Electronic Supplementary Material

Conduction Band Engineering of Half-Heusler Thermoelectrics Using Orbital Chemistry

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Table S1: Energy offset of X_3 and X_2 (eV), valence difference, electronegativity difference of X and Y atoms and n-type conductivity effective mass (m_c^* , m_e) with carrier concentration of 10^{20} cm^{-3} at 900 K for 69 half-Heusler compounds.

Compound	E_{X_3}-E_{X_2} (eV)	valence difference	electronegativity difference	m_c^* (m_e)
HfCoAs	-1.0168	5	0.58	1.0171
HfCoBi	-1.1033	5	0.58	1.0880
HfCoSb	-1.0052	5	0.58	1.2459
HfIrSb	0.057246	5	0.90	0.4607
HfNiGe	-1.7973	6	0.61	0.6433
HfNiSn	-1.7219	6	0.61	0.5226
HfPdSn	-1.1252	6	0.90	0.5357
HfRhBi	-0.50297	5	0.98	0.4422
HfRhSb	-0.36829	5	0.98	1.1816
NbCoGe	0.052254	4	0.28	1.1234
NbCoSi	0.24413	4	0.28	0.5589
NbCoSn	-0.035925	4	0.28	1.3253
NbFeAs	0.77251	3	0.23	0.4229
NbFeP	0.95904	3	0.23	0.3790
NbFeSb	0.65265	3	0.23	0.4497
NbIrGe	1.2759	4	0.60	0.3891
NbIrSn	1.0241	4	0.60	0.3827
NbNiGa	-0.63584	5	0.31	0.3144
NbOsSb	1.772	3	0.60	0.3498
NbRhSi	0.91372	4	0.68	0.3162
NbRhSn	0.52431	4	0.68	0.3660
NbRuAs	1.4933	3	0.60	0.3856
NbRuSb	1.2937	3	0.60	0.3926
ScCoSe	-0.85577	6	0.52	0.5339
ScNiAs	-1.4379	7	0.55	0.7761
ScNiBi	-1.3557	7	0.55	0.3175
ScNiSb	-1.3978	7	0.55	0.4679
TaCoGe	-0.28823	4	0.38	1.4285
TaCoSi	-0.074663	4	0.38	1.3002
TaCoSn	-0.36272	4	0.38	1.3467
TaFeAs	0.51322	3	0.33	0.4416
TaFeSb	0.39706	3	0.33	0.4921
TaIrGe	1.0705	4	0.70	0.4538
TaIrSn	0.81574	4	0.70	0.4232
TaOsSb	1.6526	3	0.70	0.4003
TaPtGa	0.24594	5	0.70	0.4763
TaRhSn	0.28509	4	0.78	0.5073
TaRuAs	1.3335	3	0.70	0.3768
TaRuSb	1.1268	3	0.70	0.4258
TiCoAs	-0.07443	5	0.34	2.1327
TiCoBi	-0.21452	5	0.34	2.257
TiCoSb	-0.1425	5	0.34	2.0827
TiFeTe	0.39504	4	0.29	1.1599
TiIrAs	0.87557	5	0.66	0.7129
TiIrP	1.0621	5	0.66	0.7804
TiNiGe	-0.64018	6	0.37	1.0482
TiNiPb	-0.66169	6	0.37	0.6430
TiNiSn	-0.64163	6	0.37	0.8276
TiPtGe	0.27642	6	0.66	1.1188
TiRhAs	0.46848	5	0.74	1.0526
TiRhBi	0.19854	5	0.74	2.1949
VCoGe	0.44448	4	0.25	0.7608
VCoSn	0.29576	4	0.25	1.2070
VFeSb	0.8205	3	0.20	0.5902
YPdAs	-1.6939	7	0.98	0.4324

ZrCoAs	-0.69399	5	0.55	1.3396
ZrCoBi	-0.7663	5	0.55	1.2885
ZrCoSb	-0.67736	5	0.55	1.3938
ZrIrAs	0.38371	5	0.87	0.3455
ZrIrBi	0.12954	5	0.87	0.3519
ZrNiGe	-1.4015	6	0.58	0.7075
ZrNiPb	-1.3875	6	0.58	0.5407
ZrNiSn	-1.3368	6	0.58	0.6208
ZrPdGe	-0.78469	6	0.87	0.7272
ZrPdPb	-0.89481	6	0.87	0.5469
ZrPtGe	-0.32137	6	0.87	1.1035
ZrRhAs	-0.039293	5	0.95	0.7762
ZrRhBi	-0.24747	5	0.95	1.1438
ZrRuTe	0.64613	4	0.87	0.5776

