Supplementary Material: High-throughput computational screening of 2D materials for thermoelectrics

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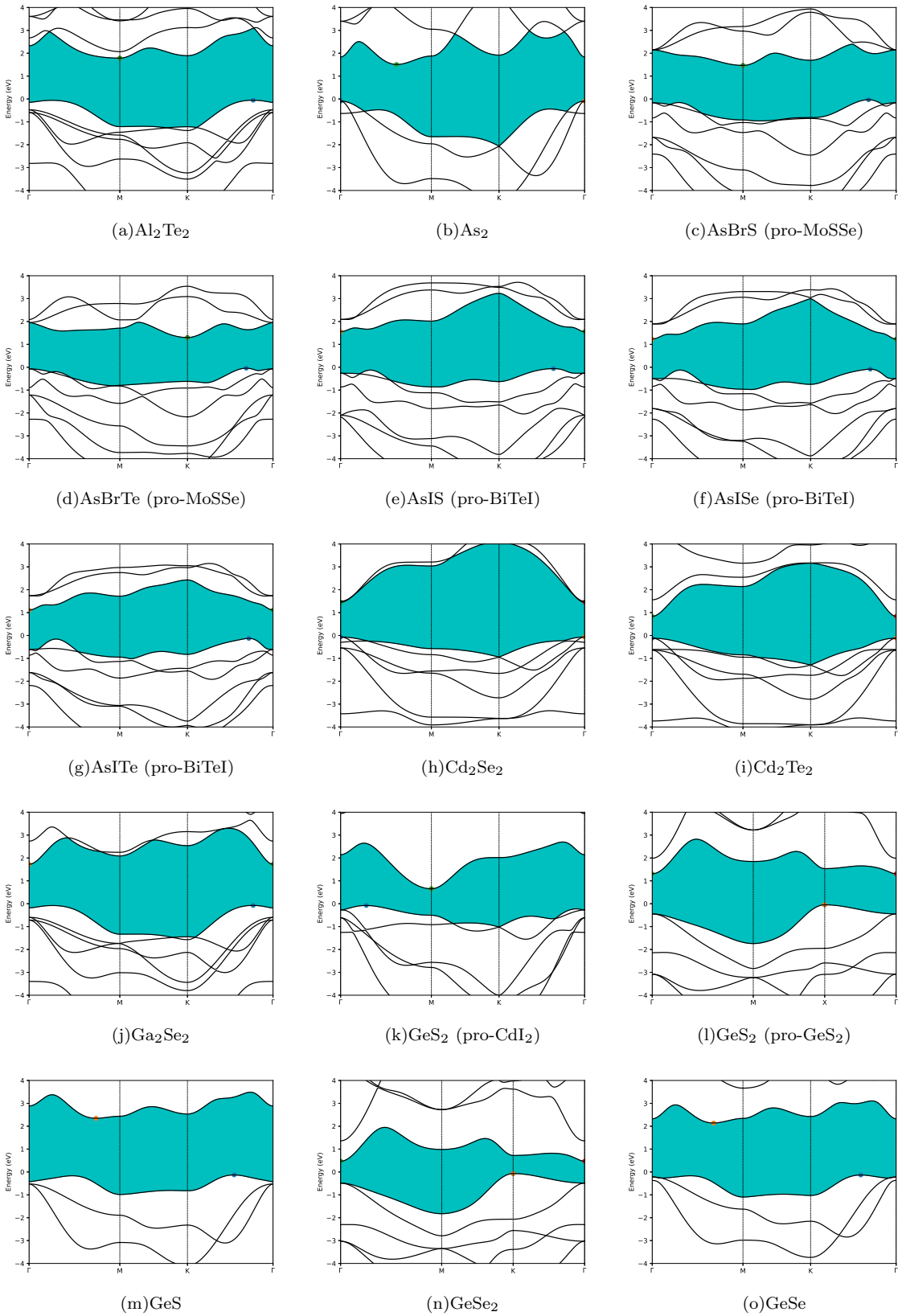
Table S1. Structural information, lattice parameters and energy band gap (E_{gap}) values of 2D isotropic materials. "D" and "ID" stand for direct and indirect energy bands, respectively.

Prototype	Material	Structure	Phase	a (Å)	E_g (eV)
pro-GaS	Al_2Te_2	P$\bar{6}$m2	-	4.12	1.84 (ID)
pro-C	As_2	P$\bar{3}$m1	Xene	3.60	1.60 (ID)
pro-MoSSe	AsBrS	P3m1	MXY Janus	3.62	1.50 (ID)
pro-MoSSe	AsBrTe	P3m1	2H	3.88	1.34 (ID)
pro-BiTeI	AsIS	P3m1	MXY Janus		1.61 (ID)
pro-BiTeI	AsISe	P3m1	MXY Janus	3.93	1.32 (ID)
pro-BiTeI	AsITe	P3m1	MXY Janus	4.08	1.24 (ID)
pro-CH	Cd_2Se_2	P$\bar{1}$	-	4.45	1.52 (D)
pro-CH	Cd_2Te_2	P$\bar{1}$	-	4.67	0.95 (D)
pro-GaS	Ga_2Se_2	P$\bar{6}$m2	-	3.82	1.8 (ID)
pro-CdI_2	GeS_2	P$\bar{3}$m1	1T	3.45	0.73 (ID)
pro-GeS_2	GeS_2	P$\bar{4}$m2	-	3.52	1.56 (ID)
pro-GeSe	GeS	P3m1	-	3.49	2.47 (ID)
pro-GeS_2	$GeSe_2$	P$\bar{4}$m2	-	3.72	0.54 (ID)
pro-GeSe	GeSe	P3m1	-	3.67	2.27 (ID)
pro-GeSe	GeTe	P3m1	-	3.96	1.78 (ID)
pro-Ti_2CO_2	Hf_2CO_2	P$\bar{3}$m1	MXene	3.26	1.02 (ID)
pro-MoS_2	$HfBr_2$	P$\bar{6}$m2	2H	3.49	0.86 (ID)
pro-MoS_2	$HfCl_2$	P$\bar{6}$m2	2H	3.34	1.01 (ID)
pro-MoS_2	HfI_2	P$\bar{6}$m2	2H	3.76	0.78 (ID)
pro-CdI_2	HfS_2	P$\bar{3}$m1	1T	3.64	1.28 (ID)
pro-BiTeI	HfSSe	P3m1	MXY Janus	3.69	0.81 (ID)
pro-CdI_2	$HfSe_2$	P$\bar{3}$m1	1T	3.76	0.60 (ID)
pro-MoS_2	$HfTe_2$	P$\bar{6}$m2	2H	3.90	0.38 (ID)
pro-MoSSe	ISbSe	P3m1	MXY Janus	4.05	1.27 (ID)
pro-MoSSe	ISbTe	P3m1	MXY Janus	4.19	1.21 (ID)
pro-MoS_2	MoS_2	P$\bar{6}$m2	2H	3.18	1.67 (D)
pro-MoS_2	$MoSe_2$	P$\bar{6}$m2	2H	3.32	1.44 (D)
pro-CdI_2	NiS_2	P$\bar{3}$m1	1T	3.35	0.60 (ID)
pro-PbS	Pb_2Se_2	Pmn2_1	-	4.40	1.27 (ID)
pro-CdI_2	PdS_2	P$\bar{3}$m1	1T	3.55	1.26 (ID)
pro-CdI_2	$PdSe_2$	P$\bar{3}$m1	1T	3.73	0.72 (ID)
pro-CdI_2	PtS_2	P$\bar{3}$m1	1T	3.57	1.81 (ID)
pro-CdI_2	$PtSe_2$	P$\bar{3}$m1	1T	3.75	1.40 (ID)
pro-CdI_2	$PtTe_2$	P$\bar{3}$m1	1T	4.02	0.76 (ID)
pro-CdI_2	$SnSe_2$	P$\bar{3}$m1	1T	3.87	0.79 (ID)
pro-GeSe	SnTe	P3m1	-	4.18	1.89 (ID)
pro-Ti_2CO_2	Ti_2CO_2	P$\bar{3}$m1	MXene	3.03	0.26 (ID)
pro-MoS_2	WS_2	P$\bar{6}$m2	2H	3.18	1.81 (D)
pro-MoS_2	WSe_2	P$\bar{6}$m2	2H	3.31	1.54 (D)
pro-CH	Zn_2Se_2	P$\bar{1}$	-	4.08	1.74 (D)
pro-CH	Zn_2Te_2	P$\bar{1}$	-	4.33	0.87 (D)
pro-Ti_2CO_2	Zr_2CO_2	P$\bar{3}$m1	MXene	3.31	0.97 (ID)
pro-CdI_2	ZrS_2	P$\bar{3}$m1	1T	3.68	1.20 (ID)
pro-BiTeI	ZrSSe	P3m1	MXY Janus	3.74	0.73 (ID)
pro-CdI_2	$ZrSe_2$	P$\bar{3}$m1	1T	3.80	0.50 (ID)

