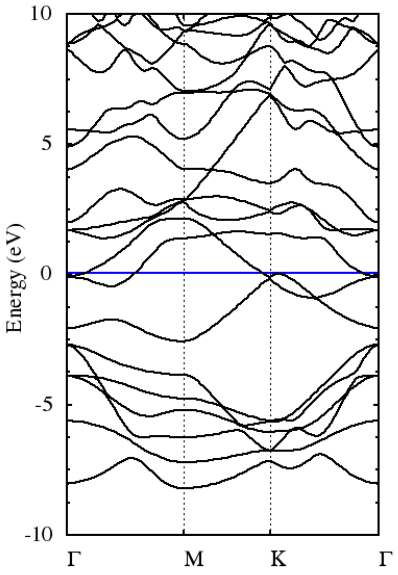
$TaBr_2$



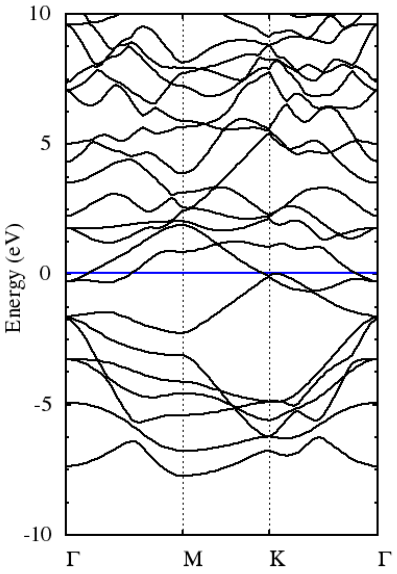
TaI_2



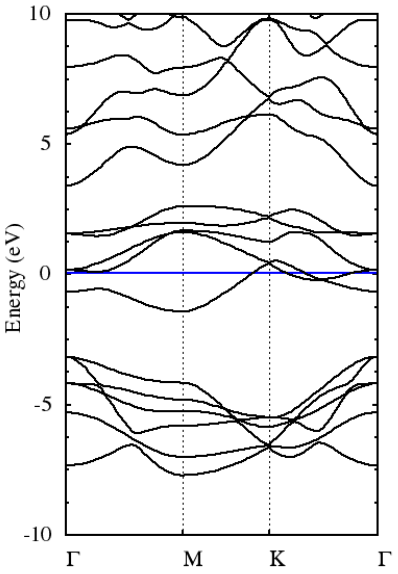
$TiCl_2$



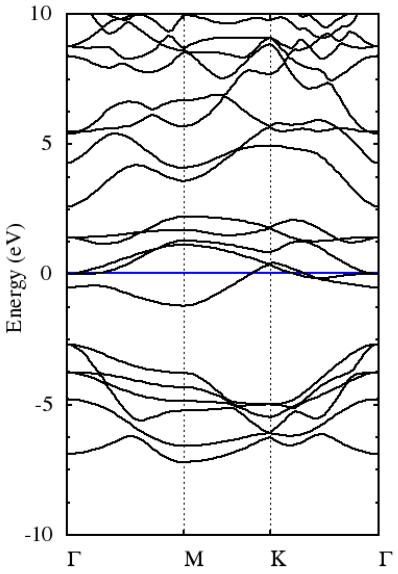
$TiBr_2$



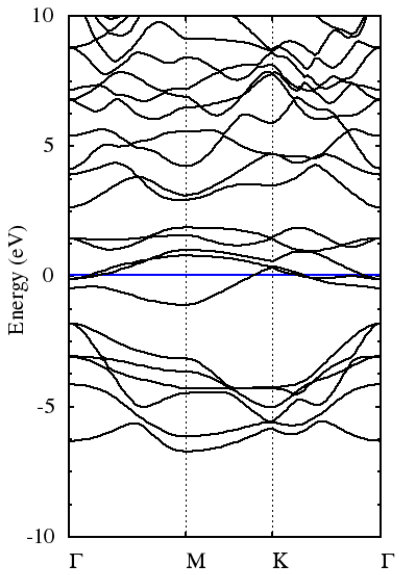
TiI_2



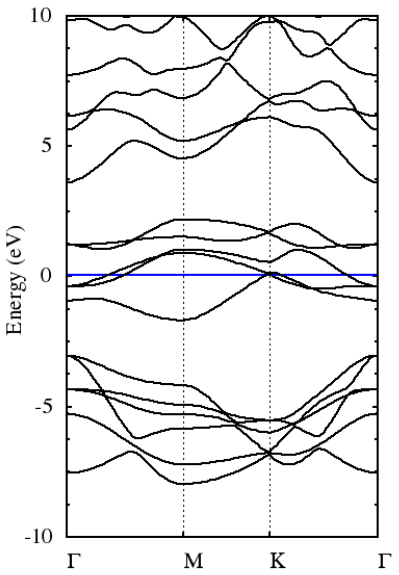
VCl_2



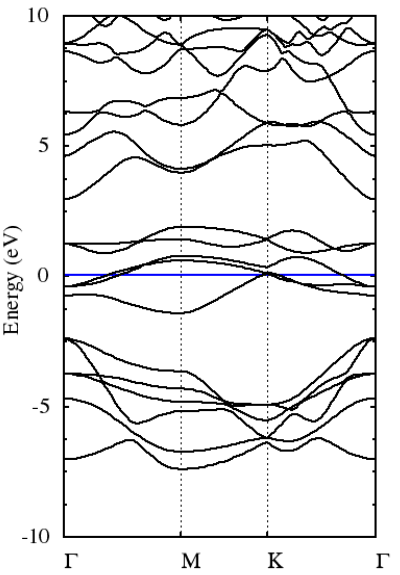
