

## *Supporting Information*

### **Controllable topological phase transition via ferroelectric-paraelectric switching in ferromagnetic single-layer $M_I M_{II} \text{Ge}_2 \text{X}_6$ family**

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**Table SI.** Wyckoff sites of atoms in ferroelectric (FE) and paraelectric (PE) phases of 11 2D multiferroic materials.

Materials	PE	FE
ReIrGe <sub>2</sub> S <sub>6</sub>	S (6I) (0.32983, 0.03906, 0.42971) Ir (1b) (0.00000, 0.00000, 0.50000) Re (1f) (0.66667, 0.33333, 0.50000) Ge (2h) (0.33333, 0.66667, 0.55602)	S1 (3d) (0.33108,0.04411,0.45785) S2 (3d) (0.98402,0.66965,0.53975) Ir (1a) (0.00000,0.00000,0.49884) Re (1c) (0.66667,0.33333,0.49755) Ge (1b) (0.33333,0.66667,0.515790) Ge (1b) (0.33333,0.66667,0.43195)
ReIrGe <sub>2</sub> Se <sub>6</sub>	S (6I) (0.32936,0.04187,0.42584) Ir (1b) (0.00000,0.00000,0.50000) Re (1f) (0.66667,0.33333,0.50000) Ge (2h) (0.33333,0.66667,0.55680)	Se1 (3d) (0.32997,0.04946,0.45454) Se2 (3d) (0.98100,0.66994,0.54285) Ir (1a) (0.00000,0.00000,0.49940) Re (1c) (0.66667,0.33333,0.49805) Ge (1b) (0.33333,0.66667,0.51518) Ge (1b) (0.33333,0.66667,0.43213)
ReAlGe <sub>2</sub> Se <sub>6</sub>	Se (6I) (0.33813,0.04085,0.42319) Al (1b) (0.00000,0.00000,0.50000) Re (1f) (0.66667,0.33333,0.50000) Ge (2h) (0.33333,0.66667,0.55641)	Se1 (3d) (0.33245,0.04762,0.45279) Se2 (3d) (0.98008,0.65584,0.54483) Al (1a) (0.00000,0.00000,0.50299) Re (1c) (0.66667,0.33333,0.49761) Ge (1b) (0.33333,0.66667,0.51383) Ge (1b) (0.33333,0.66667,0.42964)
ReBiGe <sub>2</sub> Se <sub>6</sub>	S (6I) (0.37520,0.03798,0.43527) Bi (1b) (0.00000,0.00000,0.50000) Re (1f) (0.66667,0.33333,0.50000) Ge (2h) (0.33333,0.66667,0.54659)	Se1 (3d) (0.37126,0.03889,0.42896) Se2 (3d) (0.96119,0.62884,0.55843) Bi (1a) (0.00000,0.00000,0.49365) Re (1c) (0.66667,0.33333,0.49372) Ge (1b) (0.33333,0.66667,0.59437) Ge (1b) (0.33333,0.66666,0.39302)
ReRhGe <sub>2</sub> Se <sub>6</sub>	Se (6I) (0.32955,0.04165,0.42522) Rh (1b) (0.00000,0.00000,0.50000) Re (1f) (0.66667,0.33333,0.50000) Ge (2h) (0.33333,0.66667,0.55699)	Se1 (3d) (0.32950,0.04877,0.45425) Se2 (3d) (0.98025,0.66870,0.54304) Rh (1a) (0.00000,0.00000,0.49960) Re (1c) (0.66667,0.33333,0.49818) Ge (1b) (0.33333,0.66667,0.51512) Ge (1b) (0.33333,0.66667,0.43215)
ReSnGe <sub>2</sub> S <sub>6</sub>	S (6I) (0.36300,0.04025,0.43634) Sn (1b) (0.00000,0.00000,0.50000) Re (1f) (0.66667,0.33333,0.50000) Ge (2h) (0.33333,0.66666,0.54862)	S1 (3d) (0.35381,0.05032,0.45815) S2 (3d) (0.97866,0.62496,0.53792) Sn (1a) (0.00000,0.00000,0.50178) Re (1c) (0.66667,0.33333,0.49656) Ge (1b) (0.33333,0.66667,0.51280) Ge (1b) (0.33333,0.66667,0.43757)
TcIrGe <sub>2</sub> S <sub>6</sub>	S (6I) (0.32882,0.03756,0.43995) Ir (1b) (0.00000,0.00000,0.50000) Tc (1f) (0.66667,0.33333,0.50000) Ge (2h) (0.33333,0.66667,0.54705)	S1 (3d) (0.33116,0.03889,0.45833) S2 (3d) (0.98425,0.67090,0.53951) Ir (1a) (0.00000,0.00000,0.49871) Tc (1c) (0.66667,0.33333,0.49735) Ge (1b) (0.33333,0.66667,0.51617)