Table S2. Structural information, lattice parameters and energy band gap (E_{gap}) values of 2D anisotropic materials. "D" and "ID" stand for direct and indirect energy bands, respectively.

Prototype	Material	Structure	Phase	a (Å)	b (Å)	E_g (eV)
pro-AuSe	Ag_2S_2	Pm	-	3.57	6.08	0.98 (ID)
pro-AuSe	Ag_2Se_2	Pm	-	3.76	5.99	0.86 (ID)
pro-AuSe	Ag_2Te_2	Pm	-	4.09	6.30	0.65 (ID)
pro-FeOCl	$Al_2Br_2O_2$	Pmmn	-	3.65	3.31	4.17 (ID)
pro-FeOCl	$Al_2Br_2S_2$	Pmmn	-	4.89	3.51	2.28 (D)
pro-FeOCl	$Al_2Br_2Se_2$	Pmmn	-	5.24	3.61	1.54 (ID)
pro-FeOCl	$Al_2Cl_2S_2$	Pmmn	-	4.89	3.40	2.35 (D)
pro-FeOCl	$Al_2I_2S_2$	Pmmn	-	4.85	3.71	1.75 (D)
pro-FeOCl	$Al_2I_2Se_2$	Pmmn	-	5.21	3.79	1.51 (D)
pro-AuSe	Au_2O_2	P2/m	-	3.10	6.07	0.17 (ID)
pro-AuSe	Au_2S_2	P2/m	-	3.54	6.26	1.35 (ID)
pro-AuSe	Au_2Se_2	P2/m	-	3.72	6.35	1.21 (ID)
pro-AuSe	Au_2Te_2	Pm	-	4.01	6.66	0.96 (ID)
pro-AuSe	Cu_2S_2	Pm	-	3.36	5.52	0.63 (ID)
pro-FeOCl	$Ga_2Br_2O_2$	Pmmn	-	3.83	3.41	2.58 (ID)
pro-FeOCl	$Ga_2I_2S_2$	Pmmn	-	5.03	3.75	0.95 (D)
pro-FeOCl	$Hf_2Br_2N_2$	Pmmn	-	4.13	3.57	2.11 (D)
pro-WTe_2	Hf_2Br_4	$P2_1/m$	$1T^{'}$	3.43	6.40	0.85 (D)
pro-FeOCl	$Hf_2Cl_2N_2$	Pmmn	-	4.15	3.49	2.16 (D)
pro-WTe_2	Hf_2Cl_4	$P2_1/m$	$1T^{'}$	3.26	6.13	0.85 (D)
pro-TiS_3	Hf_2O_6	Pmmn	-	3.21	4.07	3.29 (ID)
pro-FeOCl	$Ir_2Cl_2O_2$	Pmmn	-	4.08	3.38	0.44 (ID)
pro-CrW_3S_8	MoW_3S_8	P1	TMDC-Alloy	6.37	5.51	1.76 (D)
pro-PdS_2	Ni_2S_4	$P2_1/c$	-	5.22	5.33	0.82 (ID)
pro-PdS_2	Ni_2Se_4	$P2_1/c$	-	5.50	5.70	1.02 (ID)
pro-PdS_2	Ni_2Te_4	$P2_1/c$	-	5.93	6.24	0.96 (ID)
pro-WTe_2	Os_2O_4	$P2_1/m$	$1T^{'}$	3.18	4.77	0.38 (ID)
pro-WTe_2	Os_2S_4	$P2_1/m$	$1T^{'}$	3.53	5.55	0.70 (ID)
pro-WTe_2	Os_2Se_4	$P2_1/m$	$1T^{'}$	3.67	5.77	0.77 (ID)
pro-WTe_2	Os_2Te_4	$P2_1/m$	$1T^{'}$	3.88	6.13	0.76 (ID)
pro-P	P_4	Pmna	-	3.30	4.62	0.91 (D)
pro-PdS_2	Pd_2S_4	$P2_1/c$	-	5.47	5.57	1.17 (ID)
pro-PdS_2	Pd_2Se_4	$P2_1/c$	-	5.74	5.92	1.36 (ID)
pro-PdS_2	Pd_2Te_4	$P2_1/c$	-	6.14	6.43	1.27 (D)
pro-PdS_2	Pt_2Te_4	$P2_1/c$	-	6.11	6.41	1.38 (ID)
pro-WTe_2	Ru_2S_4	$P2_1/m$	$1T^{'}$	3.45	5.56	0.79 (ID)
pro-WTe_2	Ru_2Se_4	$P2_1/m$	$1T^{'}$	3.60	5.79	0.83 (ID)
pro-WTe_2	Ru_2Te_4	$P2_1/m$	$1T^{'}$	3.82	6.15	0.69 (ID)
pro-FeOCl	$Sc_2Br_2Se_2$	Pmmn	-	5.37	3.82	1.53 (ID)
pro-FeOCl	$Sc_2Cl_2Se_2$	Pmmn	-	5.37	3.74	1.37 (ID)
pro-FeOCl	$Sc_2I_2S_2$	Pmmn	-	5.08	3.90	1.71 (D)
pro-FeOCl	$Sc_2I_2Se_2$	Pmmn	-	5.37	3.96	1.47 (ID)
pro-WTe_2	Zr_2Br_4	$P2_1/m$	$1T^{'}$	3.50	6.50	0.58 (ID)
pro-WTe_2	Zr_2Cl_4	$P2_1/m$	$1T^{'}$	3.34	6.24	0.59 (D)
pro-TiS_3	Zr_2O_6	Pmmn	-	3.26	4.11	3.42 (ID)



(a)Al_2Te_2 (b)As_2 (c)AsBrS (pro-MoSSe)

