

Tunable electronic structures upon Janus $\text{In}_2\text{Ge}_2\text{X}_3\text{Y}_3$ (X, Y =S, Se and Te) monolayers by external fields

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Table S1. The Mulliken charge distributions of monolayer $\text{In}_2\text{Ge}_2\text{S}_3\text{Se}_3$

Biaxial strain	Mulliken charge distributions e				
	In	Ge1	Ge2	S	Se
-8%	0.63	0.43	0.24	-0.39	-0.25
-6%	0.64	0.44	0.23	-0.4	-0.25
-4%	0.64	0.44	0.23	-0.4	-0.25
-2%	0.65	0.46	0.28	-0.42	-0.27
0%	0.66	0.47	0.32	-0.42	-0.28
2%	0.65	0.48	0.31	-0.42	-0.27
4%	0.65	0.49	0.32	-0.43	-0.27
6%	0.63	0.49	0.37	-0.43	-0.28
8%	0.56	0.62	0.22	-0.44	-0.21

Table S2. The Mulliken charge distributions of monolayer $\text{In}_2\text{Ge}_2\text{S}_3\text{Te}_3$

Biaxial strain	Mulliken charge distributions e				
	In	Ge1	Ge2	S	Te
-8%	0.50	0.47	0.24	-0.43	-0.14
-6%	0.48	0.46	0.15	-0.4	-0.12
-4%	0.49	0.47	0.16	-0.41	-0.13
-2%	0.51	0.48	0.18	-0.42	-0.14
0%	0.50	0.49	0.23	-0.42	-0.15
2%	0.51	0.48	0.21	-0.43	-0.14
4%	0.51	0.48	0.22	-0.43	-0.14
6%	0.50	0.47	0.23	-0.43	-0.14
8%	0.56	0.62	0.22	-0.44	-0.21

Table S3. The Mulliken charge distributions of monolayer $\text{In}_2\text{Ge}_2\text{Se}_3\text{Te}_3$

Biaxial strain	Mulliken charge distributions e				
	In	Ge1	Ge2	Se	Te
-8%	0.33	0.40	0.12	-0.28	-0.11
-6%	0.34	0.42	0.13	-0.29	-0.12
-4%	0.35	0.43	0.14	-0.30	-0.13
-2%	0.35	0.44	0.14	-0.30	-0.13
0%	0.33	0.44	0.13	-0.30	-0.12
2%	0.35	0.44	0.15	-0.30	-0.12
4%	0.35	0.40	0.17	-0.30	-0.12
6%	0.36	0.40	0.16	-0.30	-0.12
8%	0.36	0.39	0.17	-0.30	-0.12

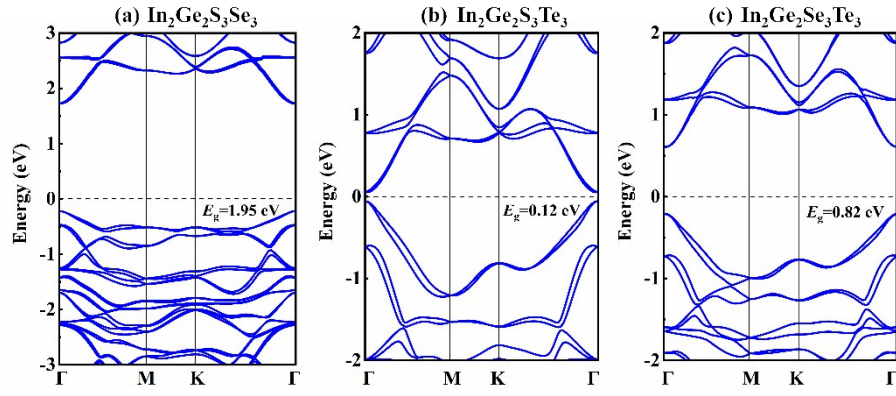


Fig. S1 Electronic band structures of monolayer $\text{In}_2\text{Ge}_2\text{X}_3\text{Y}_3$ using the HSE06 hybrid functional with SOC. The Fermi level is set to zero presented by the black dash line.