VBr_2



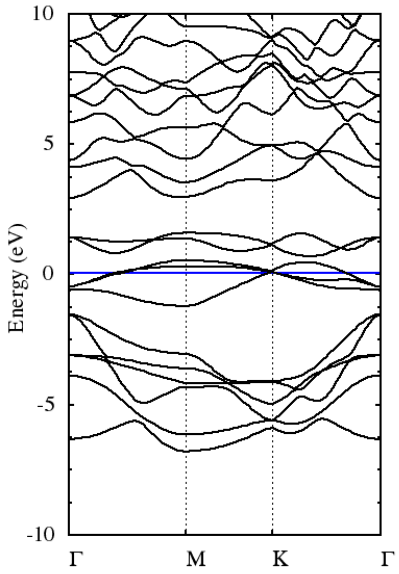
VI_2



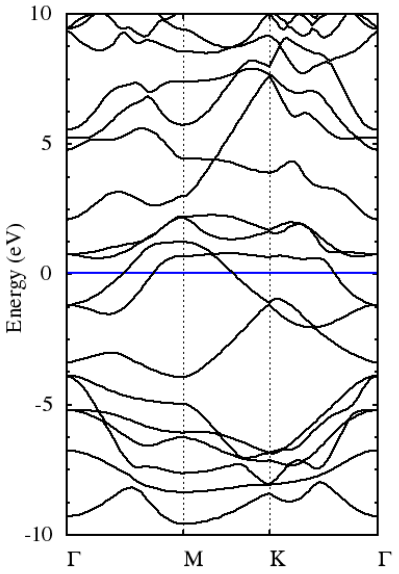
WCl_2



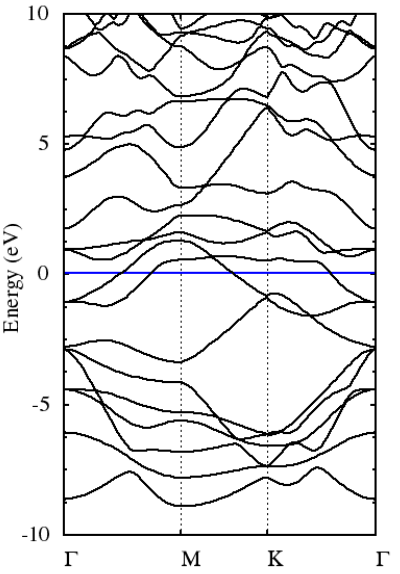
WBr_2



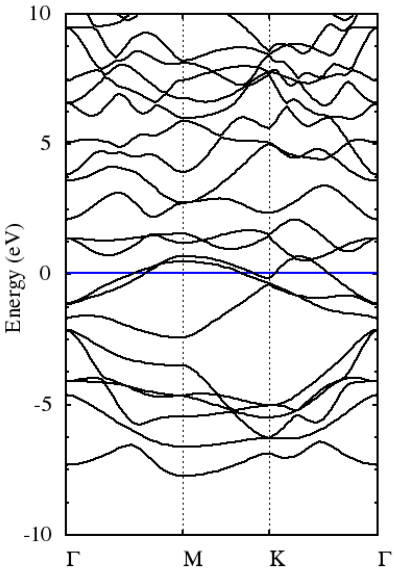
WI_2



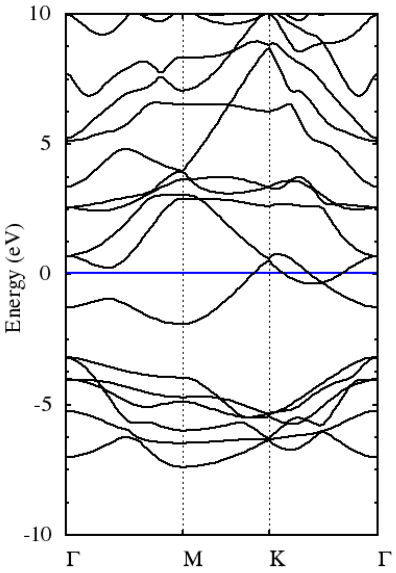
$ZrCl_2$



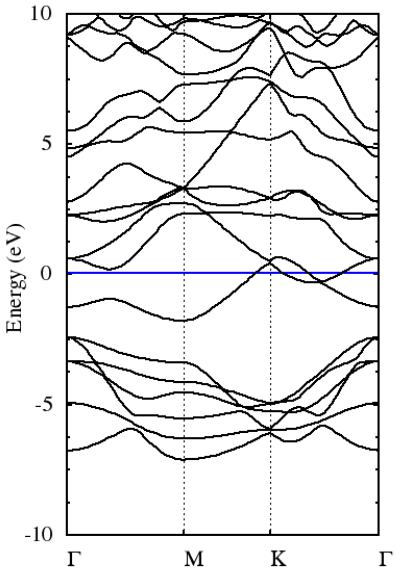
$ZrBr_2$



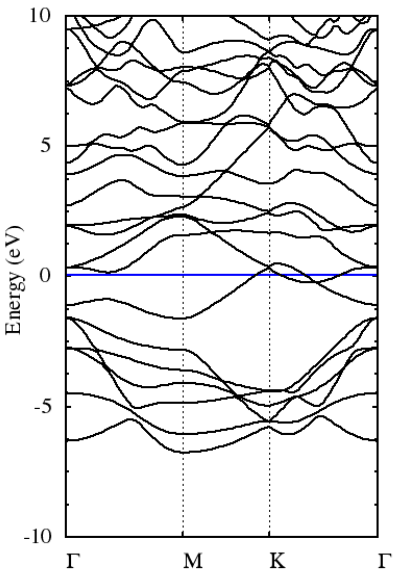