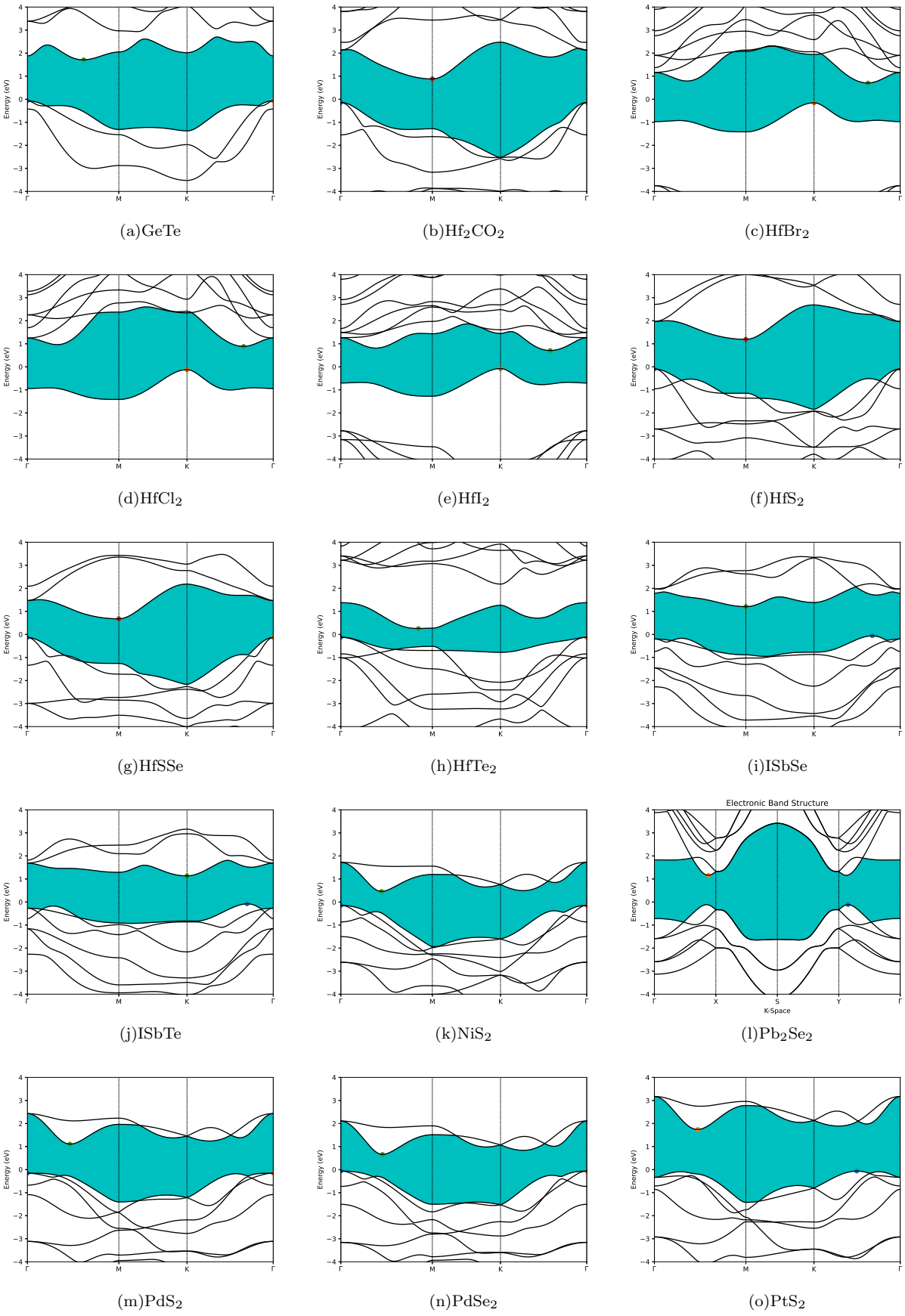
(d)AsBrTe (pro-MoSSe) (e)AsIS (pro-BiTeI) (f)AsISe (pro-BiTeI)

(g)AsITe (pro-BiTeI) (h)Cd_2Se_2 (i)Cd_2Te_2

(j)Ga_2Se_2 (k)GeS_2 (pro-CdI_2) (l)GeS_2 (pro-GeS_2)