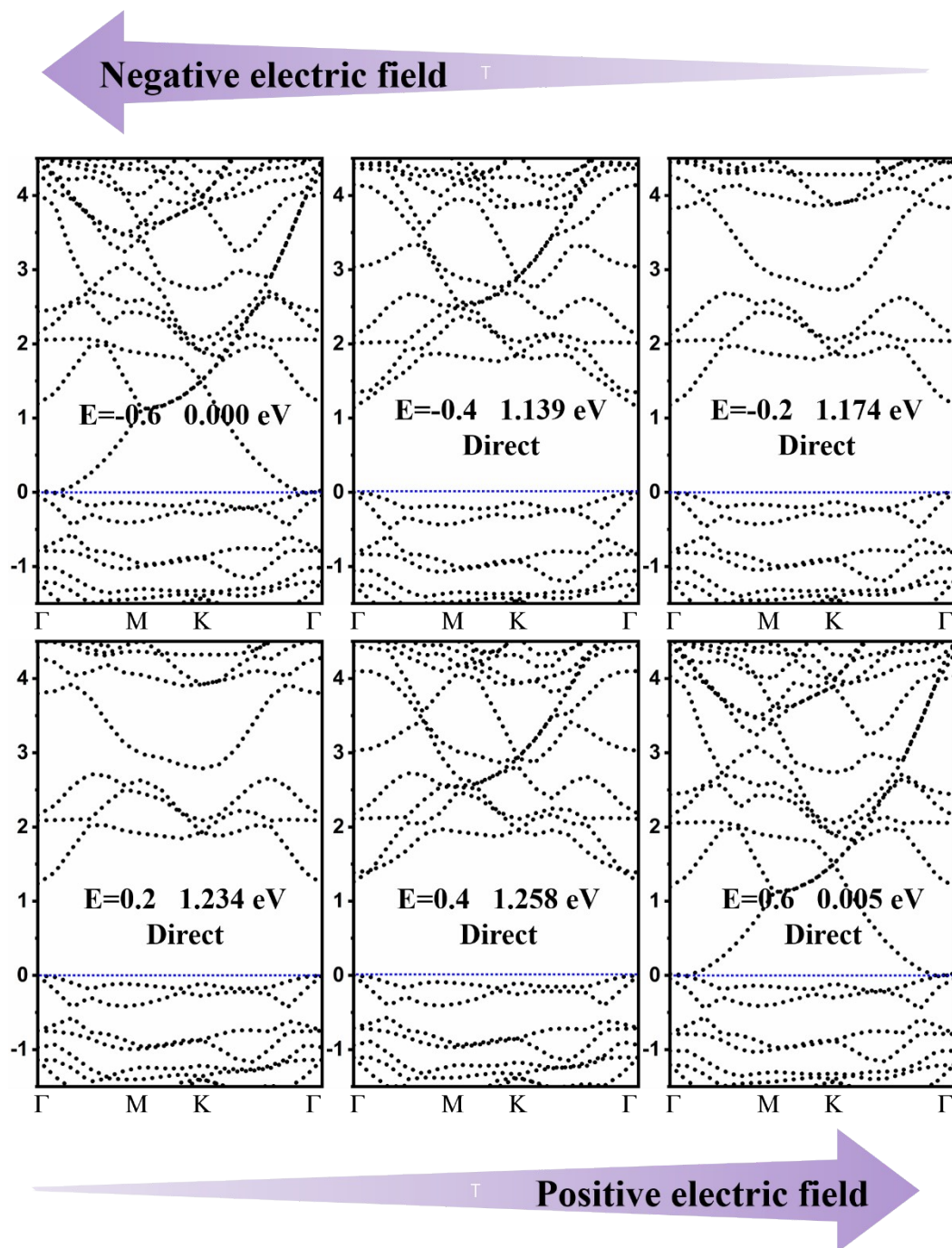


Fig. S2 Electronic band structures of monolayer $\text{In}_2\text{Ge}_2\text{S}_3\text{Se}_3$ with various electric fields using the PBE functional. The Fermi level is set to zero presented by the blue dash line.