$CoCl_2$



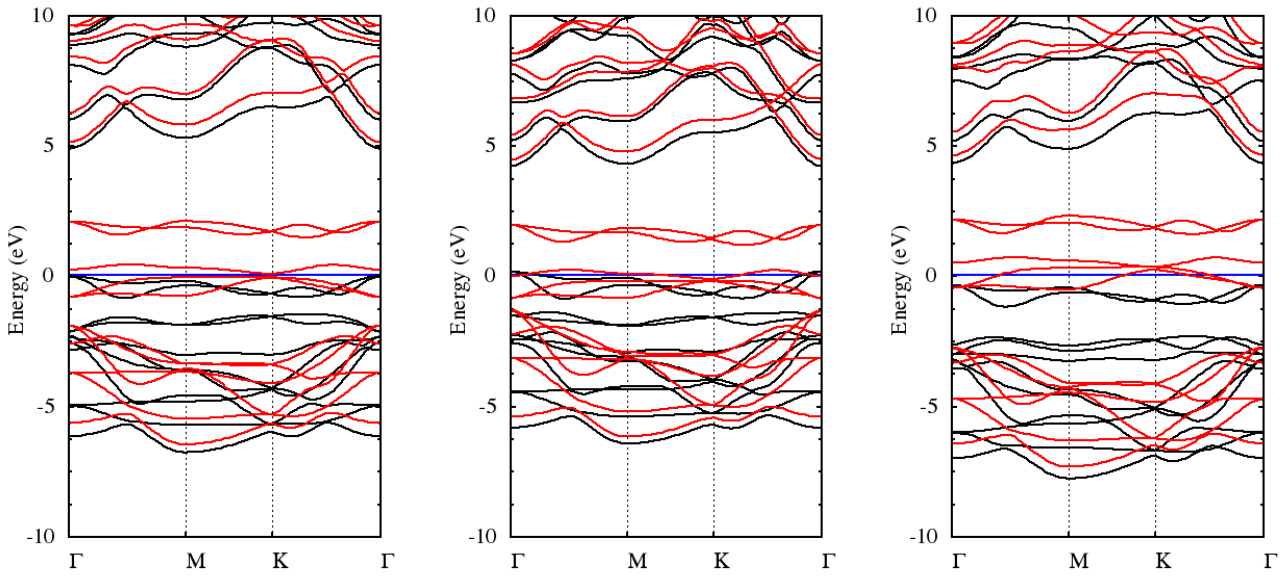
$CoBr_2$



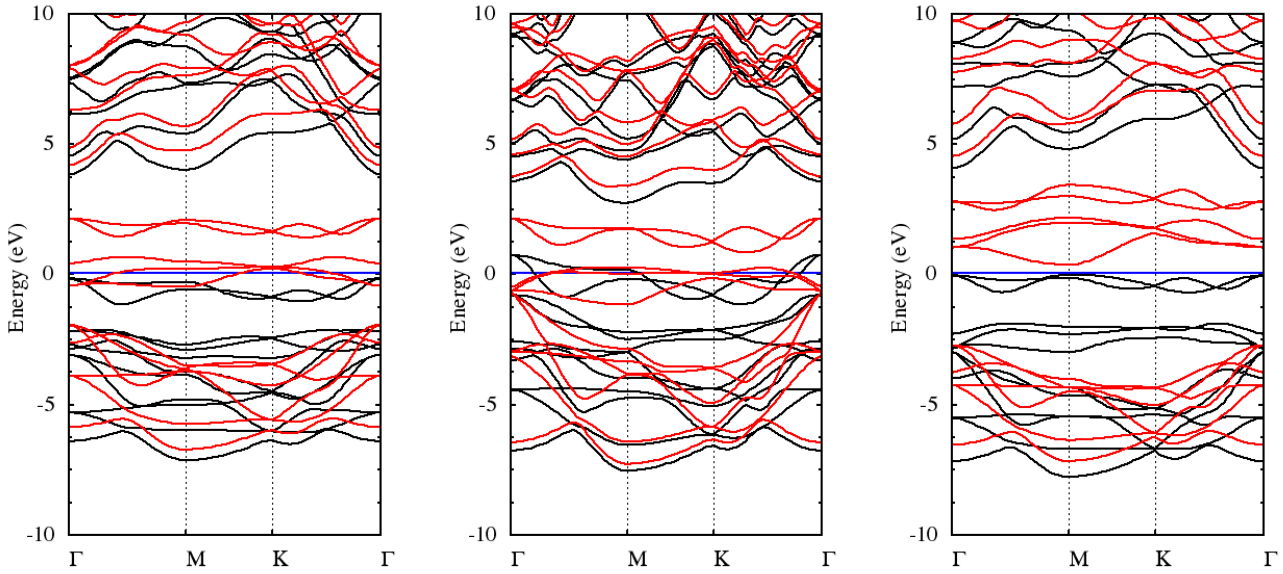
$FeCl_2$



ZrI_2



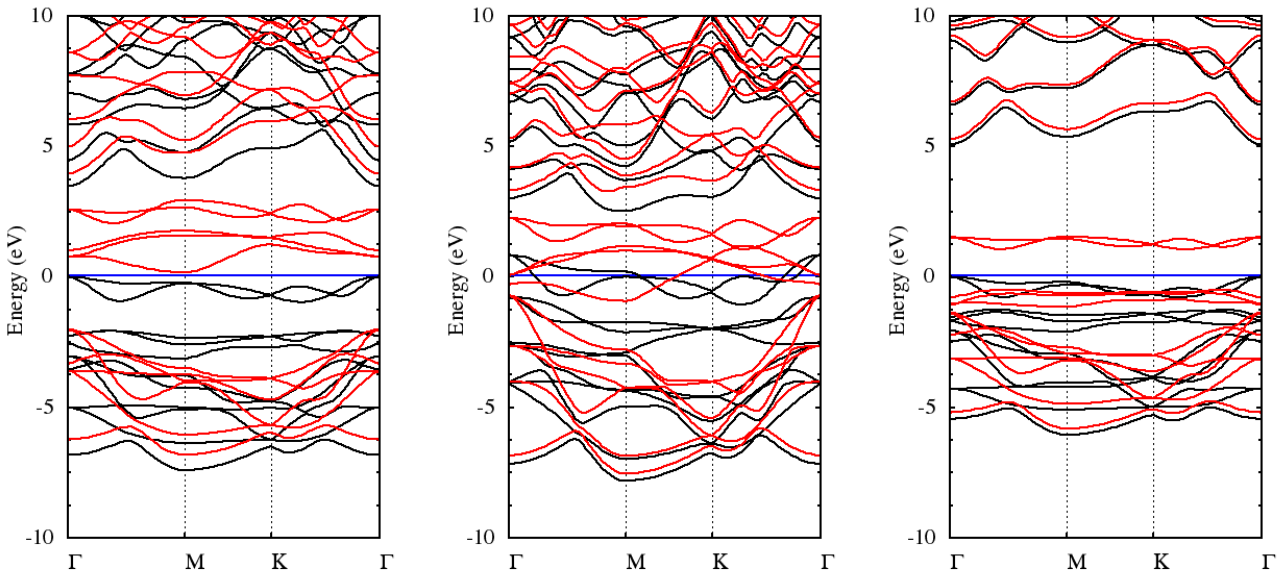
$FeBr_2$ FeI_2 $MnCl_2$



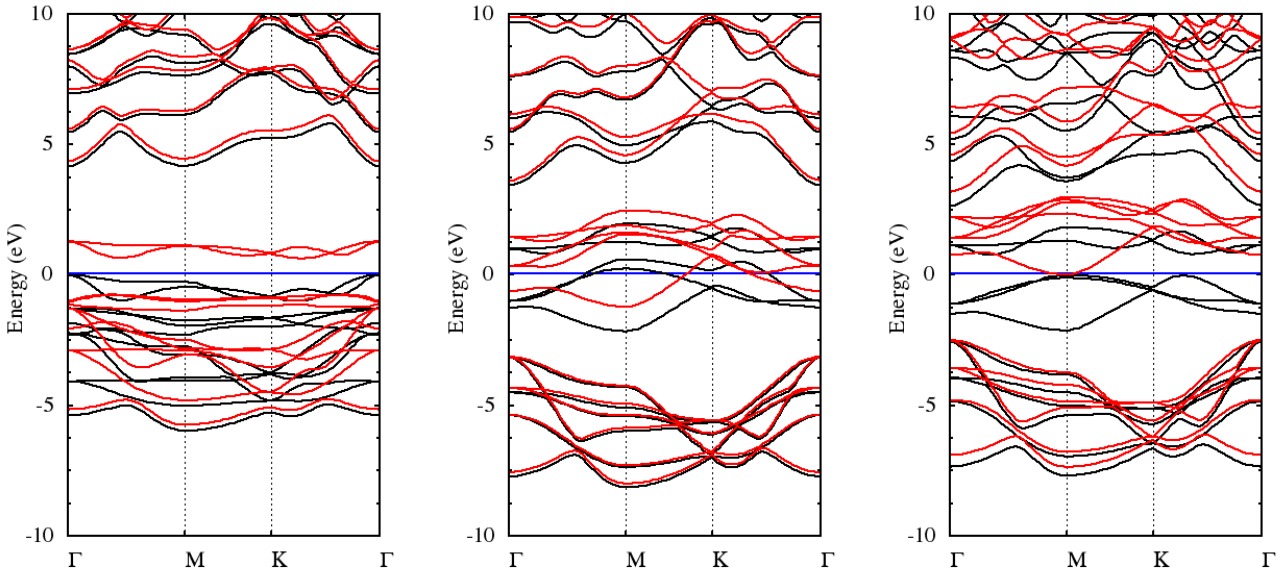
5

10

$MnBr_2$ MnI_2 $NiCl_2$



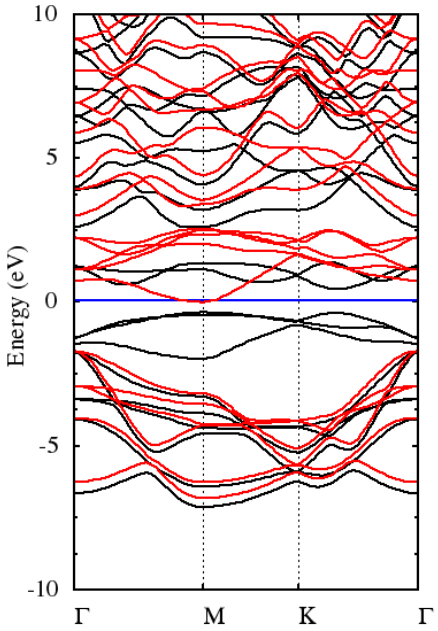
$NiBr_2$ VCl_2 VBr_2