(m)GeS (n)$GeSe_2$ (o)GeSe

Figure S1. (Color online) Electronic band structures of isotropic 2D materials



(a)GeTe (b)Hf_2CO_2 (c)$HfBr_2$

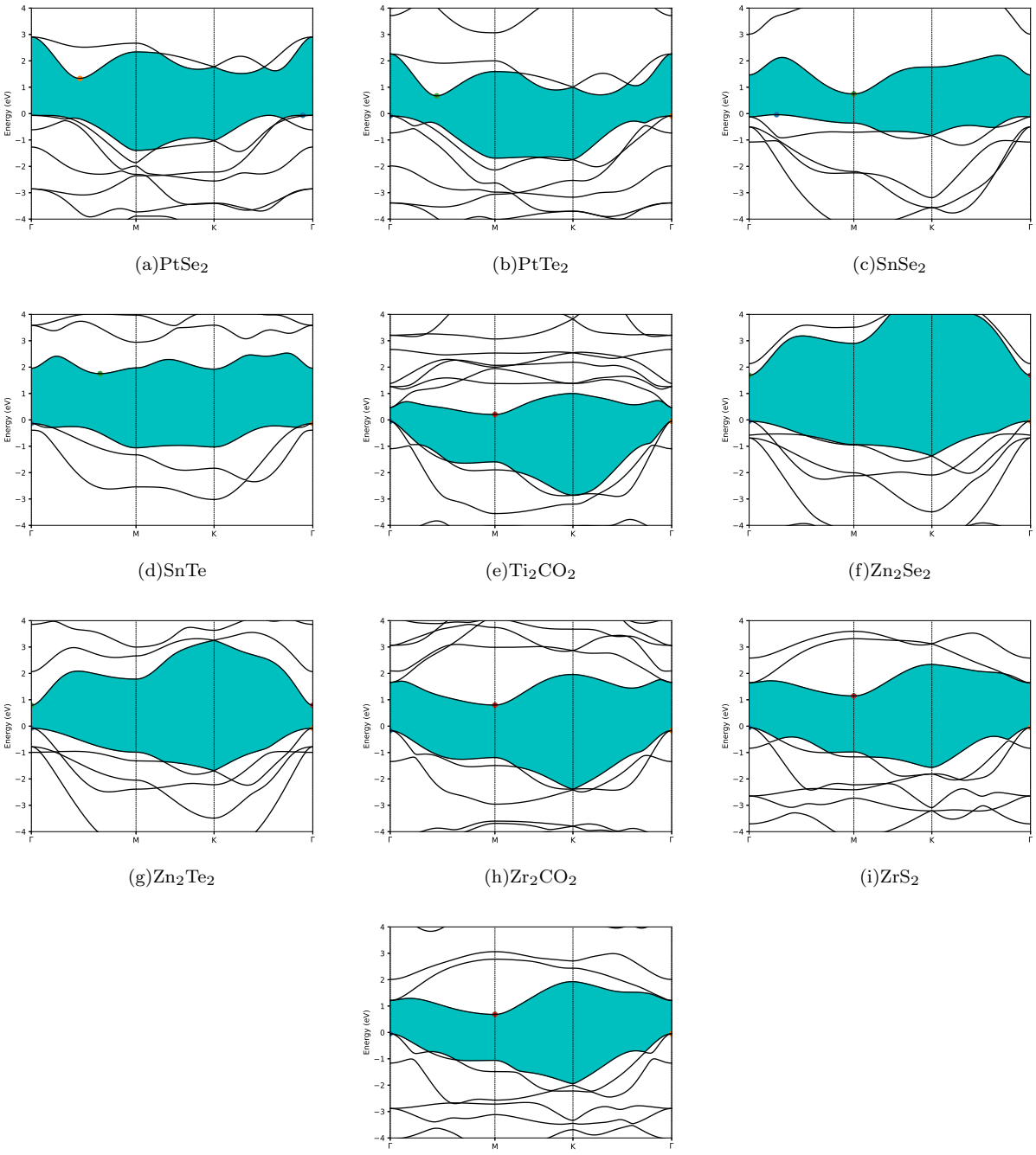
(d)$HfCl_2$ (e)HfI_2 (f)HfS_2

(g)HfSSe (h)$HfTe_2$ (i)ISbSe

(j)ISbTe (k)NiS_2 (l)Pb_2Se_2

(m)PdS_2 (n)$PdSe_2$ (o)PtS_2

Figure S2. (Color online) Electronic band structures of isotropic 2D materials



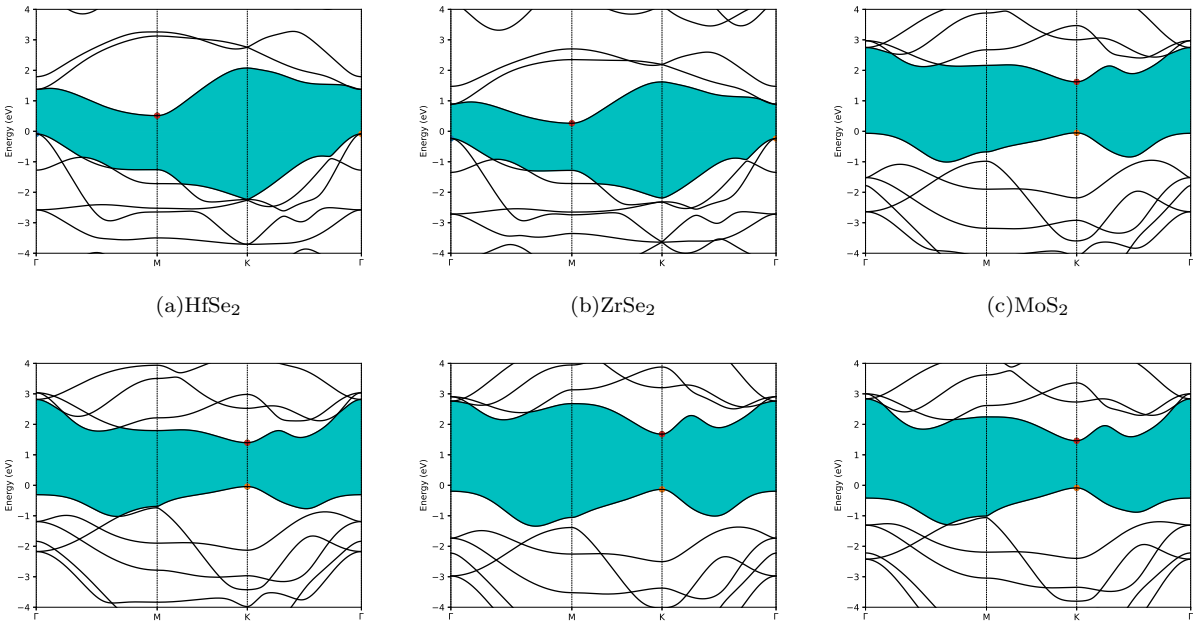
(a)$PtSe_2$ (b)$PtTe_2$ (c)$SnSe_2$

(d)SnTe (e)Ti_2CO_2 (f)Zn_2Se_2

(g)Zn_2Te_2 (h)Zr_2CO_2 (i)ZrS_2

(j)ZrSSe

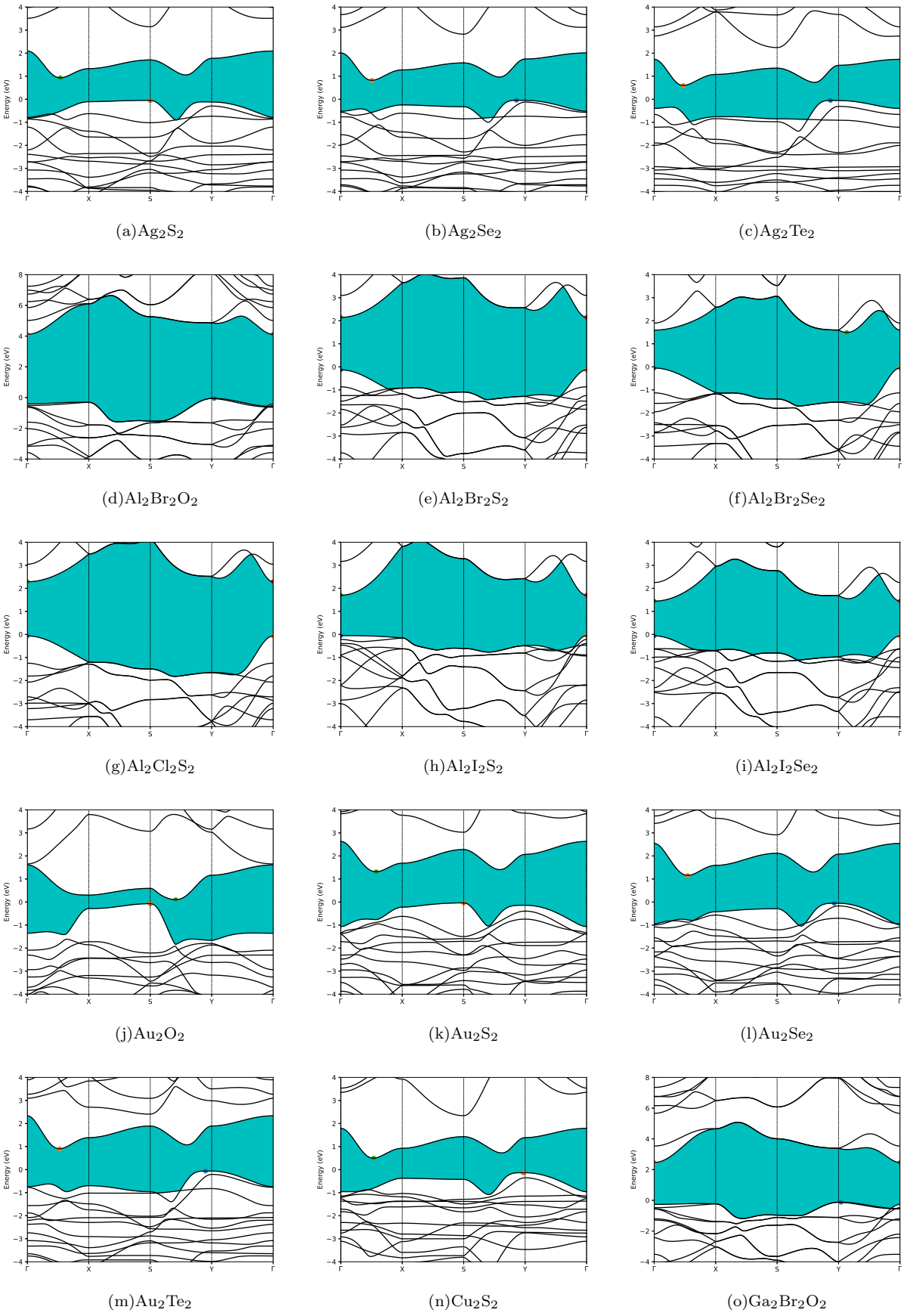
Figure S3. (Color online) Electronic band structures of isotropic 2D materials



(a)$HfSe_2$ (b)$ZrSe_2$ (c)MoS_2

(d)$MoSe_2$ (e)WS_2 (f)WSe_2

Figure S4. (Color online) Electronic band structures of MX_2 (M=Mo,W; X=S, Se) monolayers.