		Ge ( <i>1b</i> ) (0.33333,0.66667, 0.43119)
TcIrGe <sub>2</sub> Se <sub>6</sub>	Se ( <i>6I</i> ) (0.32841,0.04052,0.42790) Ir ( <i>1b</i> ) (0.00000,0.00000,0.50000) Tc ( <i>1f</i> ) (0.66667,0.33333,0.50000) Ge ( <i>2h</i> ) (0.33333,0.66667,0.55444)	Se1 ( <i>3d</i> ) (0.32970,0.04649,0.45088) Se2 ( <i>3d</i> ) (0.98113,0.67074,0.54755) Ir ( <i>1a</i> ) (0.00000,0.00000,0.49993) Tc ( <i>1c</i> ) (0.66667,0.33333,0.49834) Ge ( <i>1b</i> ) (0.33333,0.66667,0.51762) Ge ( <i>1b</i> ) (0.33333,0.66667,0.42577)
WIrGe <sub>2</sub> S <sub>6</sub>	S ( <i>6I</i> ) (0.32375,0.03188 ,0.42803) Ir ( <i>1b</i> ) (0.00000,0.00000,0.50000) W ( <i>1f</i> ) (0.66667,0.33333,0.50000) Ge ( <i>2h</i> ) (0.33333,0.66667,0.55453)	S1 ( <i>3d</i> ) (0.32970,0.04649,0.45088) S2 ( <i>3d</i> ) (0.98113,0.67074,0.54755) Ir ( <i>1a</i> ) (0.00000,0.00000,0.49993) W ( <i>1c</i> ) (0.66667,0.33333,0.49834) Ge ( <i>1b</i> ) (0.33333,0.66667,0.51762) Ge ( <i>1b</i> ) (0.33333,0.66667,0.42577)
WAlGe <sub>2</sub> Se <sub>6</sub>	Se ( <i>6I</i> ) (0.33265,0.03360,0.42464) Al ( <i>1b</i> ) (0.00000,0.00000,0.50000) W ( <i>1f</i> ) (0.66667,0.33333,0.50000) Ge ( <i>2h</i> ) (0.33333,0.66667,0.55466)	Se1 ( <i>3d</i> ) (0.34337,0.01809,0.45481) Se2 ( <i>3d</i> ) (0.95702,0.66433,0.54672) Al ( <i>1a</i> ) (0.00000,0.00000,0.49776) W ( <i>1c</i> ) (0.66667,0.33333,0.50068) Ge ( <i>1b</i> ) (0.33333,0.66667,0.57297) Ge ( <i>1b</i> ) (0.33333,0.66667,0.48708)
WPtGe <sub>2</sub> Te <sub>6</sub>	Te ( <i>6I</i> ) (0.32964,0.04144,0.42129) Pt ( <i>1b</i> ) (0.00000,0.00000,0.50000) Re ( <i>1f</i> ) (0.66667,0.33333,0.50000) Ge ( <i>2h</i> ) (0.33333,0.66667,0.55828)	Te1 ( <i>3d</i> ) (0.32956,0.05872,0.44866) Te2 ( <i>3d</i> ) (0.98337,0.67228,0.54713) Pt ( <i>1a</i> ) (0.00000,0.00000,0.49941) W ( <i>1c</i> ) (0.66667,0.33333,0.49818) Ge ( <i>1b</i> ) (0.33333,0.66666,0.51568) Ge ( <i>1b</i> ) (0.33333,0.66667,0.43633)

**Table SII.** Lattice constants of ferroelectric (FE) and paraelectric (PE) phases for 11 2D multiferroic materials.

Materials	PE	FE
ReIrGe <sub>2</sub> S <sub>6</sub>	a=b=6.11 Å	a=b=6.26 Å
ReIrGe <sub>2</sub> Se <sub>6</sub>	a=b=6.44 Å	a=b=6.57 Å
ReAlGe <sub>2</sub> Se <sub>6</sub>	a=b=6.43 Å	a=b=6.52 Å
ReBiGe <sub>2</sub> Se <sub>6</sub>	a=b=6.37 Å	a=b=6.51 Å
ReRhGe <sub>2</sub> Se <sub>6</sub>	a=b=6.42 Å	a=b=6.55 Å
ReSnGe <sub>2</sub> S <sub>6</sub>	a=b=6.33 Å	a=b=6.45 Å
TcIrGe <sub>2</sub> S <sub>6</sub>	a=b=6.08 Å	a=b=6.23 Å
TcIrGe <sub>2</sub> Se <sub>6</sub>	a=b=6.41 Å	a=b=6.55 Å

WIrGe <sub>2</sub> S <sub>6</sub>	a=b=6.08 Å	a=b=6.29 Å
WAlGe <sub>2</sub> Se <sub>6</sub>	a=b=6.47 Å	a=b=6.55 Å
WPtGe <sub>2</sub> Te <sub>6</sub>	a=b=7.03 Å	a=b=7.09 Å

**Table III.** Ferroelectric transition barriers for the SL M<sub>I</sub>M<sub>II</sub>Ge<sub>2</sub>X<sub>6</sub> family.

Materials	Energy barrier (eV)	Materials	Energy barrier (eV)
ReIrGe <sub>2</sub> S <sub>6</sub>	0.62	ReIrGe <sub>2</sub> Se <sub>6</sub>	0.23
TcIrGe <sub>2</sub> S <sub>6</sub>	0.49	ReRhGe <sub>2</sub> Se <sub>6</sub>	0.19
ReAlGe <sub>2</sub> Se <sub>6</sub>	0.07	WPtGe <sub>2</sub> Te <sub>6</sub>	0.16
WIrGe <sub>2</sub> S <sub>6</sub>	0.77	WAlGe <sub>2</sub> Se <sub>6</sub>	0.22
ReSnGe <sub>2</sub> Se <sub>6</sub>	0.20	ReBiGe <sub>2</sub> Se <sub>6</sub>	0.24