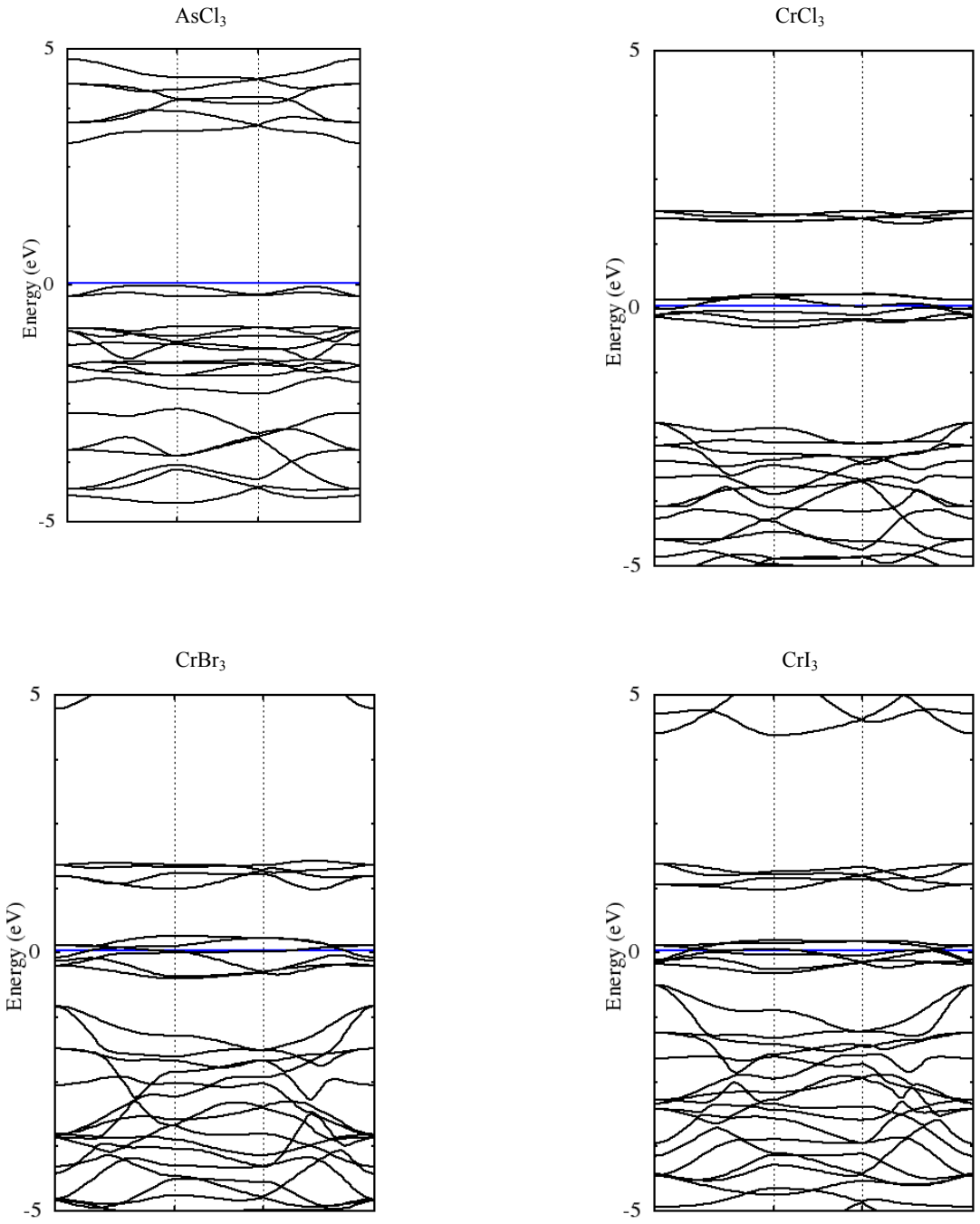
5

10

VI_2


10
5
0
-5
-10
Energy (eV)
Γ
M
K
Γ

3.7. Transition metal halides (MY_3)



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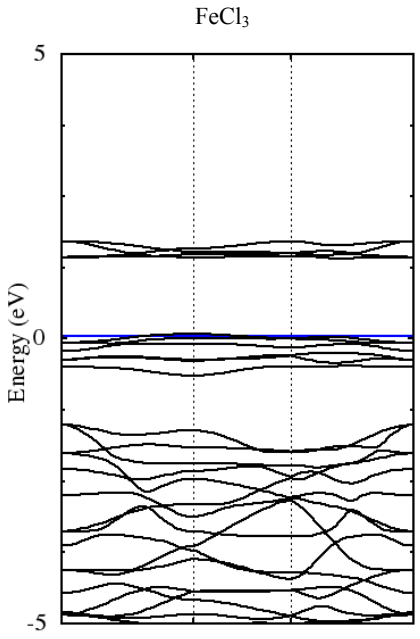
FeCl3
5
0
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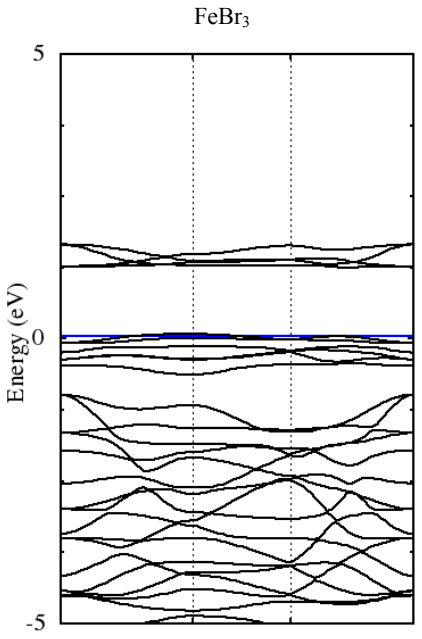
Energy (eV)


FeBr3