(a)Ag_2S_2 (b)Ag_2Se_2 (c)Ag_2Te_2

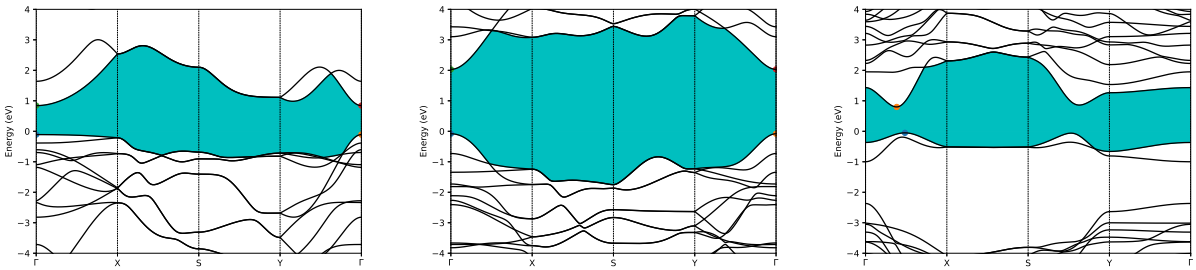
(d)$Al_2Br_2O_2$ (e)$Al_2Br_2S_2$ (f)$Al_2Br_2Se_2$

(g)$Al_2Cl_2S_2$ (h)$Al_2I_2S_2$ (i)$Al_2I_2Se_2$

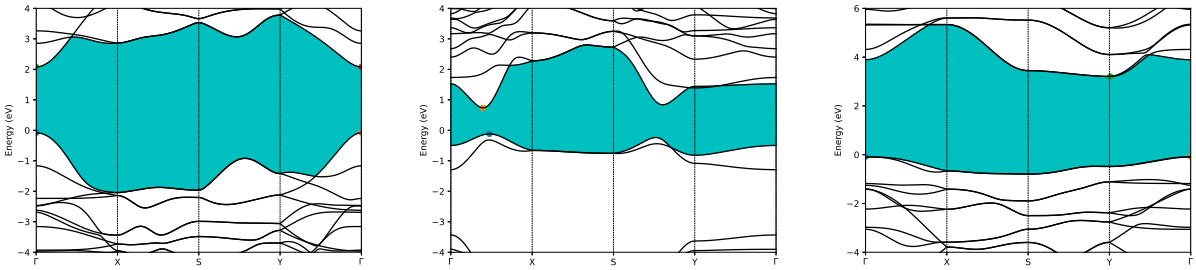
(j)Au_2O_2 (k)Au_2S_2 (l)Au_2Se_2

(m)Au_2Te_2 (n)Cu_2S_2 (o)$Ga_2Br_2O_2$

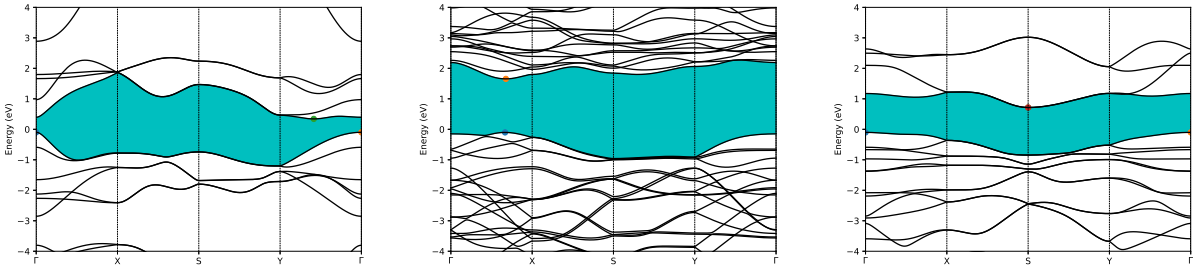
Figure S5. (Color online) Electronic band structures of anisotropic 2D materials



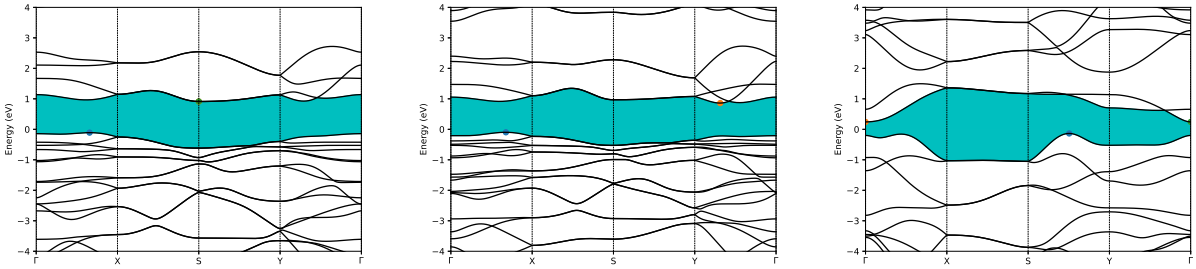
(a)$Ga_2I_2S_2$ (b)$Hf_2Br_2N_2$ (c)Hf_2Br_4