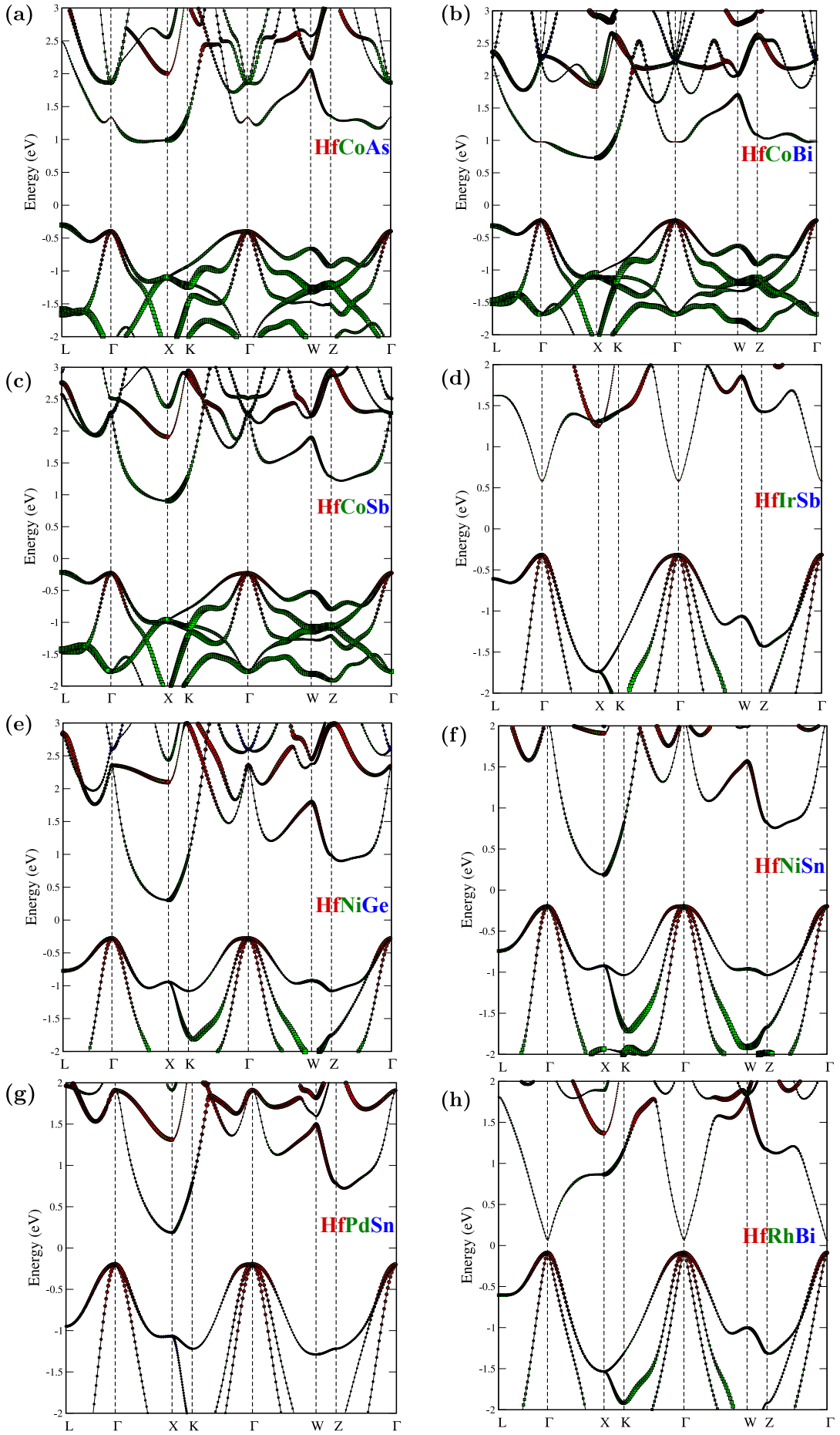

Fig. S1: The projected band structures of (a) HfCoAs, (b) HfCoBi, (c) HfCoSb, (d) HfIrSb, (e) HfNiGe, (f) HfNiSn, (g) HfPdSn and (h) HfRhBi.