**Table IV.** Magnetic ground states of ferroelectric (FE) phase for 11 2D multiferroic materials.

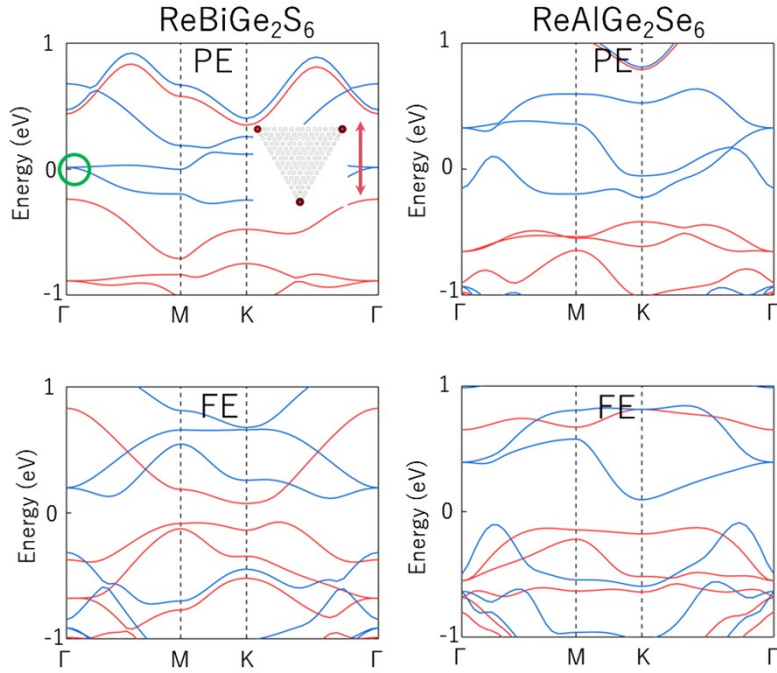
Materials	FM (eV)	AFM1 (eV)	AFM2 (eV)
ReIrGe <sub>2</sub> S <sub>6</sub>	-226.32145395	-226.14374067	-226.14374197
ReIrGe <sub>2</sub> Se <sub>6</sub>	-222.62311261	-222.15396648	-222.14701290
ReAlGe <sub>2</sub> Se <sub>6</sub>	-204.84004770	-204.45416126	-204.45347128
ReBiGe <sub>2</sub> Se <sub>6</sub>	-204.84004770	-204.45416126	-204.45347128
ReRhGe <sub>2</sub> Se <sub>6</sub>	-195.76309287	-195.51162751	-195.51162879
ReSnGe <sub>2</sub> S <sub>6</sub>	-210.25680034	-210.12374933	-210.12349296
TcIrGe <sub>2</sub> S <sub>6</sub>	-187.83463627	-187.57906846	-187.57906987
TcIrGe <sub>2</sub> Se <sub>6</sub>	-203.81887192	-203.68401305	-203.68445755
WIrGe <sub>2</sub> S <sub>6</sub>	-232.32182864	-232.13392289	-232.13392147
WAlGe <sub>2</sub> Se <sub>6</sub>	-198.86190839	-198.63532164	-198.63591126
WPtGe <sub>2</sub> Te <sub>6</sub>	-205.93188200	-205.54534612	-205.54534552

**Table SV.** Fractional corner charges of SL-ReBiGe<sub>2</sub>S<sub>6</sub>, SL-WIrGe<sub>2</sub>S<sub>6</sub>, SL-TcIrGe<sub>2</sub>S<sub>6</sub>, SL-TcIrGe<sub>2</sub>Se<sub>6</sub>, and SL-ReIrGe<sub>2</sub>S<sub>6</sub>.

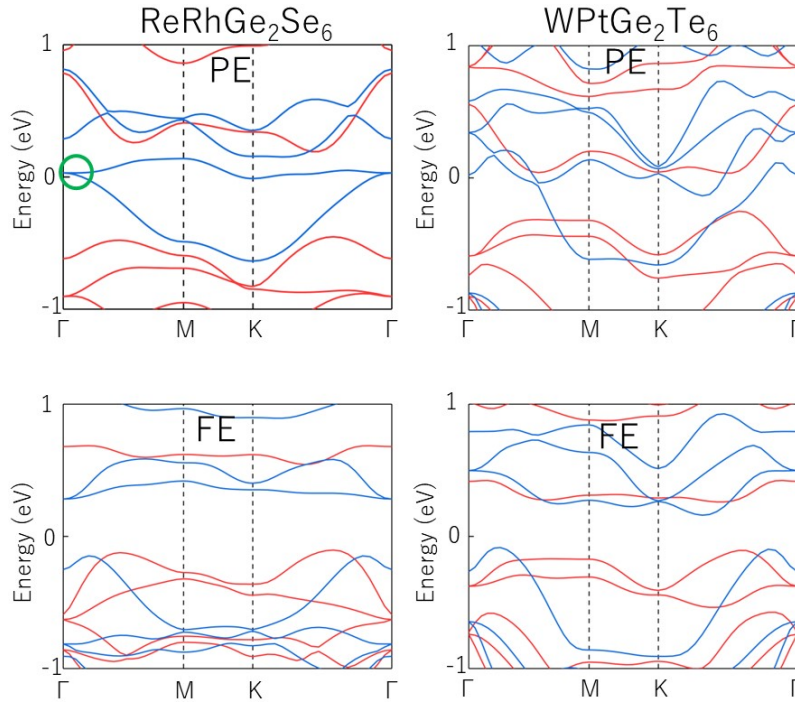
2D multiferroic materials		Spin-up			Spin-down		
		#K <sub>2↑</sub> <sup>3</sup>	#Γ <sub>2↑</sub> <sup>3</sup>	Q <sub>c↑</sub> <sup>(3)</sup>	#K <sub>2↓</sub> <sup>3</sup>	#Γ <sub>2↓</sub> <sup>3</sup>	Q <sub>c↓</sub> <sup>(3)</sup>
ReBiGe <sub>2</sub> S <sub>6</sub>	PE	14	15	2e/3	-	-	-
	FE	-	-	-	-	-	-
WIrGe <sub>2</sub> S <sub>6</sub>	PE	-	-	-	12	13	2e/3
	FE	-	-	-	12	13	2e/3
TcIrGe <sub>2</sub> S <sub>6</sub>	PE	13	15	e/3	-	-	-
	FE	13	15	e/3	13	14	2e/3

TcIrGe <sub>2</sub> Se <sub>6</sub>	PE	14	15	2e/3	-	-	-
	FE	14	15	2e/3	12	13	2e/3