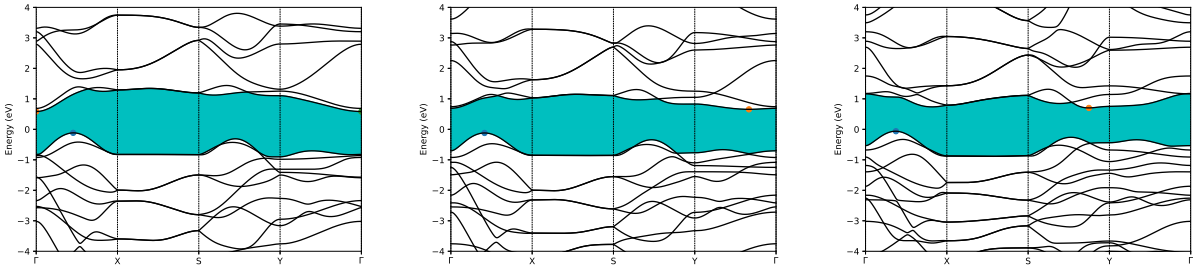
(d)$Hf_2Cl_2N_2$ (e)Hf_2Cl_4 (f)Hf_2O_6



(g)$Ir_2Cl_2O_2$ (h)MoW_3S_8 (i)Ni_2S_4

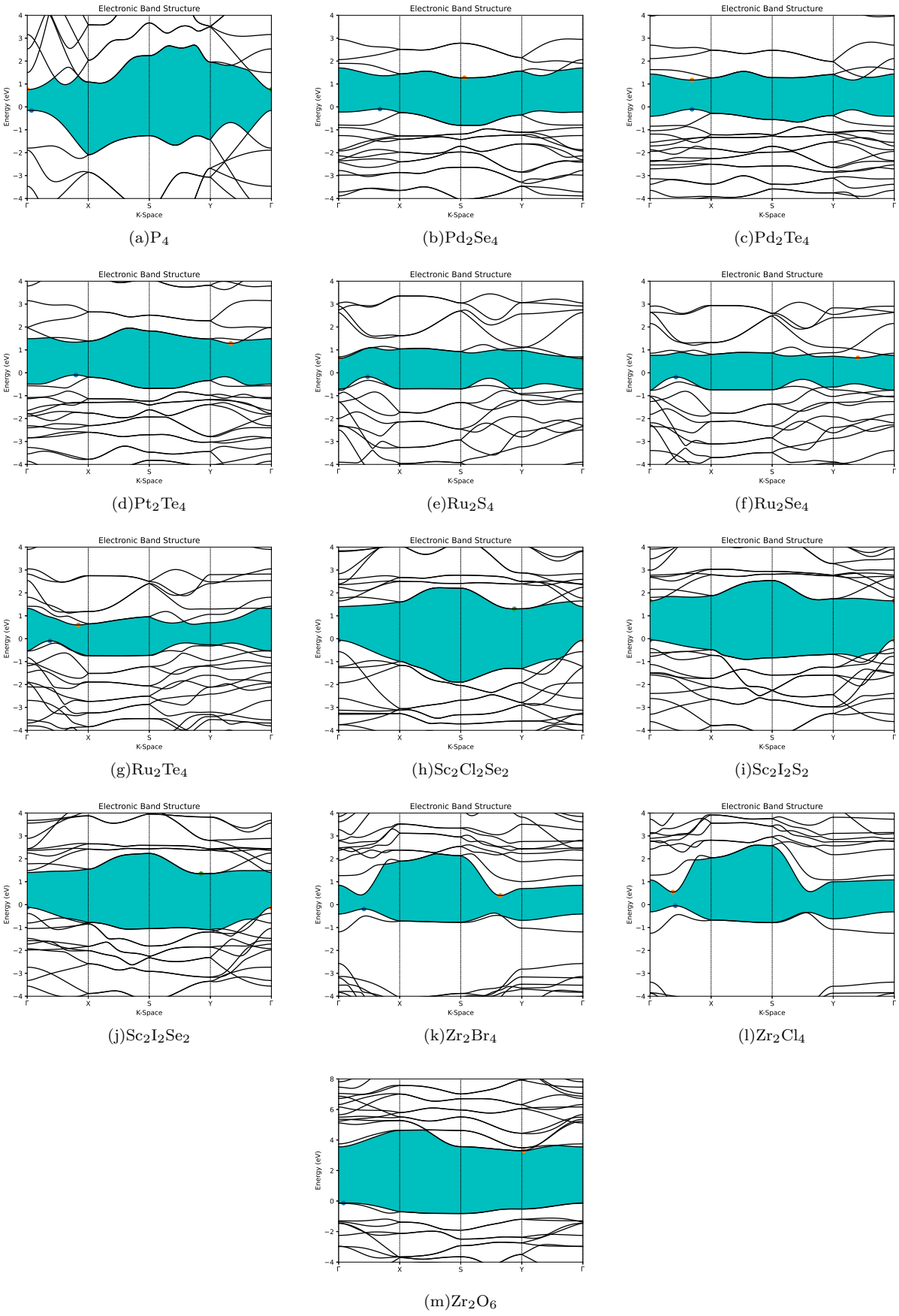


(j)Ni_2Se_4 (k)Ni_2Te_4 (l)Os_2O_4



(m)Os_2S_4 (n)Os_2Se_4 (o)Os_2Te_4

Figure S6. (Color online) Electronic band structures of anisotropic 2D materials



(a)P_4 (b)Pd_2Se_4 (c)Pd_2Te_4

(d)Pt_2Te_4 (e)Ru_2S_4 (f)Ru_2Se_4

(g)Ru_2Te_4 (h)$Sc_2Cl_2Se_2$ (i)$Sc_2I_2S_2$

(j)$Sc_2I_2Se_2$ (k)Zr_2Br_4 (l)Zr_2Cl_4

(m)Zr_2O_6

Figure S7. (Color online) Electronic band structures of anisotropic 2D materials

Table S3. Calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) for p-type carrier concentration of 2D isotropic materials at T=300 K.

p-type		T=300 K				p-type		T=300 K			
Prototype	Material	EFF$_{max}$	ρ	S	S$^2\sigma/\tau$	Prototype	Material	EFF$_{max}$	ρ	S	S$^2\sigma/\tau$
pro-PbS	Pb_2Se_2	0.41	0.30	507.52	0.22	pro-MoSSe	BiBrS	0.17	2.92	508.23	0.41
pro-CdI_2	GeS_2	0.30	1.72	508.66	0.53	pro-MoS_2	WTe_2	0.17	0.55	507.21	0.13
pro-Ti_2CO_2	Ti_2CO_2	0.27	0.95	330.82	0.32	pro-BiTeI	BiIS	0.17	3.90	509.04	0.50
pro-CdI_2	**$ZrSe_2$**	**0.25**	**0.26**	**501.86**	**0.12**	**pro-MoS_2**	**WS_2**	**0.17**	**0.87**	**507.13**	**0.18**
pro-MoSSe	ISbTe	0.25	1.46	510.17	0.38	pro-BiTeI	BrSbTe	0.17	3.06	510.36	0.42
pro-BiTeI	AsITe	0.25	2.45	510.22	0.52	pro-CH	$Pb2Te_2$	0.17	1.81	507.62	0.30
pro-CdI_2	**$HfSe_2$**	**0.24**	**0.26**	**501.51**	**0.12**	pro-MoSSe	ZrClI	0.17	0.67	504.94	0.15
pro-MoSSe	AsBrS	0.24	1.89	506.86	0.43	pro-BiTeI	AsClTe	0.17	3.88	505.71	0.48
pro-BiTeI	AsISe	0.24	2.84	507.23	0.55	pro-GeS_2	ZnI_2	0.17	3.16	506.57	0.42
pro-BiTeI	ZrSSe	0.24	0.30	503.55	0.12	pro-MoSSe	ISSb	0.16	2.76	500.07	0.38
pro-Ti_2CO_2	Zr_2CO_2	0.23	0.39	507.74	0.14	pro-GeS_2	GeS_2	0.16	1.38	507.24	0.23
pro-MoSSe	ISbSe	0.23	1.70	507.95	0.39	pro-MoSSe	WSSe	0.16	0.87	507.81	0.17
pro-MoSSe	AsBrTe	0.23	1.77	511.27	0.41	pro-MoSSe	BiBrTe	0.16	1.41	510.06	0.23
pro-MoS_2	HfI_2	0.23	0.39	509.36	0.14	pro-GeSe	GeTe	0.16	0.40	507.62	0.10
pro-Ti_2CO_2	Hf_2CO_2	0.23	0.42	505.54	0.15	pro-BN	BN	0.16	0.81	508.56	0.16
pro-CdI_2	$SnSe_2$	0.23	1.82	512.95	0.42	pro-MoSSe	BiClSe	0.16	2.87	511.64	0.36
pro-BiTeI	HfSSe	0.23	0.30	504.66	0.12	pro-CH2Si	CH2Si	0.15	0.81	502.73	0.16
pro-BiTeI	AsIS	0.22	3.25	509.67	0.57	pro-CdI_2	PtS_2	0.15	5.99	512.55	0.59
pro-MoSSe	BrSbTe	0.22	1.85	510.59	0.39	pro-MoS_2	TiI_2	0.15	0.72	508.15	0.14
pro-CdI_2	SnS_2	0.22	2.43	510.94	0.48	pro-CH	In_2I_2	0.15	2.73	507.91	0.33
pro-BiTeI	ISSb	0.22	2.92	508.71	0.51	pro-MoSSe	BiClS	0.15	3.43	509.47	0.39
pro-BiTeI	ISbSe	0.22	2.53	509.95	0.47	pro-$ScPSe_3$	Sc2P2Se6	0.15	1.23	508.95	0.20
pro-BiTeI	ISbTe	0.22	2.32	508.85	0.44	pro-MoSSe	WSeTe	0.15	0.72	507.58	0.14
pro-MoS_2	$HfBr_2$	0.22	0.46	508.86	0.15	pro-BiTeI	ClSbTe	0.14	3.93	508.47	0.42
pro-BiTeI	AsBrSe	0.22	2.68	509.55	0.48	pro-BiTeI	ClSbSe	0.14	3.75	508.87	0.40
pro-CdI_2	ZrS_2	0.21	0.37	503.82	0.13	pro-MoS_2	$TiBr_2$	0.14	0.81	507.44	0.14
pro-BiTeI	AsBrS	0.21	2.91	507.15	0.50	pro-MoS_2	$TiCl_2$	0.14	0.83	507.49	0.15
pro-MoS_2	$HfCl_2$	0.21	0.50	505.91	0.15	pro-BiTeI	BiBrSe	0.14	3.40	508.02	0.37
pro-CdI_2	HfS_2	0.21	0.37	504.92	0.13	pro-BiTeI	BiBrS	0.14	3.88	507.80	0.41
pro-MoSSe	HfBrI	0.21	0.47	507.90	0.15	pro-GeS_2	$ZnBr_2$	0.14	5.08	507.33	0.48
pro-MoSSe	BrSbSe	0.21	2.29	507.33	0.42	pro-GeS_2	SnS_2	0.14	1.76	508.04	0.23
pro-BiTeI	AsBrTe	0.21	2.96	508.59	0.49	pro-MoSSe	TiBrCl	0.14	0.88	505.89	0.15
pro-MoSSe	HfBrCl	0.21	0.50	507.54	0.15	pro-MoSSe	TiBrI	0.14	0.84	508.54	0.14
pro-MoS_2	ZrI_2	0.20	0.50	507.59	0.15	pro-MoS_2	$HfTe_2$	0.14	1.84	444.18	0.24
pro-CH	C_2H_2	0.20	0.60	502.99	0.17	**pro-MoS_2**	**$MoSe_2$**	**0.14**	**0.86**	**506.88**	**0.14**
pro-MoSSe	BrSSb	0.20	2.53	507.51	0.43	pro-CH	Ag_2Cl_2	0.13	1.05	503.95	0.16
pro-MoS_2	$ZrBr_2$	0.19	0.55	508.13	0.15	pro-$MnPSe_3$	$Zn_2P_2S_6$	0.13	0.66	509.17	0.12
pro-MoSSe	HfClI	0.19	0.56	506.35	0.15	pro-CH	Zn_2Te_2	0.13	0.80	500.67	0.13
pro-MoS_2	$ZrCl_2$	0.19	0.59	504.47	0.15	pro-CdI_2	$ZnBr_2$	0.13	4.10	510.59	0.41
pro-MoSSe	ZrBrI	0.19	0.57	507.35	0.15	pro-BiTeI	BiBrTe	0.13	3.48	507.90	0.34
pro-MoSSe	ZrBrCl	0.18	0.60	505.17	0.15	pro-MoSSe	HfSeTe	0.13	3.78	366.49	0.35
pro-C	As_2	0.18	0.33	503.76	0.10	pro-GeSe	SnTe	0.12	1.11	510.16	0.16
pro-MoSSe	BiBrSe	0.18	2.44	511.54	0.38	pro-CdI_2	$PtTe_2$	0.12	1.11	502.36	0.16
pro-GeS_2	$GeSe_2$	0.18	1.18	505.60	0.23	pro-MoS_2	$MoTe_2$	0.12	0.89	510.71	0.13
pro-BiTeI	AsClS	0.18	3.15	510.36	0.45	pro-MoSSe	TiClI	0.12	1.21	507.76	0.16
pro-BiTeI	BrSSb	0.18	3.29	508.00	0.45	pro-MoSSe	ZrSTe	0.12	1.98	442.76	0.22
pro-BiTeI	AsClSe	0.18	3.27	507.65	0.45	pro-TiCl3	Mo_2Cl_6	0.12	1.02	505.31	0.14
pro-CdI_2	GeI_2	0.18	3.55	506.96	0.48	pro-MoSSe	ZrSeTe	0.12	1.12	495.72	0.15
pro-MoS_2	**WSe_2**	**0.18**	**0.56**	**509.41**	**0.14**	pro-CdI_2	CdI_2	0.12	4.29	501.67	0.38
pro-BiTeI	BrSbSe	0.18	3.06	508.35	0.43	pro-CdI_2	$PtSe_2$	0.12	7.68	507.88	0.54
pro-BiTeI	BiISe	0.18	3.16	507.79	0.44	**pro-MoS_2**	**MoS_2**	**0.12**	**2.26**	**508.40**	**0.24**
pro-BiTeI	BiITe	0.18	2.73	507.96	0.40	pro-CdI_2	NiS_2	0.12	1.30	503.26	0.16
pro-CdI_2	ZnI_2	0.17	2.43	510.14	0.38	pro-BiTeI	BiClS	0.12	4.10	510.48	0.34