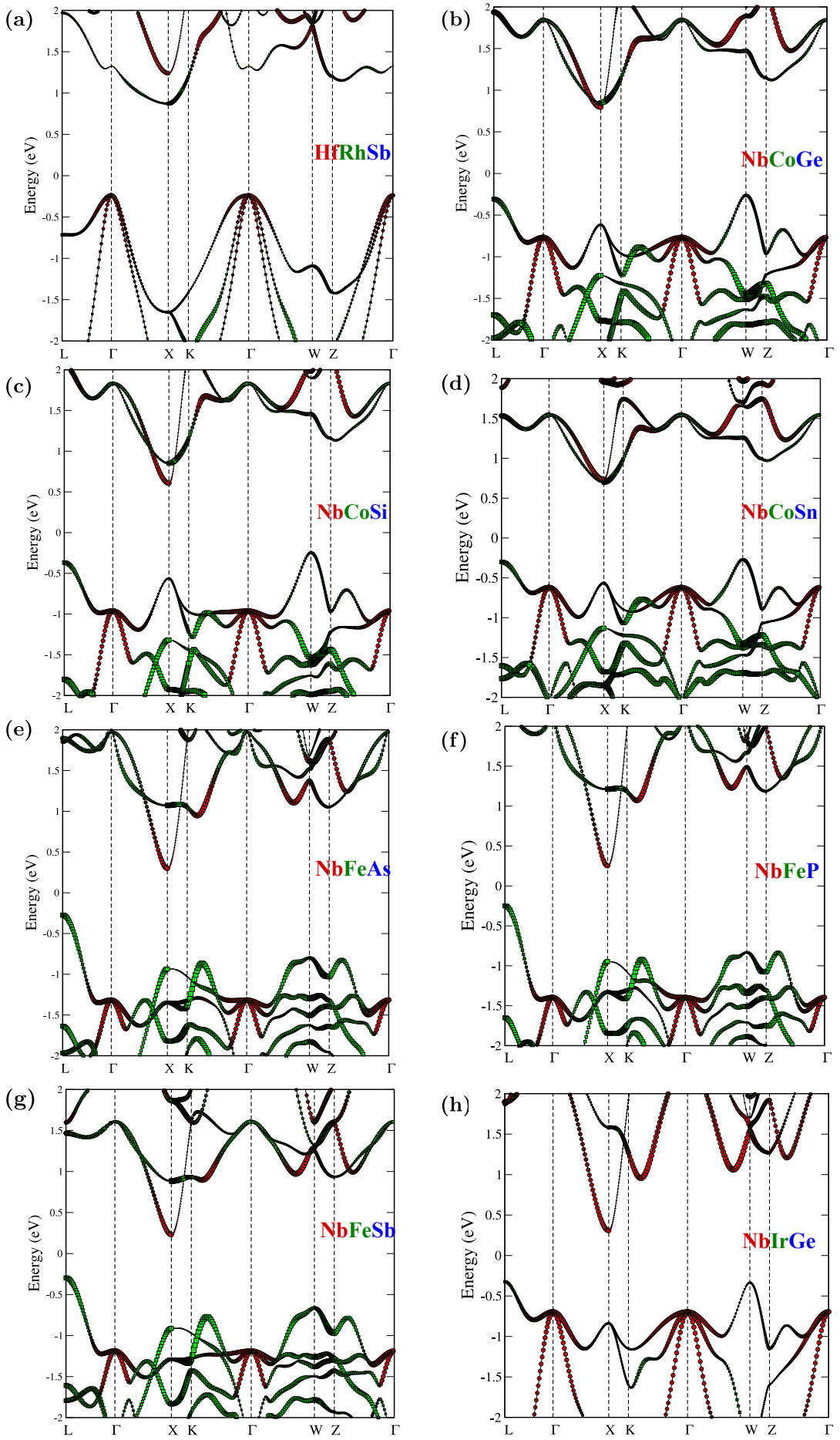

Fig. S2: The projected band structures of (a) HfRhSb, (b) NbCoGe, (c) NbCoSi, (d) NbCoSn, (e) NbFeAs, (f) NbFeP, (g) NbFeSb and (h) NbIrGe.