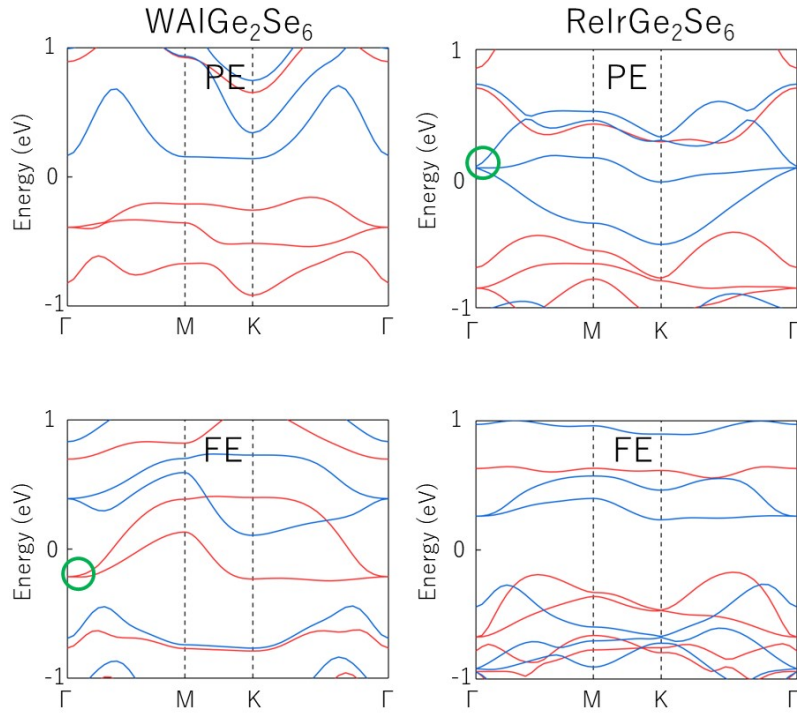
ReIrGe <sub>2</sub> S <sub>6</sub>	K <sub>1</sub>	K <sub>2</sub>	K <sub>1</sub> '	K <sub>2</sub> '	Q <sub>conner</sub>
Spin-up	-2	0	-	-	e/3
Spin-dn	-2	0	-	-	e/3



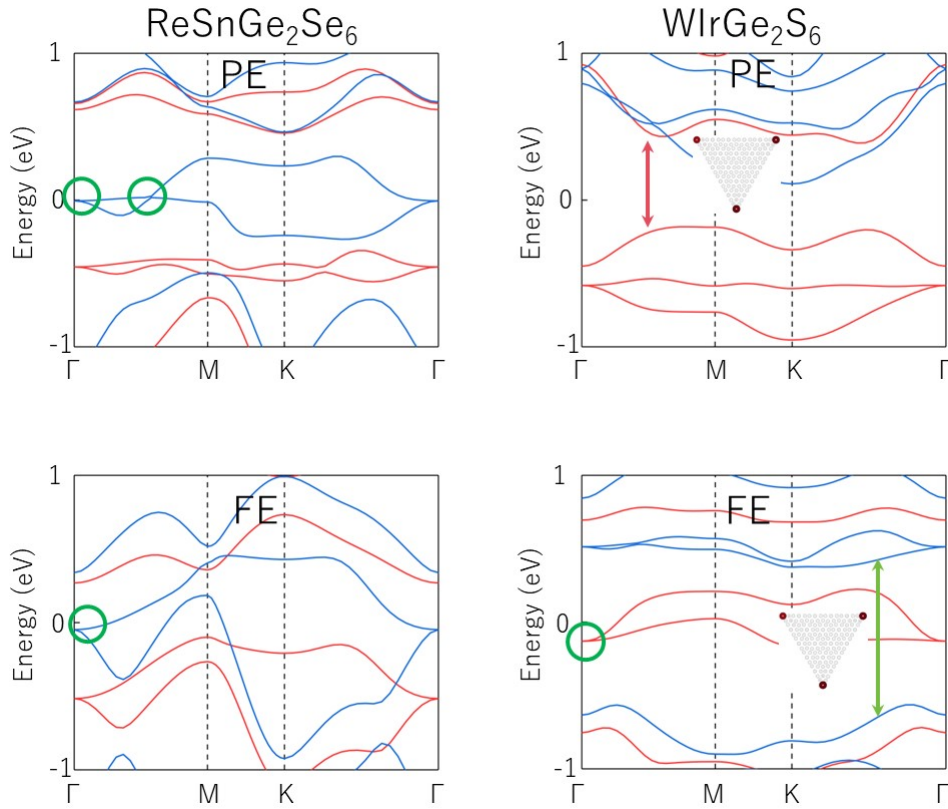
**Fig. S 1** Electronic band structures of PE and FE phases for ReBiGe<sub>2</sub>S<sub>6</sub> and ReAlGe<sub>2</sub>Se<sub>6</sub>.



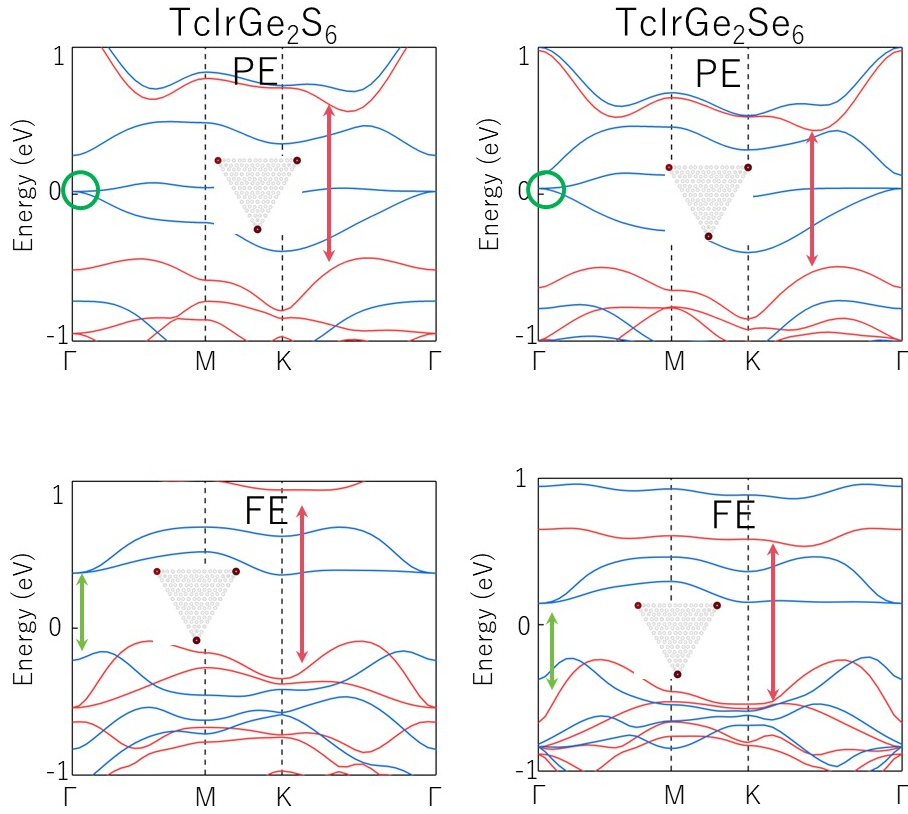
**Fig. S 2** Electronic band structures of PE and FE phases for ReRhGe<sub>2</sub>Se<sub>6</sub> and WPtGe<sub>2</sub>Te<sub>6</sub>.