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0
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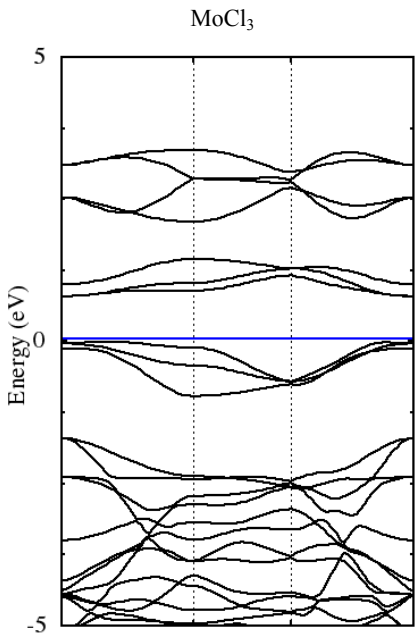
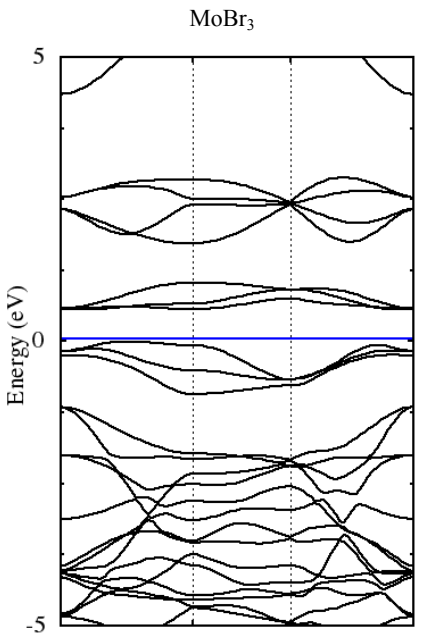
Energy (eV)


MoCl3
5
0
-5
Energy (eV)


MoBr3
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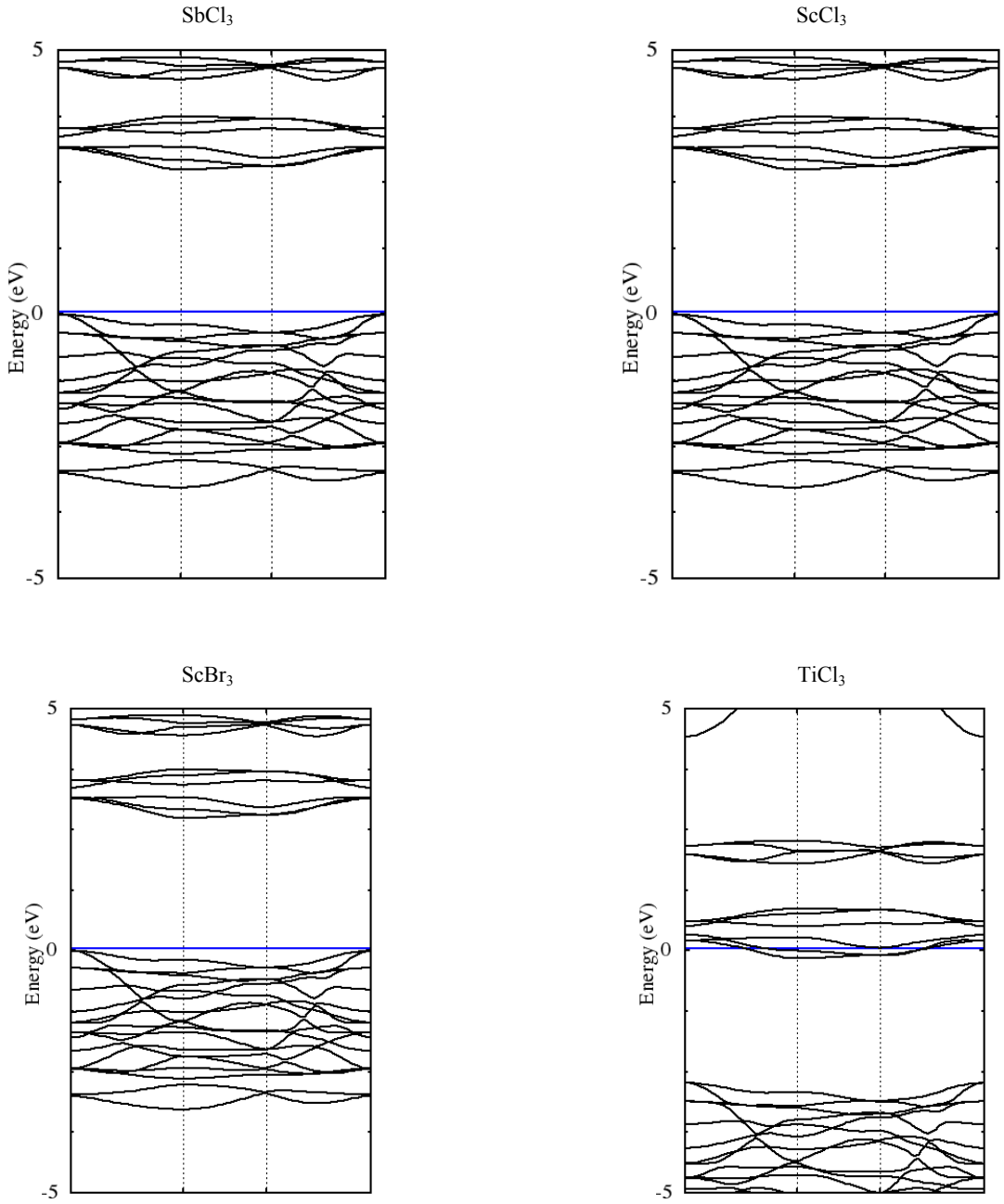
0
-5
Energy (eV)