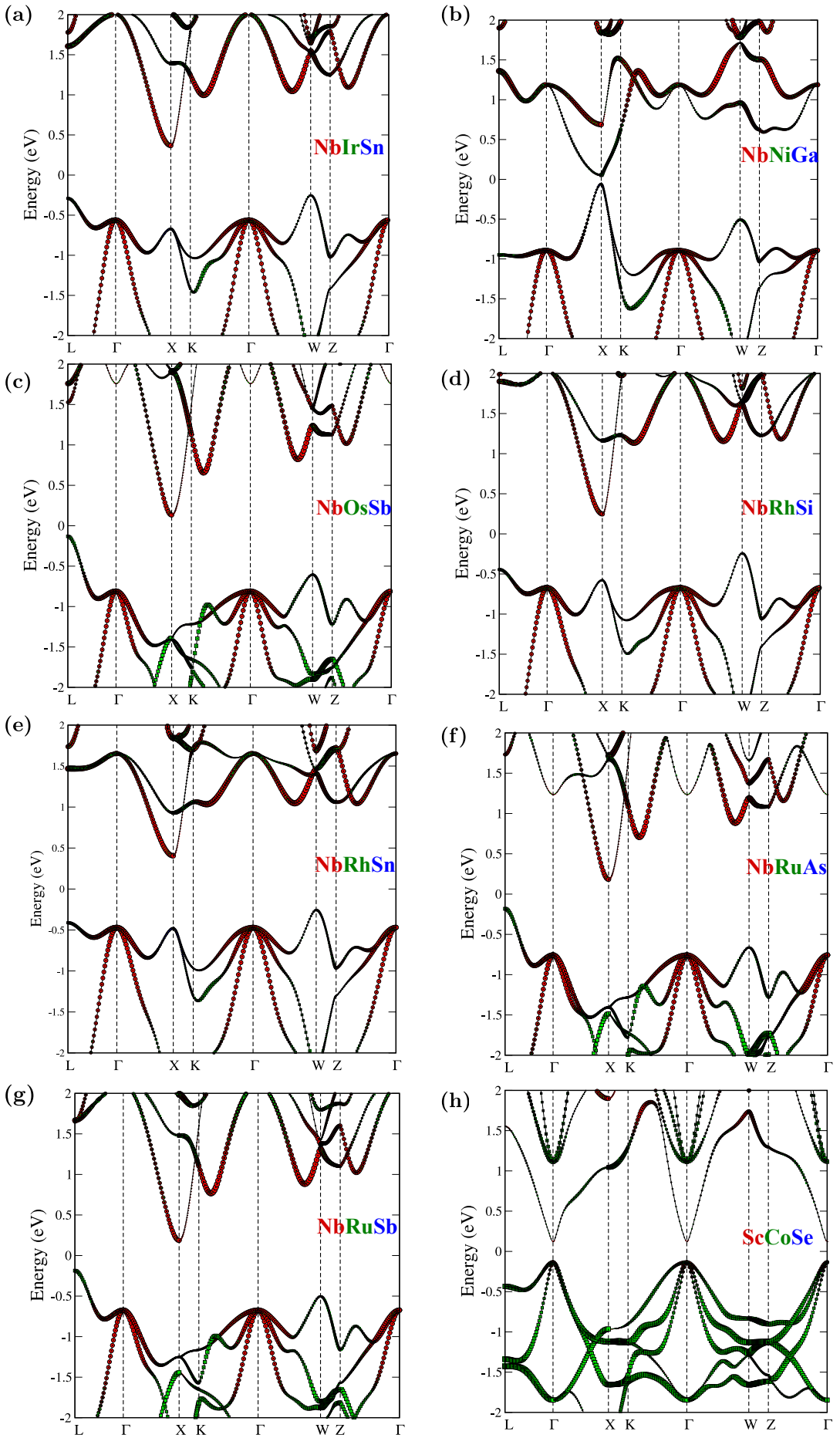

Fig. S3: The projected band structures of (a) NbIrSn, (b) NbNiGa, (c) NbOsSb, (d) NbRhSi, (e) NbRhSn, (f) NbRuAs, (g) NbRuSb and (h) ScOsSe.

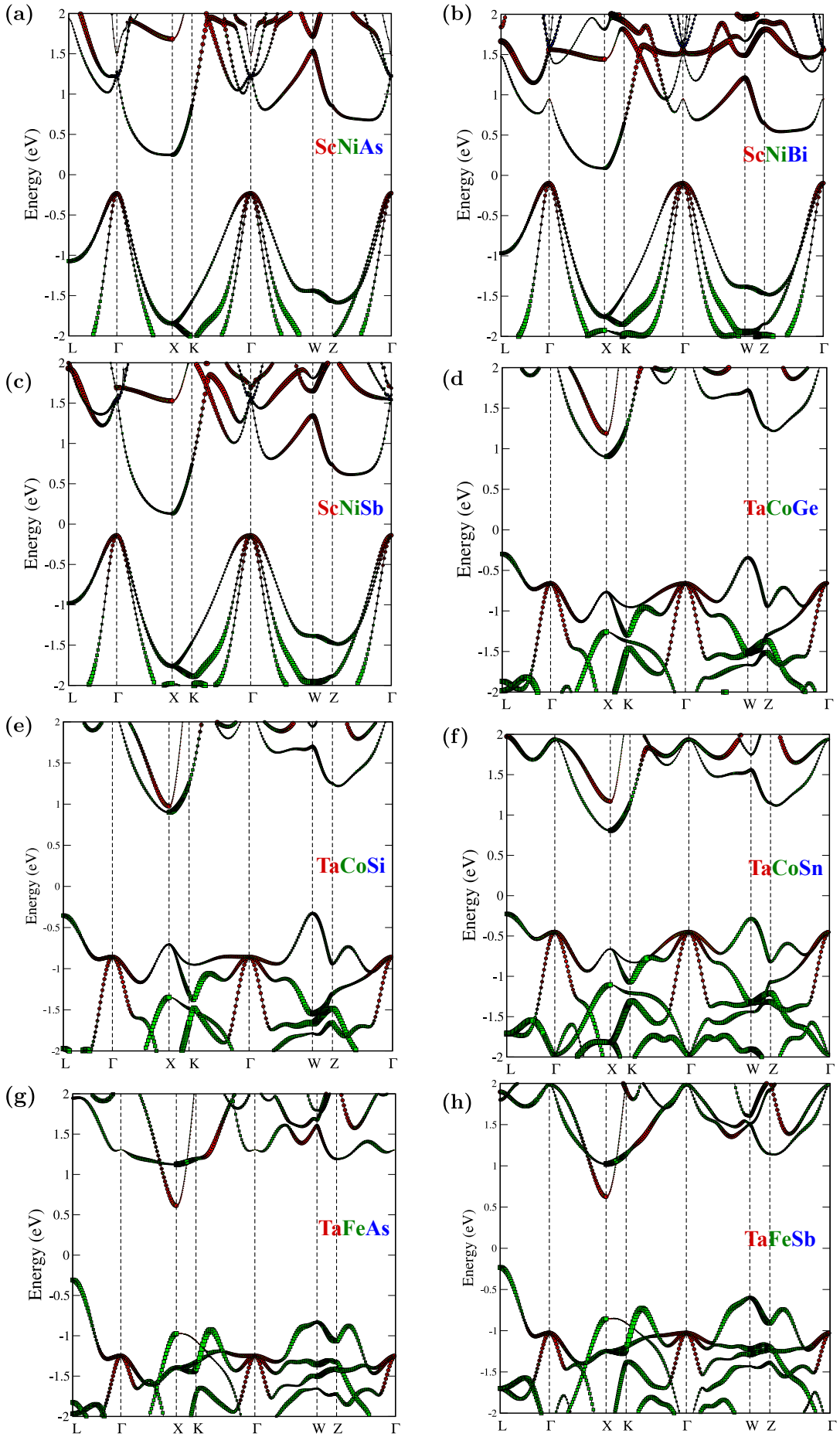

Fig. S4: The projected band structures of (a) ScNiAs, (b) ScNiBi, (c) ScNiSb, (d) TaCoGe, (e) TaCoSi, (f) TaCoSn, (g) TaFeAs and (h) TaFeSb.