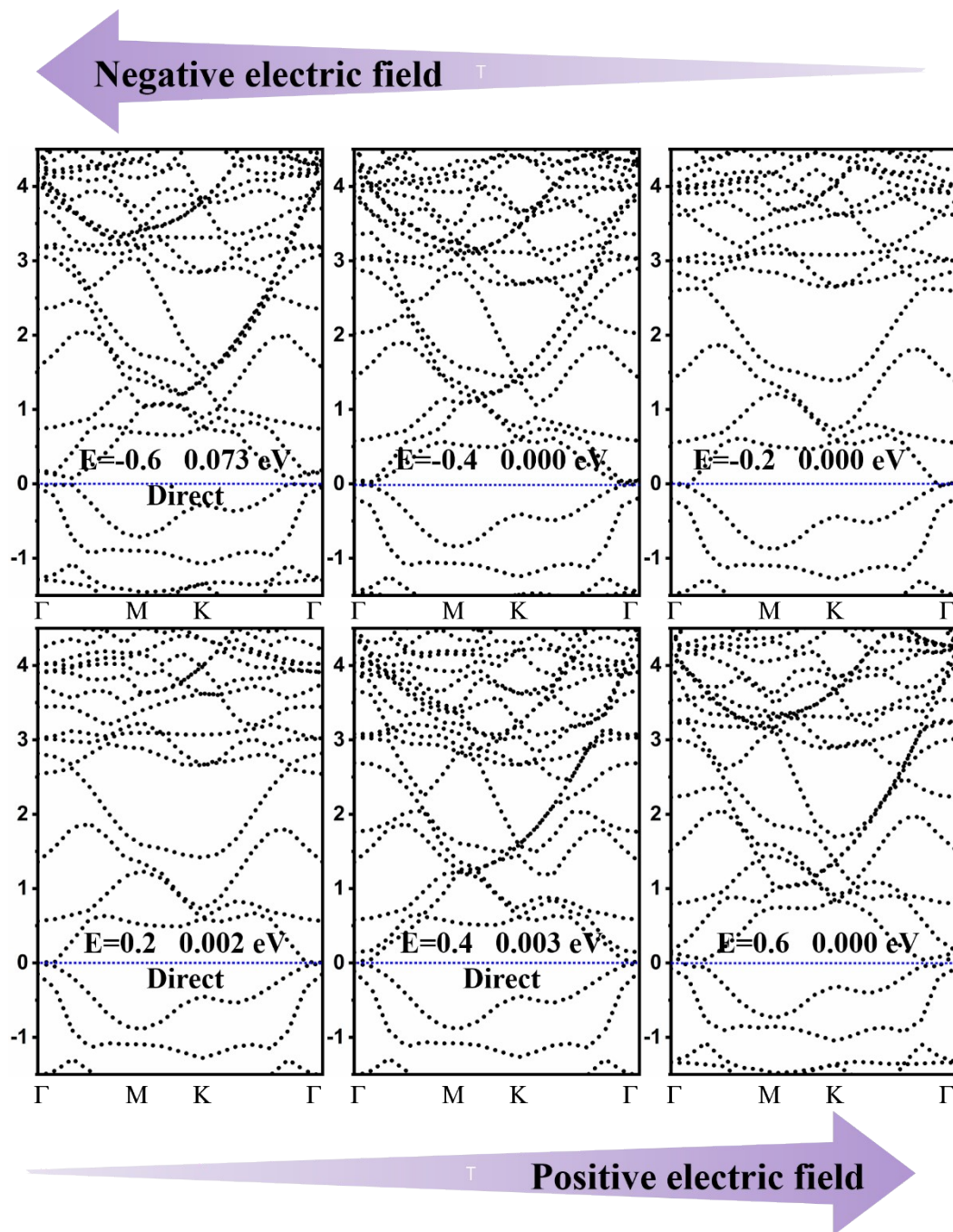


Fig. S3 Electronic band structures of monolayer $\text{In}_2\text{Ge}_2\text{S}_3\text{Te}_3$ with various electric fields using the PBE functional. The Fermi level is set to zero presented by the blue dash line.