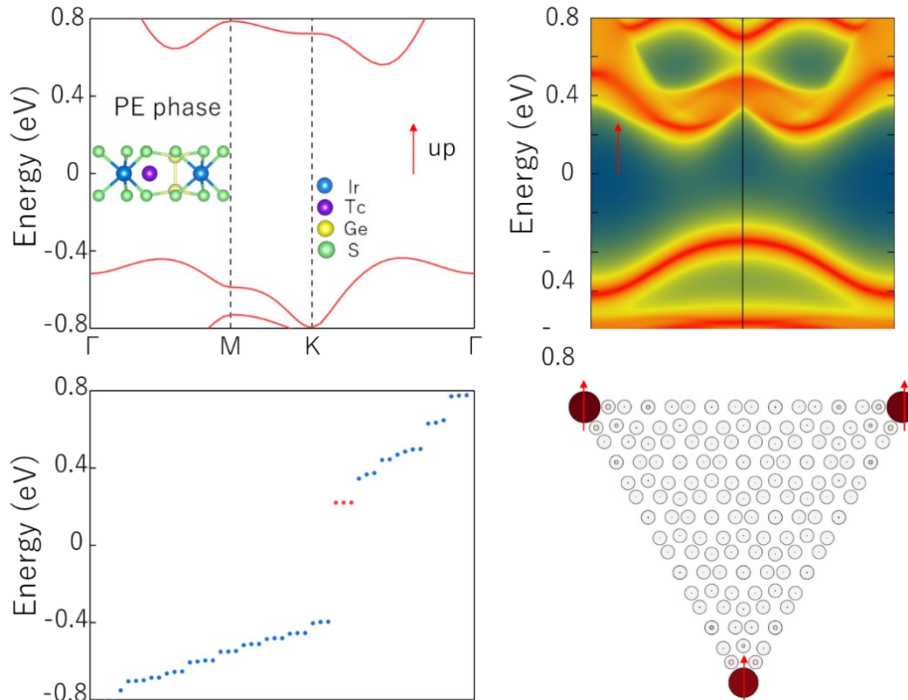
**Fig. S 3** Electronic band structures of PE and FE phases for  $\text{WAIGe}_2\text{Se}_6$  and  $\text{ReIrGe}_2\text{Se}_6$ .



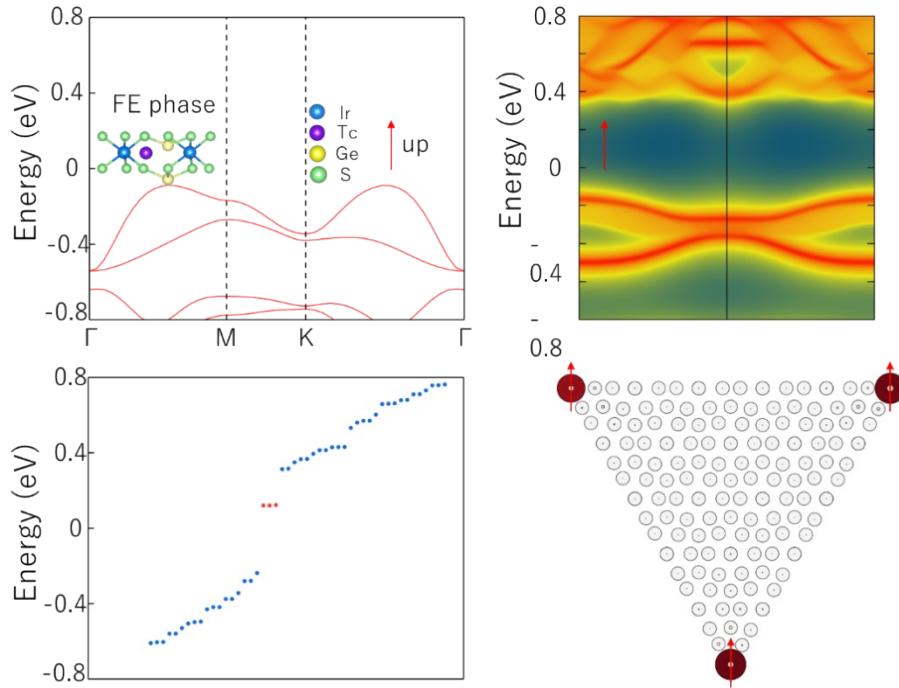
**Fig. S 4** Electronic band structures of PE and FE phases for  $\text{ReSnGe}_2\text{Se}_6$  and  $\text{WIrGe}_2\text{S}_6$ .