5

10


SbCl3
ScCl3
ScBr3
TiCl3
Energy (eV)
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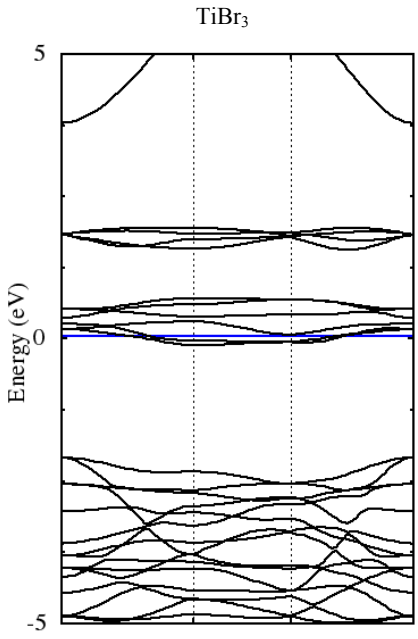
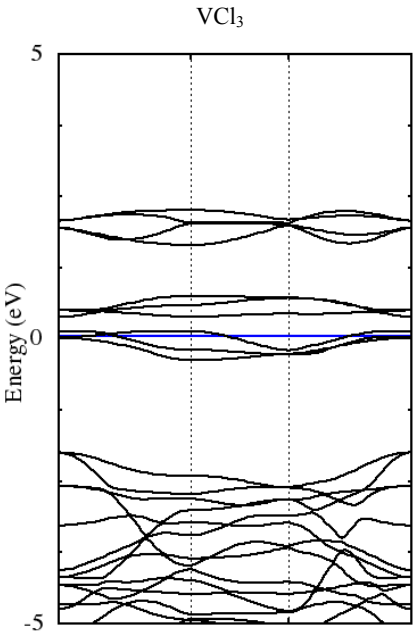
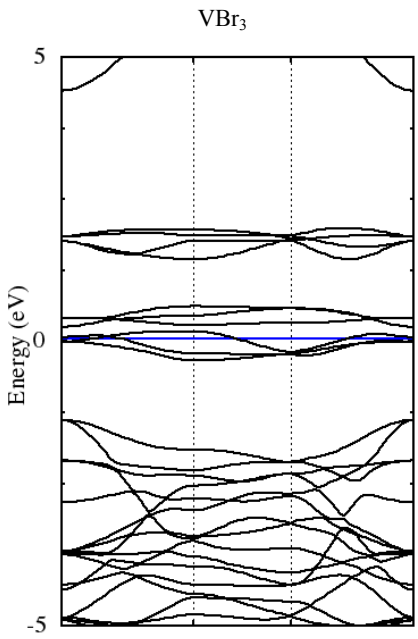
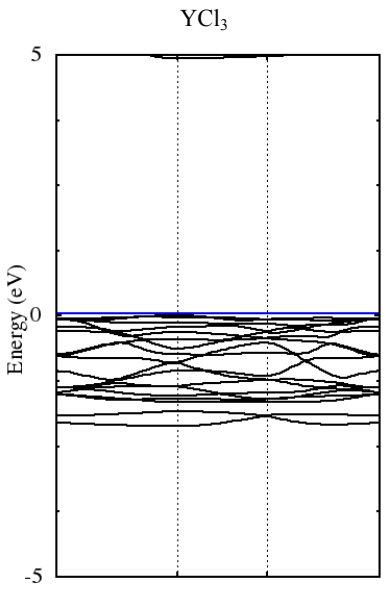
0
-5

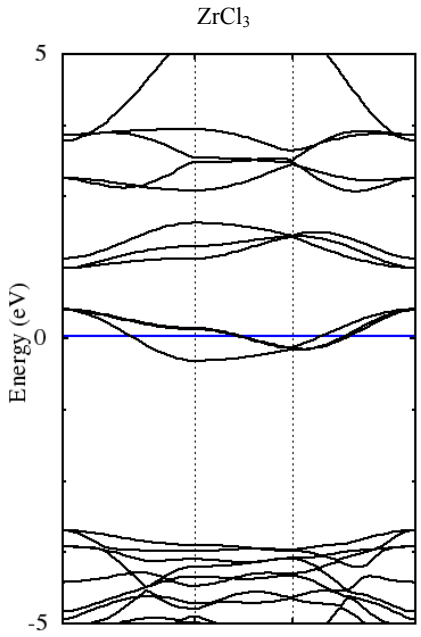

TiBr3
5
0
-5
Energy (eV)


VCl3
5
0
-5
Energy (eV)


VBr3
5
0
-5
Energy (eV)


YCl3
5
0
-5
Energy (eV)

5


ZrCl3
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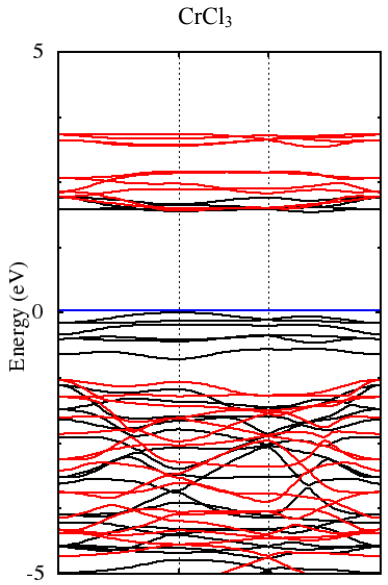
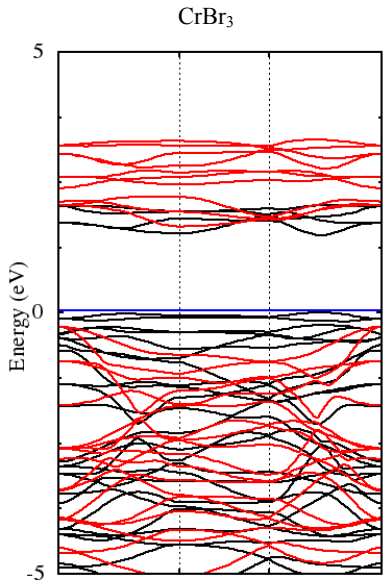
0
-5
Energy (eV)


CrCl3
5
0
-5
Energy (eV)