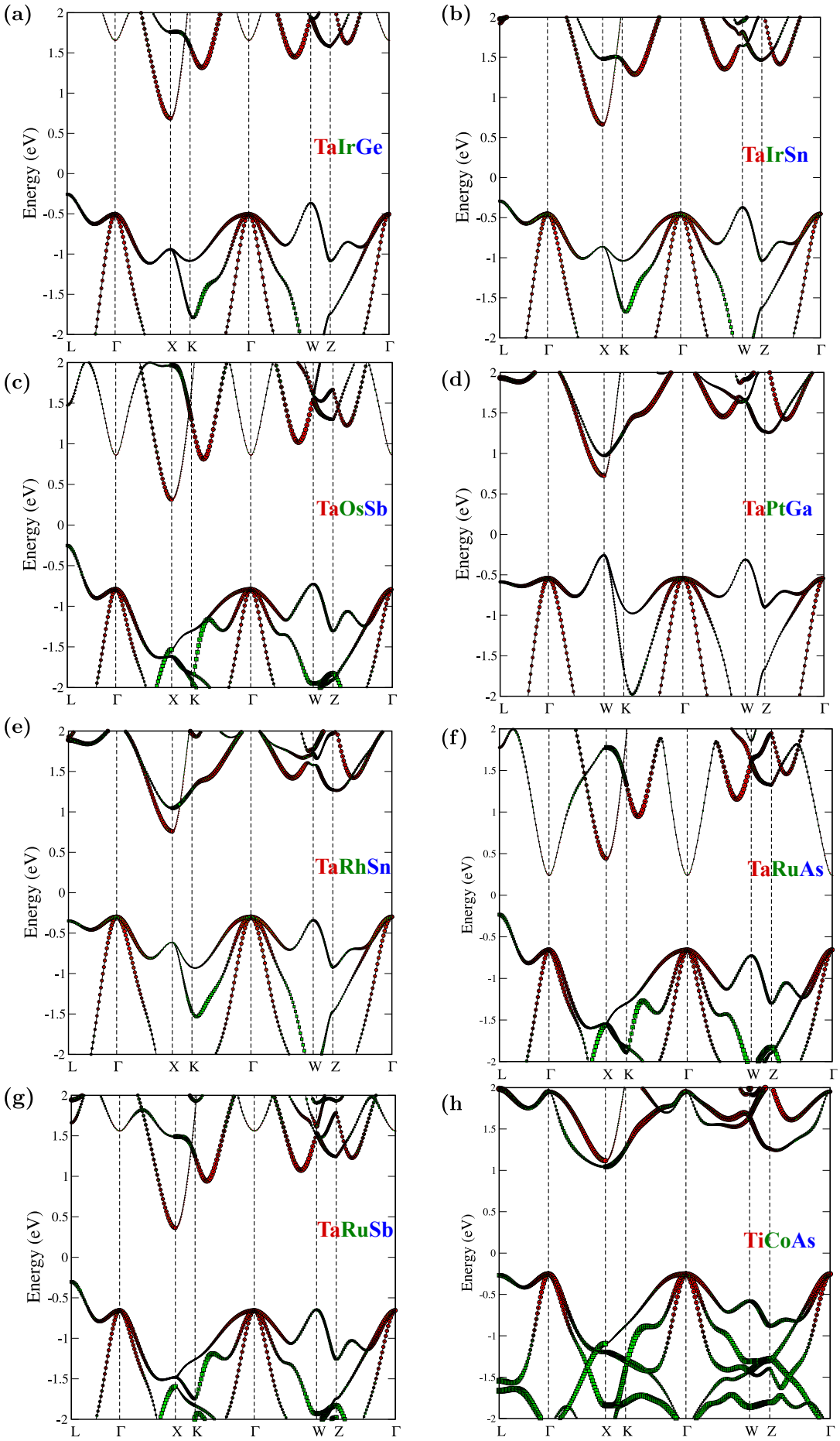

Fig. S5: The projected band structures of (a) TaIrGe, (b) TaIrSn, (c) TaOsSb, (d) TaPtGa, (e) TaRhSn, (f) TaRuAs, (g) TaRuSb and (h) TiCoAs.