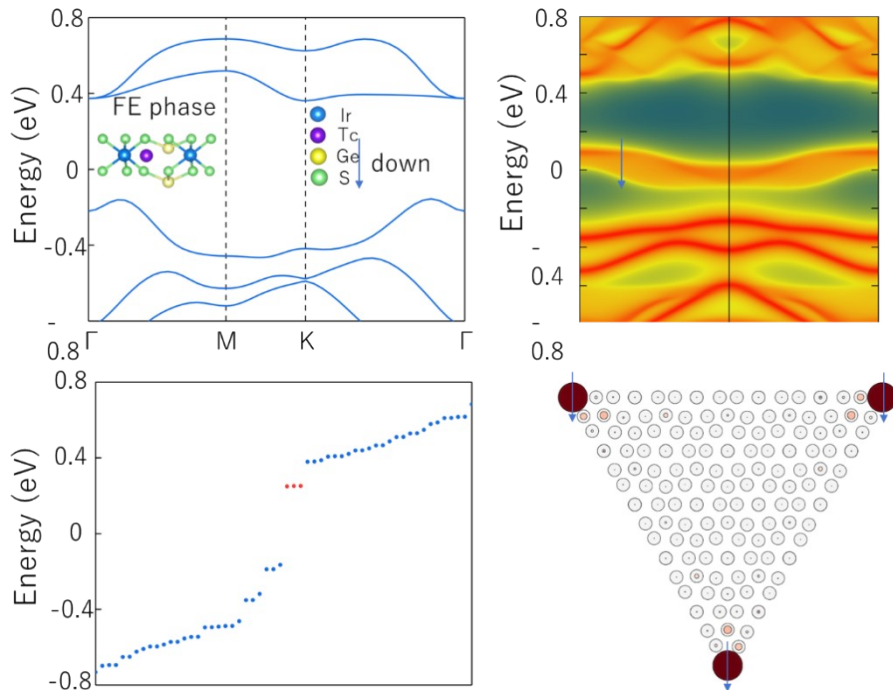
**Fig. S 5** Electronic band structures of PE and FE phases for  $\text{TcIrGe}_2\text{S}_6$  and  $\text{TcIrGe}_2\text{Se}_6$ .



**Fig. S 6** (a) Electronic band structures of PE phases in spin-up channel for  $\text{TcIrGe}_2\text{S}_6$ . (b) Projected spectrum in spin-up channel for  $\text{TcIrGe}_2\text{S}_6$ . (c) The corresponding energy levels in spin-up channel for  $\text{TcIrGe}_2\text{S}_6$ . (d) The charge distribution of the finite-sized nanodisks.

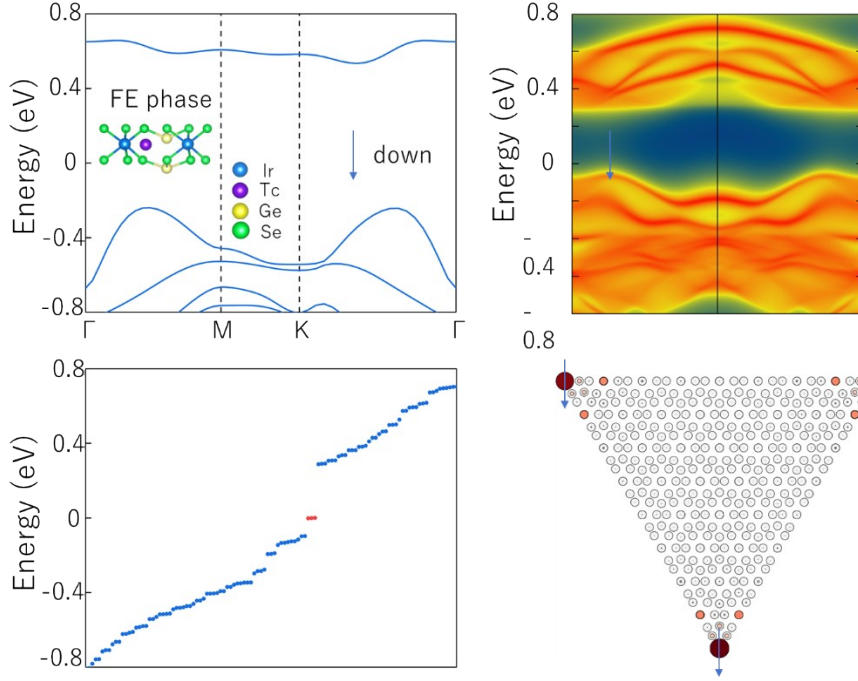


**Fig. S 7** (a) Electronic band structures of FE phases in spin-up channel for  $\text{TcIrGe}_2\text{S}_6$ . (b) Projected spectrum in spin-up channel for  $\text{TcIrGe}_2\text{S}_6$ . (c) The corresponding energy levels in spin-up channel for  $\text{TcIrGe}_2\text{S}_6$ . (d) The charge distribution of the finite-sized nanodisks.

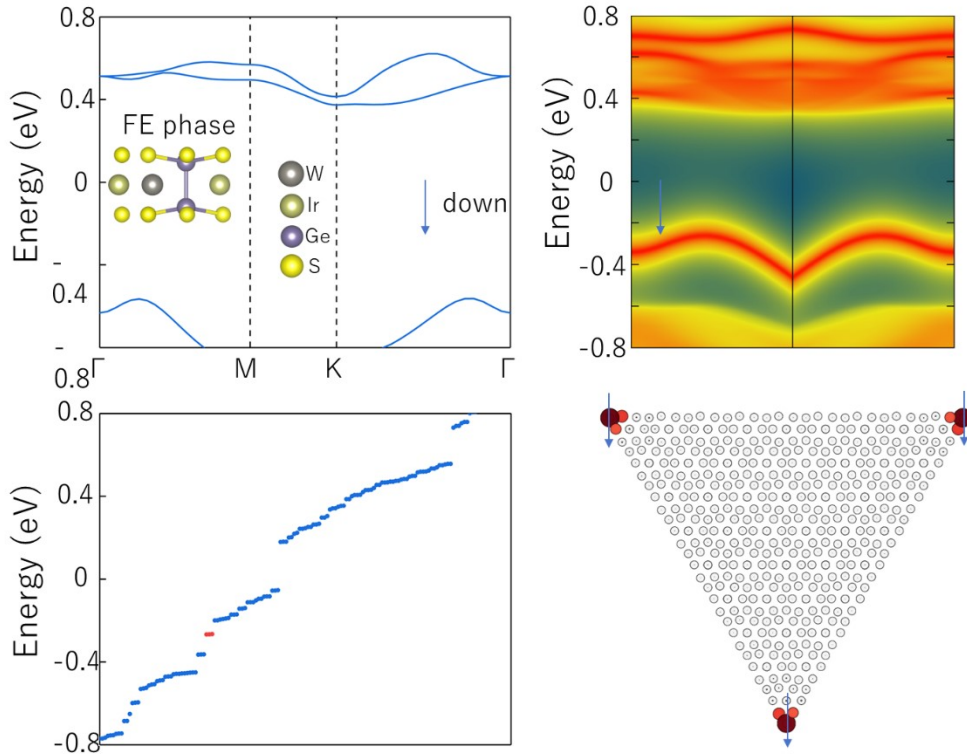


**Fig. S 8** (a) Electronic band structures of FE phases in spin-down channel for  $\text{TcIrGe}_2\text{S}_6$ . (b) Projected spectrum in spin-down channel for  $\text{TcIrGe}_2\text{S}_6$ . (c) The corresponding energy levels in spin-down channel for  $\text{TcIrGe}_2\text{S}_6$ . (d) The charge distribution of the finite-sized nanodisks.