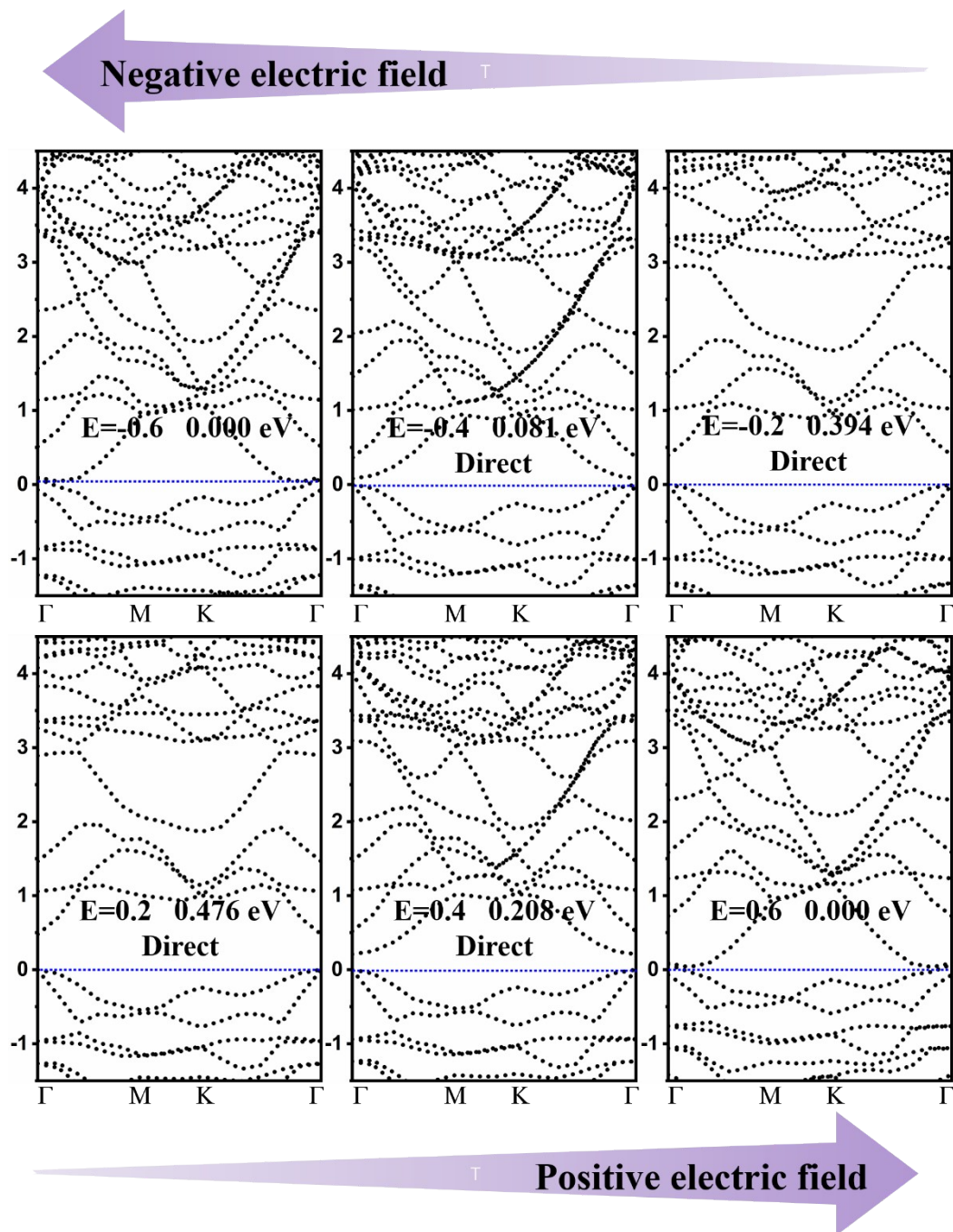


Fig. S4 Electronic band structures of monolayer $\text{In}_2\text{Ge}_2\text{Se}_3\text{Te}_3$ with various electric fields using the PBE functional. The Fermi level is set to zero presented by the blue dash line.

Table S4. The Mulliken charge distributions of monolayer $\text{In}_2\text{Ge}_2\text{S}_3\text{Se}_3$

Electric field (eV/Å/e)	Mulliken charge distributions e				
	In	Ge1	Ge2	S	Se
-0.6	0.69	0.26	0.30	-0.44	-0.21
-0.4	0.64	0.46	0.30	-0.44	-0.24
-0.2	0.64	0.46	0.30	-0.43	-0.25
0	0.65	0.46	0.28	-0.42	-0.27
0.2	0.65	0.47	0.31	-0.41	-0.29
0.4	0.65	0.48	0.31	-0.40	-0.30
0.6	0.66	0.48	0.50	-0.37	-0.39

Table S5. The Mulliken charge distributions of monolayer $\text{In}_2\text{Ge}_2\text{S}_3\text{Te}_3$

Electric field (eV/Å/e)	Mulliken charge distributions e				
	In	Ge1	Ge2	S	Te
-0.6	0.66	0.03	0.21	-0.44	-0.07
-0.4	0.54	0.36	0.21	-0.45	-0.11
-0.2	0.51	0.47	0.21	-0.44	-0.13
0	0.50	0.49	0.23	-0.42	-0.15
0.2	0.52	0.48	0.21	-0.42	-0.17
0.4	0.53	0.49	0.22	-0.40	-0.19
0.6	0.55	0.47	0.58	-0.38	-0.32

Table S6. The Mulliken charge distributions of monolayer $\text{In}_2\text{Ge}_2\text{Se}_3\text{Te}_3$

Electric field (eV/Å/e)	Mulliken charge distributions e				
	In	Ge1	Ge2	Se	Te
-0.6	0.36	0.68	0.14	-0.46	-0.03
-0.4	0.34	0.48	0.15	-0.35	-0.09
-0.2	0.34	0.45	0.15	-0.32	-0.11
0	0.33	0.44	0.13	-0.30	-0.12
0.2	0.34	0.44	0.15	-0.28	-0.15
0.4	0.34	0.44	0.16	-0.26	-0.17
0.6	0.35	0.43	0.45	-0.23	-0.29