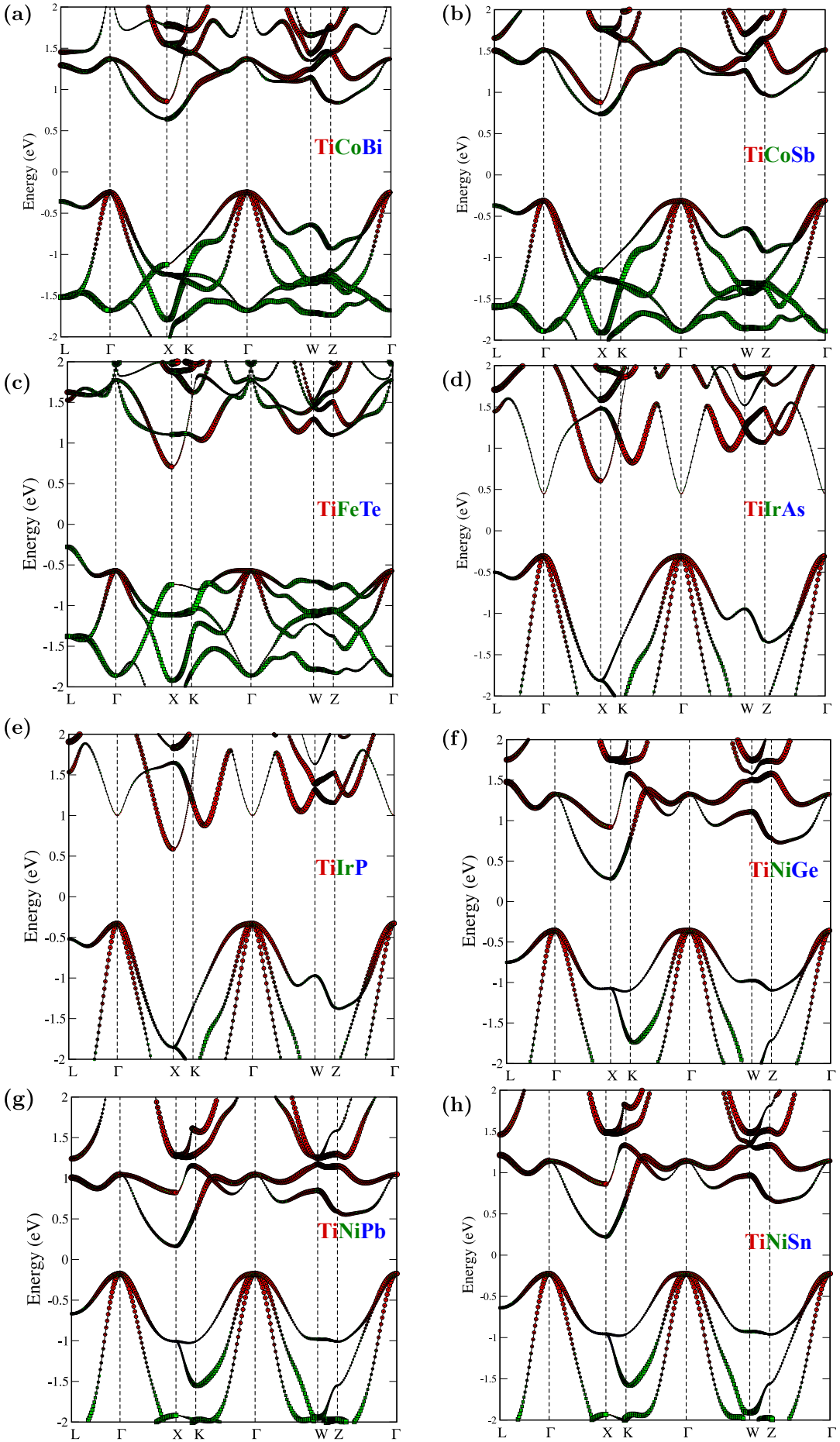

Fig. S6: The projected band structures of (a) TiCoBi, (b) TiCoSb, (c) TiFeTe, (d) TiIrAs (e) TiIrP, (f) TiNiGe, (g) TiNiPb and (h) TiNiSn.