CrBr3
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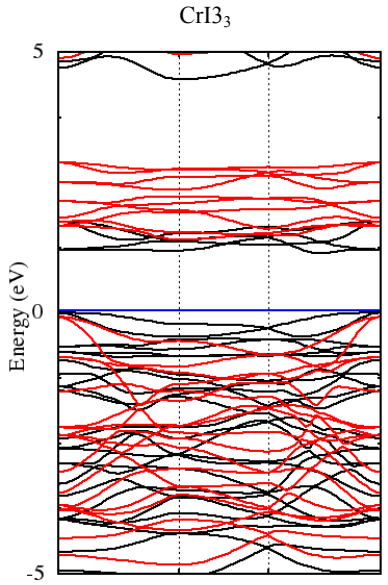
0
-5
Energy (eV)


CrI33
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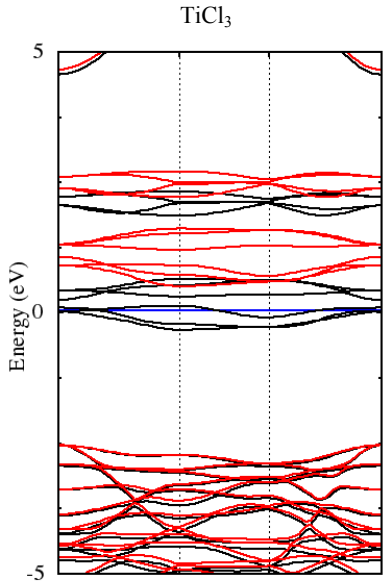
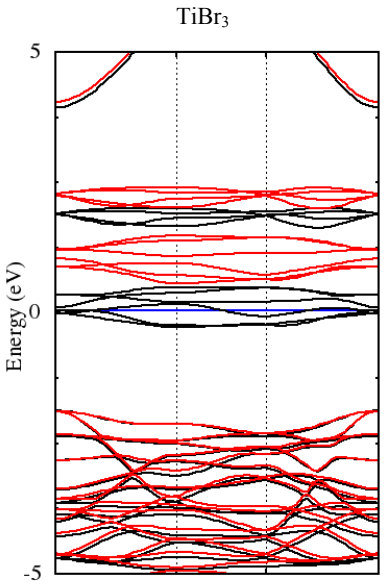
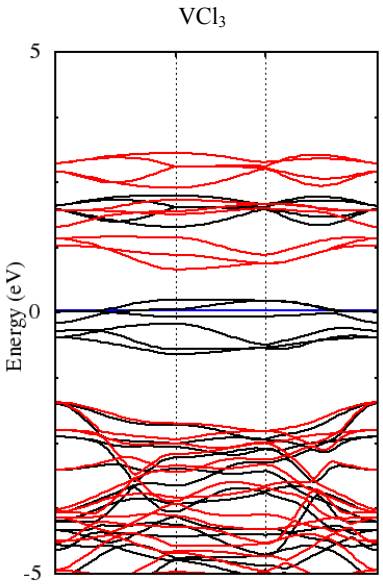
0
-5
Energy (eV)

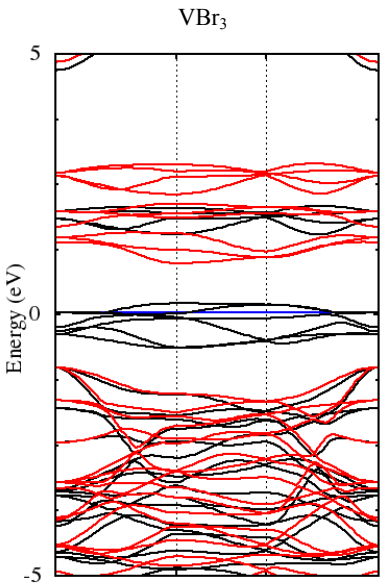

TiCl3
5
0
-5
Energy (eV)

5

10


TiBr3
5
0
-5
Energy (eV)


VCl3
5
0
-5
Energy (eV)


VBr3
5
0
-5
Energy (eV)

4. Effective Masses (GLLB-SC)

4.1. Atomically thin 2D materials

X		Effective mass		
Material	**Unit Cell Formula**	m_{lh+}	m_{hh}	m_{e-}
Graphene	C	-	-	-
Graphane	CH	-0.249	-0.249	0.983
Fluorographene	CF	-0.338	-0.338	0.466
Clorographene	CCl	-0.307	-0.309	0.283
Silicene	Si	-	-	-
Silicane	SiH	-0.129	-0.128	3.838
Fluorosilicene	SiF	-0.128	-0.128	0.235
Germanene	Ge	-	-	-
Germanane	GeH	-0.062	-0.061	0.063
Fluorogermanene	GeF	-0.017	-0.017	0.017
Clorogermanene	GeCl	-0.034	-0.035	0.034
Silicon Carbide	SiC		-0.549	0.645
Boron Nitride	BN		-0.792	1.175

Y		Effective mass		
Material	**Unit Cell Formula**	m_{lh+}	m_{hh}	m_{e-}
Graphene	C	-	-	-
Graphane	CH	-0.627	-0.626	0.983
Fluorographene	CF	-0.986	-0.983	0.462
Clorographene	CCl	-1.582	-1.582	0.253
Silicene	Si	-	-	-
Silicane	SiH	-0.564	-0.562	0.120
Fluorosilicene	SiF	-0.638	-0.640	0.233
Germanene	Ge	-	-	-
Germanane	GeH	-0.512	-0.505	0.063
Fluorogermanene	GeF	-0.597	-0.641	0.017
Clorogermanene	GeCl	-0.553	-1.603	0.034
Silicon Carbide	SiC	-	-0.550	0.644
Boron Nitride	BN	-	-0.792	1.168

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4.2. Atomically thin transition metal chalcogenides

X	Effective mass		
Material	m_{lh+}	m_{hh}	m_{e-}
α-ZnO	-0.282	-0.791	0.325
α-ZnS	-0.134	-	0.187
α-ZnSe	-0.107	-0.529	0.126
α-ZnTe	-0.085	-0.603	0.089
α-CdO	-0.258	-0.940	0.257
α-CdS	-0.157	-0.723	0.167
α-CdSe	-0.096	-0.274	0.111
α-CdTe	-0.072	-0.141	0.079
β-ZnS	-0.176	-0.178	0.187
β-ZnSe	-0.114	-0.141	0.139
β-ZnTe	-0.103	-0.645	0.108
β-CdO	-0.259	-1.041	0.258
β-CdS	-0.157	-0.751	0.165
β-CdSe	-0.094	-0.141	0.127
β-CdTe	-0.108	-0.113	0.115