Table S4. Calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) for n-type carrier concentration of 2D isotropic materials at T=300 K.

n-type		T=300 K				n-type		T=300 K			
Prototype	Material	EFF$_{max}$	ρ	S	S$^2\sigma/\tau$	Prototype	Material	EFF$_{max}$	ρ	S	S$^2\sigma/\tau$
pro-C	As_2	0.49	0.99	509.25	0.54	pro-MoSSe	BiClSe	0.22	3.59	506.45	0.57
pro-CdI_2	$PtTe_2$	0.47	1.95	505.12	0.83	pro-CdI_2	$ZnBr_2$	0.21	1.23	508.08	0.28
pro-PbS	Pb_2Se_2	0.44	0.29	508.47	0.22	pro-GaS	Al_2S_2	0.21	1.26	507.91	0.27
pro-GeSe	GeTe	0.43	1.14	506.23	0.52	pro-MoSSe	BiBrSe	0.21	2.19	507.72	0.39
pro-GeSe	SnTe	0.40	1.25	508.53	0.51	pro-CdI_2	SrI_2	0.21	1.50	508.25	0.31
pro-CdI_2	$PdSe_2$	0.39	1.05	505.65	0.45	pro-MoSSe	BrSSb	0.21	1.37	508.70	0.29
pro-GeSe	GeSe	0.38	1.43	506.63	0.53	pro-MoS_2	HfI_2	0.21	2.76	507.00	0.45
pro-CdI_2	NiS_2	0.36	2.78	512.10	0.80	pro-CdI_2	$RuBr_2$	0.21	2.78	509.43	0.45
pro-CdI_2	$PtSe_2$	0.36	1.18	508.65	0.45	pro-MoSSe	ZrSeTe	0.21	2.63	508.74	0.44
pro-CH	Cd_2Se_2	0.35	0.16	500.26	0.12	pro-MoS_2	MoO_2	0.20	0.58	507.92	0.15
pro-CdI_2	**$HfSe_2$**	**0.35**	**1.19**	**509.40**	**0.43**	pro-GeSe	SnS	0.20	2.36	508.18	0.39
pro-GaS	Al_2Te_2	0.33	1.32	506.20	0.44	pro-CdI_2	CaI_2	0.20	1.60	508.18	0.30
pro-MoS_2	$HfTe_2$	0.33	1.95	494.27	0.58	pro-MoS_2	$HfBr_2$	0.20	2.99	508.81	0.45
pro-GeSe	GeS	0.32	1.98	507.66	0.57	pro-MoSSe	HfBrI	0.20	2.95	507.07	0.45
pro-CdI_2	PdS_2	0.32	1.53	507.81	0.48	pro-CdI_2	FeI_2	0.19	5.88	509.76	0.70
pro-CdI_2	GeS_2	0.32	0.70	506.38	0.28	pro-MoSSe	AsITe	0.19	0.63	507.91	0.16
pro-BiTeI	HfSSe	0.32	1.34	509.14	0.42	pro-MoSSe	BiBrS	0.19	1.68	506.73	0.30
pro-CdI_2	PtS_2	0.32	1.60	510.11	0.48	pro-MoSSe	HfBrCl	0.19	3.05	509.74	0.44
pro-CdI_2	**$ZrSe_2$**	**0.31**	**1.21**	**508.97**	**0.38**	pro-CH	In_2I_2	0.19	0.59	509.09	0.15
pro-CdI_2	$SnSe_2$	0.30	0.73	508.71	0.27	pro-MoSSe	HfClI	0.19	2.98	510.69	0.42
pro-CdI_2	HfS_2	0.29	1.46	506.02	0.41	**pro-MoS_2**	**MoS_2**	**0.19**	**0.60**	**508.02**	**0.15**
pro-GeSe	SnSe	0.28	2.22	509.79	0.53	pro-MoS_2	ZrI_2	0.18	3.06	508.37	0.43
pro-CdI_2	RuI_2	0.28	3.08	507.99	0.65	pro-MoSSe	BiClS	0.18	2.19	507.69	0.35
pro-MoSSe	AsISe	0.28	0.93	507.59	0.29	pro-GaSe	Al_2S_2	0.18	1.27	506.20	0.24
pro-BiTeI	ZrSSe	0.27	1.38	510.24	0.37	pro-MoSSe	BiBrTe	0.18	0.93	505.62	0.19
pro-GaS	Ga_2S_2	0.27	0.24	505.18	0.11	pro-GaSe	Al_2Se_2	0.18	1.48	506.28	0.26
pro-MoSSe	HfSeTe	0.27	3.73	444.08	0.73	pro-MoS_2	$HfCl_2$	0.18	3.14	510.37	0.43
pro-Ti_2CO_2	Hf_2CO_2	0.26	1.34	510.13	0.35	pro-MoSSe	ISbTe	0.18	0.71	505.36	0.16
pro-MoS_2	$ZrTe_2$	0.26	2.21	508.27	0.49	pro-MoSSe	ZrSTe	0.18	3.40	489.30	0.46
pro-CdI_2	ZnI_2	0.26	0.80	509.24	0.25	pro-MoSSe	ZrBrI	0.17	3.19	509.93	0.42
pro-CdI_2	SnS_2	0.26	0.82	510.14	0.25	pro-MoSSe	AsBrTe	0.17	0.72	508.51	0.15
pro-CdI_2	MgI_2	0.25	0.83	508.98	0.25	pro-Ti_2CO_2	Ti_2CO_2	0.17	5.58	431.78	0.60
pro-Ti_2CO_2	Y_2CF_2	0.25	1.08	506.86	0.30	pro-MoSSe	BiITe	0.17	0.81	508.59	0.16
pro-MoSSe	WSTe	0.25	2.32	504.40	0.49	pro-MoS_2	$TiSe_2$	0.17	3.53	508.95	0.44
pro-MoS_2	**WS_2**	**0.25**	**0.40**	**506.75**	**0.15**	pro-MoSSe	MoSSe	0.17	0.69	510.75	0.15
pro-MoSSe	AsBrS	0.25	1.14	508.40	0.30	pro-CdI_2	$CaBr_2$	0.17	2.03	506.31	0.30
pro-CdI_2	ZrS_2	0.24	1.47	509.64	0.35	pro-MoSSe	BrSbTe	0.17	0.76	508.90	0.15
pro-MoS_2	WTe_2	0.24	0.39	509.35	0.14	**pro-MoS_2**	**$MoSe_2$**	**0.17**	**0.73**	**507.67**	**0.15**
pro-MoS_2	**WSe_2**	**0.24**	**0.50**	**509.54**	**0.17**	pro-MoSSe	MoSTe	0.16	1.61	506.23	0.25
pro-MoSSe	ISbSe	0.24	1.09	509.85	0.28	pro-MoS_2	$ZrBr_2$	0.16	3.41	509.72	0.41
pro-MoSSe	WSSe	0.24	0.55	507.36	0.18	pro-MoSSe	ZrClI	0.16	3.27	512.68	0.40
pro-Ti_2CO_2	Sc_2CF_2	0.23	1.32	506.16	0.31	pro-MoS_2	$MoTe_2$	0.16	0.72	510.70	0.14
pro-GaS	Al_2Se_2	0.23	1.29	507.52	0.31	pro-BN	BN	0.16	2.11	504.93	0.28
pro-MoSSe	ISSb	0.23	1.09	505.64	0.27	pro-CdI_2	NiO_2	0.16	4.41	510.08	0.47
pro-Ti_2CO_2	Zr_2CO_2	0.23	1.74	507.31	0.36	pro-MoSSe	MoSeTe	0.15	0.97	507.12	0.17
pro-MoS_2	WO_2	0.23	0.48	508.74	0.15	pro-MoSSe	ZrBrCl	0.15	3.51	513.16	0.39
pro-MoSSe	WSeTe	0.22	0.66	503.61	0.19	pro-MoS_2	CaI_2	0.15	1.98	507.21	0.26
pro-MoSSe	BrSbSe	0.22	1.75	506.11	0.36	pro-MoSSe	TiSSe	0.14	3.86	513.47	0.39
pro-CdI_2	CdI_2	0.22	0.95	509.71	0.23	pro-MoS_2	$ZrCl_2$	0.14	3.76	511.31	0.37
pro-MoSSe	BiISe	0.22	1.27	509.35	0.28	pro-MoS_2	TiI_2	0.14	5.25	513.19	0.45