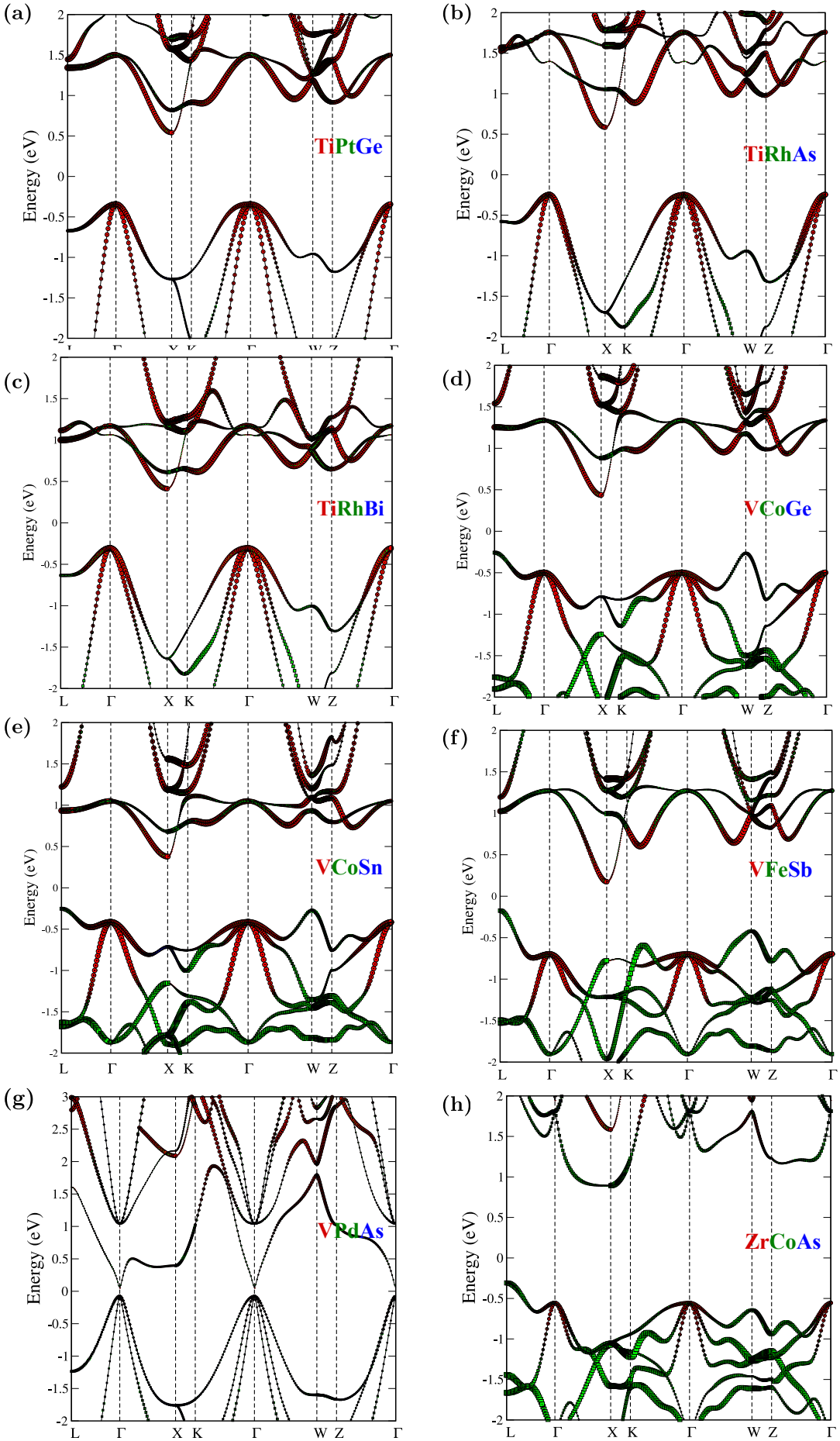

Fig. S7: The projected band structures of (a) TiPtGe, (b) TiRhAs, (c) TiRhBi, (d) VCoGe (e) VCoSn, (f) VFeSb, (g) YPdAs and (h) ZrCoAs.