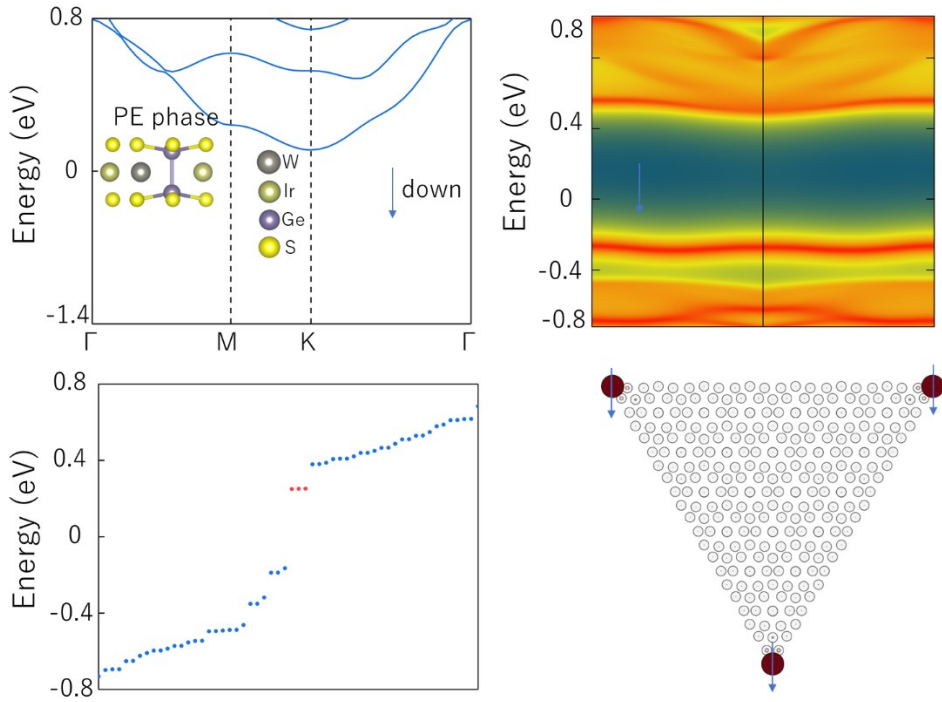




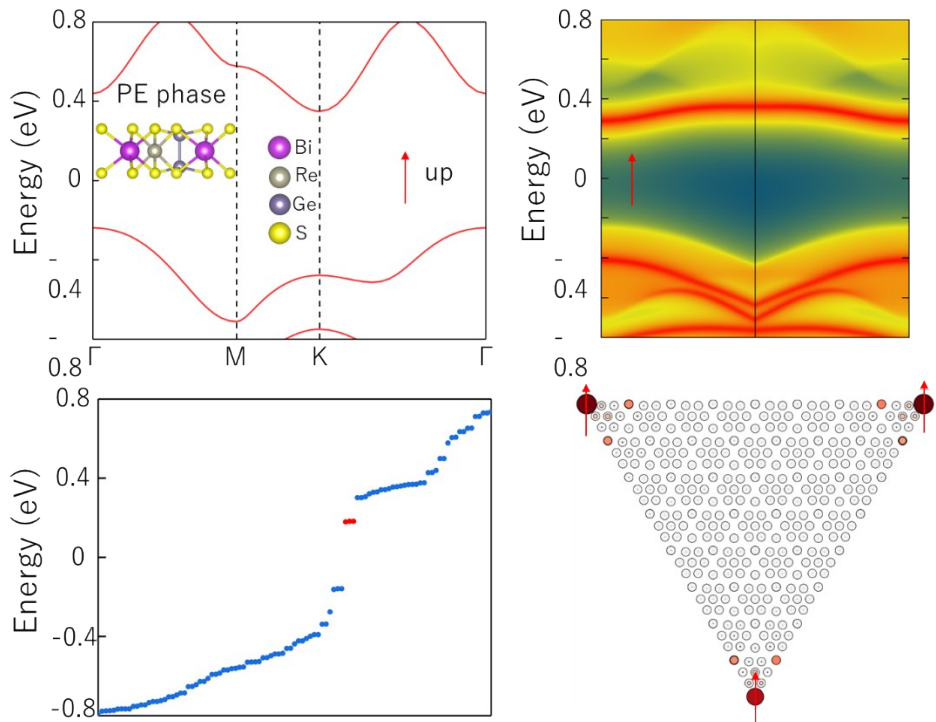
**Fig. S 9** (a) Electronic band structures of FE phases in spin-down channel for  $\text{TcIrGe}_2\text{Se}_6$ . (b) Projected spectrum in spin-down channel for  $\text{TcIrGe}_2\text{Se}_6$ . (c) The corresponding energy levels in spin-down channel for  $\text{TcIrGe}_2\text{Se}_6$ . (d) The charge distribution of the finite-sized nanodisks.