Y	Effective mass		
Material	m_{lh+}	m_{hh}	m_{e-}
α-ZnO	-0.391	-	0.325
α-ZnS	-0.375	-	0.187
α-ZnSe	-0.132	-	0.126
α-ZnTe	-0.086	-0.689	0.089
α-CdO	-0.272	-1.157	0.257
α-CdS	-0.158	-0.742	0.167
α-CdSe	-0.143	-	0.111
α-CdTe	-0.135	-1.683	0.079
β-ZnS	-0.770	-0.811	0.187
β-ZnSe	-0.578	-	0.139
β-ZnTe	-0.104	-0.687	0.108
β-CdO	-0.264	-1.122	0.258
β-CdS	-0.159	-0.798	0.165
β-CdSe	-0.454	-	0.127
β-CdTe	-0.627	-0.824	0.115

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4.3. Metalloid chalcogenides

X	Effective mass		
Material	m_{lh+}	m_{hh}	m_{e-}
GaS	-	-2.755	2.020
GaSe	-	-2.007	0.173
InS	-	-3.758	0.313
InSe	-	-3.228	0.213

Y	Effective mass		
Material	m_{lh+}	m_{hh}	m_{e-}
GaS	-	-	0.361
GaSe	-	14.013	0.173
InS	-	20.336	0.313
InSe	-	20.463	0.213

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4.4. Transition metal chalcogenides (1T)

X	Effective mass		
Material	m_{lh+}	m_{hh}	m_{e-}
HfS_2	-0.189	-0.198	1.843
$HfSe_2$	-0.122	-0.132	1.627
NiS_2	-0.302	-0.789	1.119
$NiSe_2$	-0.211	-0.226	0.947
PdS_2	-0.725	-6.368	0.407
$PdSe_2$	-0.392	-1.997	0.406
PtS_2	-2.301	-4.095	1.378
$PtSe_2$	-0.740	-3.925	1.026
$PtTe_2$	-0.245	-0.245	0.796
TiS_2	-0.126	-0.134	2.247
ZrS_2	-0.218	-0.221	1.869
$ZrSe_2$	-0.147	-0.328	1.719

Y	Effective mass		
Material	m_{lh+}	m_{hh}	m_{e-}
HfS_2	-0.515	-0.591	0.235
$HfSe_2$	-0.343	-0.438	0.155
NiS_2	-0.369	-1.501	0.421
$NiSe_2$	-0.705	-0.756	0.370
PdS_2	-0.777	-7.303	0.369
$PdSe_2$	-0.417	-2.087	0.352
PtS_2	-	-	0.382
$PtSe_2$	-1.145	-5.807	0.323
$PtTe_2$	-1.180	-1.187	0.262
TiS_2	-0.220	-0.244	0.252
ZrS_2	-0.538	-0.559	0.298
$ZrSe_2$	-0.163	-0.421	0.210

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4.5. Transition metal chalcogenides (2H)

X	Effective mass		
Material	m_{lh+}	m_{hh}	m_{e-}
HfS_2	-	-0.705	3.695
$HfSe_2$	-0.718	-0.718	2.938
$HfTe_2$	-0.622	-0.622	12.147
MoS_2	-	-0.557	0.463
$MoSe_2$	-	-0.617	0.525
$MoTe_2$	-	-0.666	0.553
TiS_2	-	-0.826	5.514
$TiSe_2$	-0.825	-0.836	4.508
$TiTe_2$	-0.803	-0.803	10.775
WS_2	-	-0.405	0.312
WSe_2	-	-0.420	0.327
WTe_2	-	-0.384	0.313
ZrS_2	-	-0.726	13.881
$ZrSe_2$	-	-0.586	8.031
$ZrTe_2$	-	-0.567	-

Y	Effective mass		
Material	m_{lh+}	m_{hh}	m_{e-}
HfS_2	-	-3.415	0.528
$HfSe_2$	-1.102	-1.102	0.305
$HfTe_2$	-0.643	-0.643	0.176
MoS_2	-	-0.558	0.463
$MoSe_2$	-	-0.618	0.524
$MoTe_2$	-	-0.668	0.552
TiS_2	-	-	0.569
$TiSe_2$	-1.539	-1.576	0.349
$TiTe_2$	-0.859	-0.858	0.129
WS_2	-	-0.406	0.312
WSe_2	-	-0.421	0.327
WTe_2	-	-0.420	0.299
ZrS_2	-	-2.519	1.029
$ZrSe_2$	-	-2.604	0.503
$ZrTe_2$	-	-0.607	0.091

5

4.6. Transition metal halides (MY_2)

X	Effective mass[a]		
Material	m_{lh+}	m_{hh}	m_{e-}
$FeCl_2$	-	-2.862	2.751
$FeBr_2$	-	-2.579	2.086
$MnCl_2$	-	-1.079	2.582
$MnBr_2$	-0.314	-0.326	2.862
$NiCl_2$	-0.490	-0.549	2.447
$NiBr_2$	-0.286	-1.154	1.988

Y	Effective mass[a]		
Material	m_{lh+}	m_{hh}	m_{e-}
$FeCl_2$	-	-	1.104
$FeBr_2$	-	-	0.837
$MnCl_2$	-	-3.824	0.551
$MnBr_2$	-1.517	-1.838	0.422
$NiCl_2$	-1.537	-2.23	1.102
$NiBr_2$	-0.338	-	0.942

[a] PBE (scalar)

5

4.7. Transition metal halides (MY_3)

X	Effective mass		
Material	m_{lh+}	m_{hh}	m_{e-}
$AsCl_3$	-	-1.198	0.741
$CrCl_3$	-	-2.248[a]	3.552[a]
$CrBr_3$	-	-2.325[a]	0.993[a]
CrI_3	-0.434[a]	-8.543[a]	0.927[a]
$MoCl_3$	-1.748	-8.239	3.291
$MoBr_3$	-0.382	-42.664	3.591
$SbCl_3$	-	-1.215	0.704
$ScCl_3$	-0.536	-1.856	4.985
$ScBr_3$	-0.331	-0.566	2.698
YCl_3	-11.665	-1.196	3.230

[a] PBE (scalar)

Y	Effective mass		
Material	m_{lh+}	m_{hh}	m_{e-}
$AsCl_3$	-	-	0.741[a]
$CrCl_3$	-	-4.858[a]	2.281[a]
$CrBr_3$	-	-2.830[a]	0.629[a]
CrI_3	-0.576	-	0.683
$MoCl_3$	8.956	-29.885	2.449
$MoBr_3$	-1.606	-	3.583
$SbCl_3$	-	-9.331	0.704
$ScCl_3$	-0.634	-3.999	1.187
$ScBr_3$	-0.642	-3.314	0.756
YCl_3	3.943	-3.686	0.883

[a] PBE (scalar)