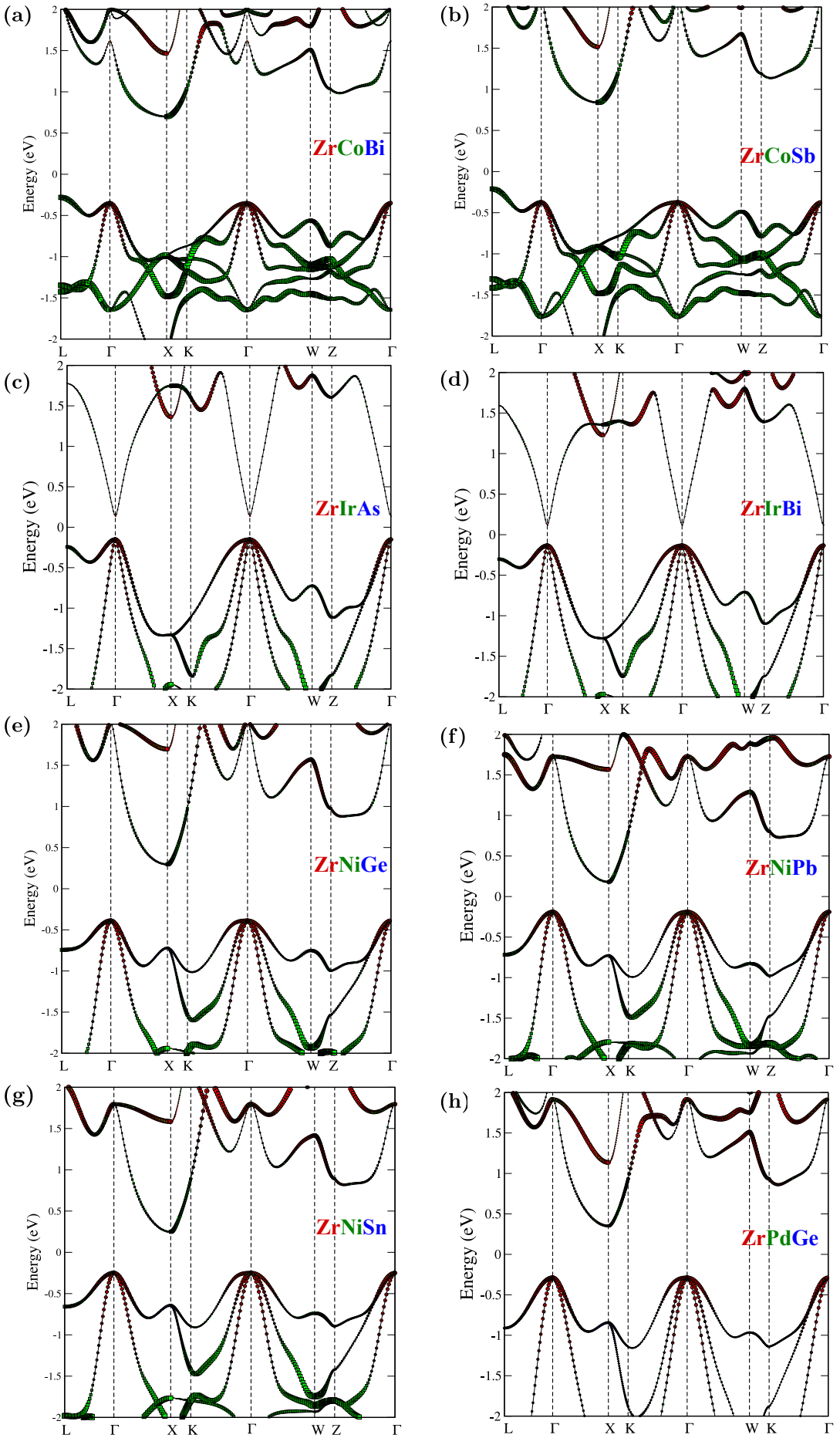

Fig. S8: The projected band structures of (a) ZrCoBi, (b) ZrCoSb, (c) ZrIrAs, (d) ZrIrBi (e) ZrNiGe, (f) ZrNiPb, (g) ZrNiSn and (h) ZrPdGe.

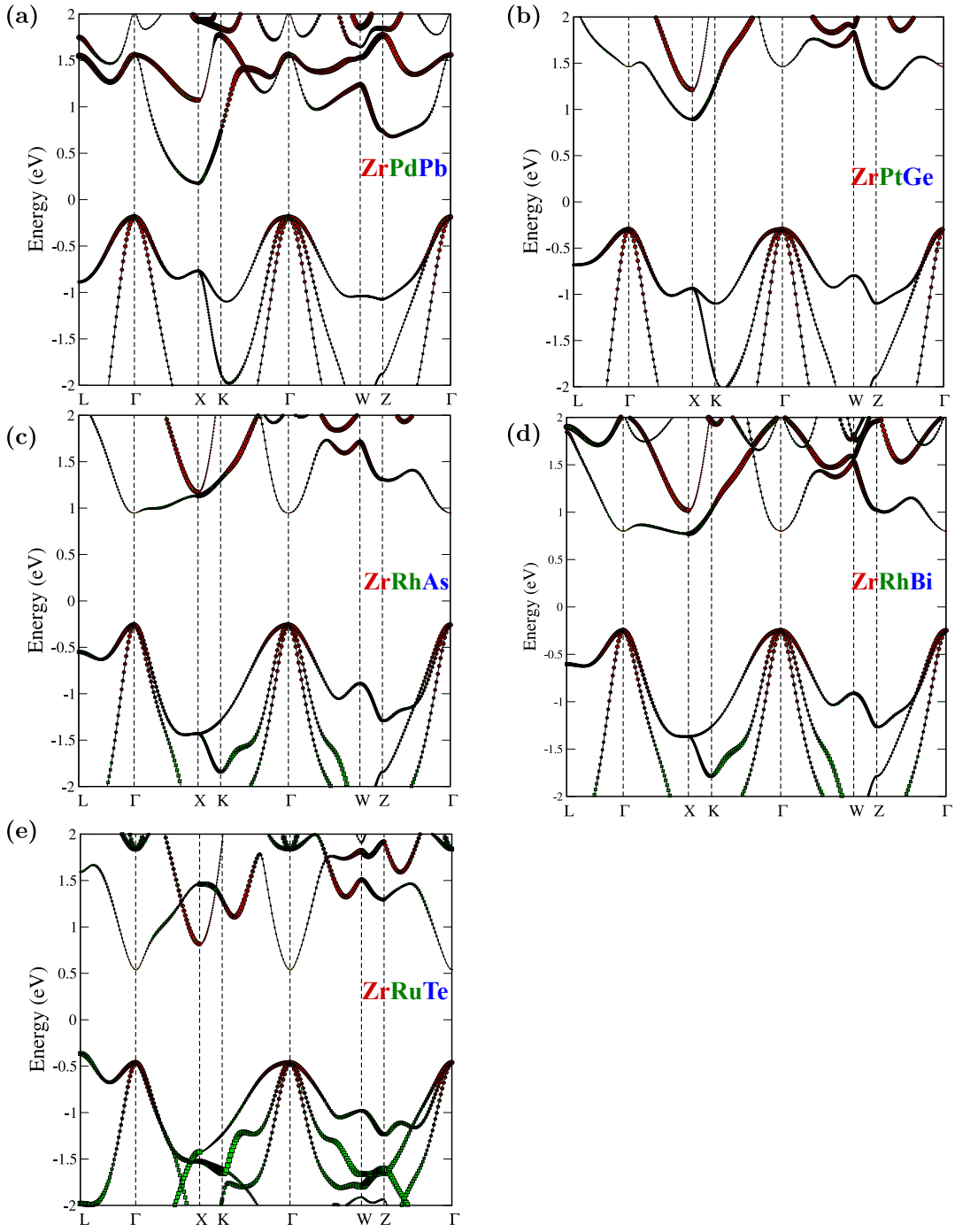

Fig. S9: The projected band structures of (a) ZrPdPb, (b) ZrPtGe, (c) ZrRhAs, (d) ZrRhBi and (h) ZrRuTe.