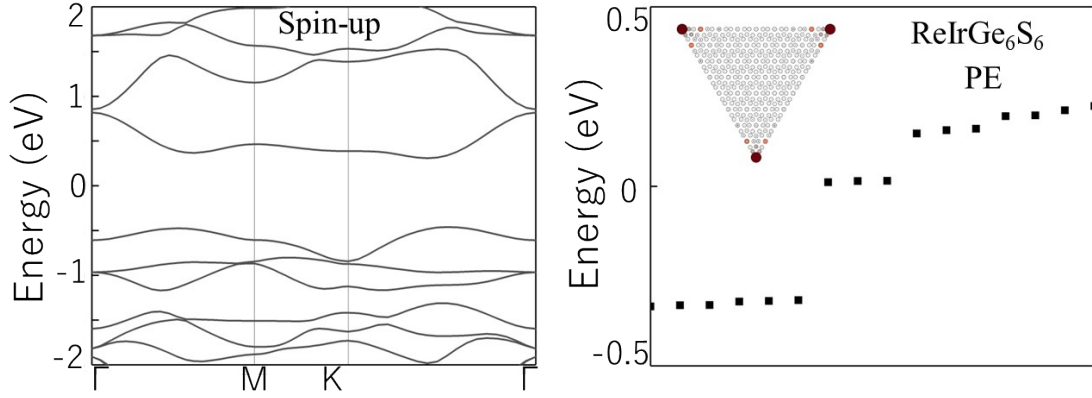
**Fig. S 10** (a) Electronic band structures of FE phases in spin-down channel for  $\text{WIrGe}_2\text{S}_6$ . (b) Projected spectrum in spin-down channel for  $\text{WIrGe}_2\text{S}_6$ . (c) The corresponding energy levels in spin-down channel for  $\text{WIrGe}_2\text{S}_6$ . (d) The charge distribution of the finite-sized nanodisks.



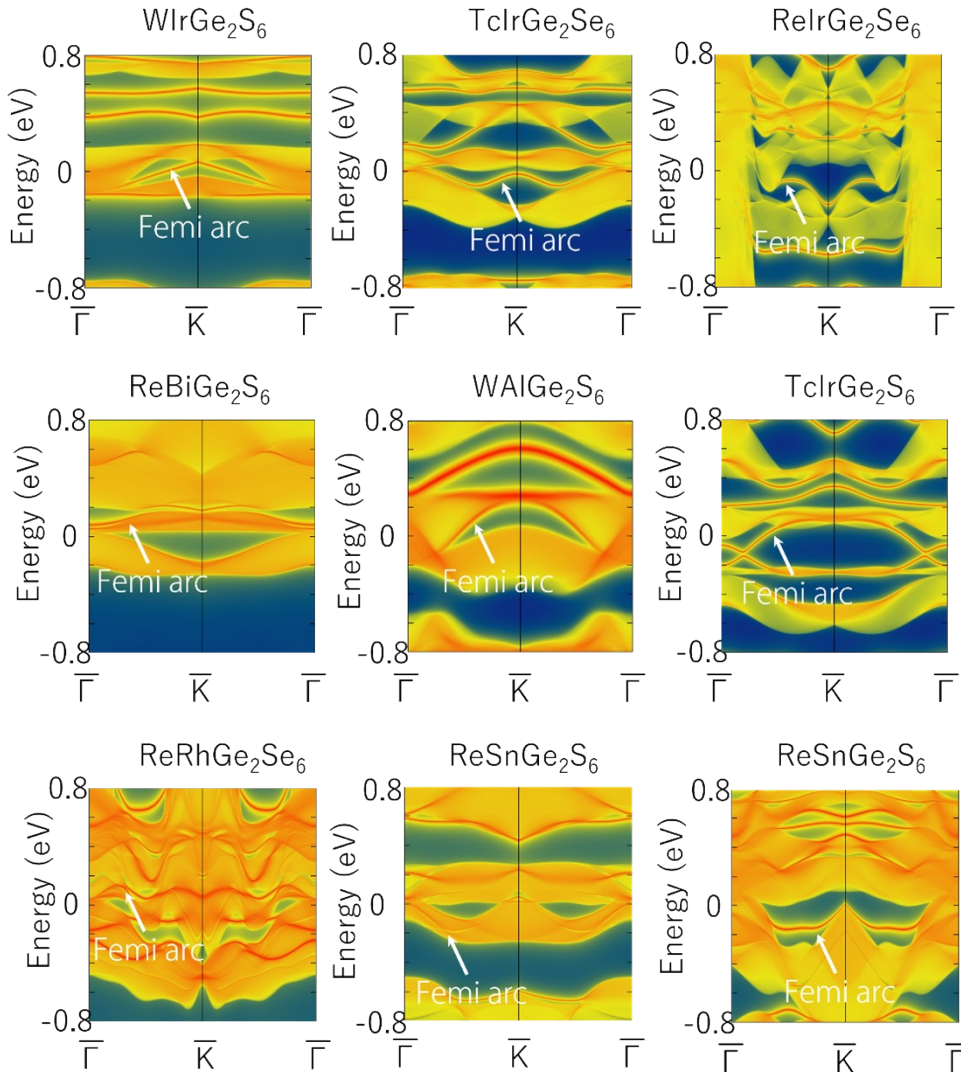
**Fig. S 11** (a) Electronic band structures of PE phases in spin-down channel for  $\text{WIrGe}_2\text{S}_6$ . (b) Projected spectrum in spin-down channel for  $\text{WIrGe}_2\text{S}_6$ . (c) The corresponding energy levels in spin-down channel for  $\text{WIrGe}_2\text{S}_6$ . (d) The charge distribution of the finite-sized nanodisks.



**Fig. S 12** (a) Electronic band structures of PE phases in spin-up channel for  $\text{ReBiGe}_2\text{S}_6$ . (b) Projected spectrum in spin-up channel for  $\text{ReBiGe}_2\text{S}_6$ . (c) The corresponding energy levels in spin-down channel for  $\text{ReBiGe}_2\text{S}_6$ . (d) The charge distribution of the finite-sized nanodisks.



**Fig. S 13** (a) Electronic band structures of PE phases in spin-up channel for  $\text{ReIrGe}_2\text{S}_6$ . (b) The corresponding energy levels in spin-up channel for  $\text{ReIrGe}_2\text{S}_6$ , and the charge distribution of the finite-sized nanodisks.



**Fig. S 14.** The band projections along the (100) direction for the  $\text{M}_I\text{M}_{II}\text{Ge}_2\text{X}_6$  family with Weyl points. Among them, the last two band projections are the edge states of PE and FE phases for  $\text{ReSnGe}_2\text{S}_6$ .