Table S5. Calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) for p-type carrier concentration of 2D isotropic materials at T=600 K.

p-type		T=600 K				p-type		T=600 K			
Prototype	Material	EFF$_{max}$	ρ	S	S$^2\sigma/\tau$	Prototype	Material	EFF$_{max}$	ρ	S	S$^2\sigma/\tau$
pro-PbS	Pb_2Se_2	0.75	0.84	511.13	0.49	pro-GeS_2	ZnI_2	0.30	5.47	510.30	0.68
pro-CdI_2	GeS_2	0.51	3.88	497.09	0.93	pro-BiTeI	BiITe	0.30	4.15	509.93	0.56
pro-BiTeI	ZrSSe	0.47	0.99	464.96	0.34	pro-BiTeI	BrSbSe	0.30	4.93	509.55	0.63
pro-BiTeI	HfSSe	0.47	0.81	485.71	0.30	**pro-MoS_2**	**WS_2**	**0.30**	**2.51**	**509.94**	**0.40**
pro-CdI_2	**$HfSe_2$**	**0.47**	**1.94**	**390.26**	**0.53**	pro-BiTeI	AsClTe	0.30	6.06	510.09	0.71
pro-Ti_2CO_2	Zr_2CO_2	0.46	0.80	505.71	0.29	pro-BiTeI	BrSbTe	0.30	4.92	511.60	0.62
pro-Ti_2CO_2	Hf_2CO_2	0.46	0.83	506.20	0.29	pro-MoSSe	ISSb	0.30	5.10	509.51	0.64
pro-CdI_2	**$ZrSe_2$**	**0.44**	**3.37**	**336.59**	**0.71**	pro-MoSSe	BiBrSe	0.30	4.28	512.34	0.56
pro-BiTeI	AsITe	0.44	3.87	510.23	0.78	pro-BiTeI	BiIS	0.29	6.38	510.48	0.73
pro-BiTeI	AsISe	0.43	4.61	508.74	0.86	pro-CH	Zn_2Te_2	0.29	1.60	502.53	0.29
pro-CdI_2	HfS_2	0.43	0.77	506.98	0.26	pro-MoS_2	WTe_2	0.29	1.10	510.29	0.22
pro-MoS_2	HfI_2	0.43	1.04	483.74	0.32	pro-CH	Ag_2Cl_2	0.29	2.74	503.21	0.41
pro-CdI_2	ZrS_2	0.42	0.79	507.43	0.26	pro-MoSSe	BiBrS	0.29	5.00	512.04	0.60
pro-MoSSe	ISbTe	0.41	2.82	511.59	0.60	pro-MoSSe	BiBrTe	0.28	4.25	511.25	0.54
pro-MoS_2	$HfBr_2$	0.41	1.05	498.08	0.30	pro-MoSSe	WSSe	0.28	2.57	512.19	0.38
pro-MoS_2	$HfCl_2$	0.40	1.00	506.21	0.29	pro-GeS_2	SnS_2	0.27	3.73	507.16	0.47
pro-CH	C_2H_2	0.40	1.12	507.95	0.31	pro-CdI_2	PtS_2	0.26	11.98	511.15	0.99
pro-MoSSe	HfBrCl	0.39	1.02	506.22	0.29	pro-MoS_2	$TiCl_2$	0.26	1.96	505.58	0.29
pro-MoSSe	HfBrI	0.39	1.06	498.10	0.29	pro-MoS_2	$TiBr_2$	0.26	2.18	488.69	0.31
pro-BiTeI	AsIS	0.39	5.61	510.30	0.89	pro-MoS_2	TiI_2	0.26	3.58	434.01	0.43
pro-BiTeI	ISSb	0.39	5.37	509.79	0.86	pro-$ScPSe_3$	Sc2P2Se6	0.25	3.86	439.04	0.46
pro-CdI_2	$SnSe_2$	0.39	4.17	504.04	0.75	pro-CdI_2	$PtTe_2$	0.25	3.40	467.49	0.41
pro-MoSSe	AsBrS	0.39	3.66	511.44	0.67	pro-CH	In_2I_2	0.25	3.71	510.15	0.43
pro-BiTeI	ISbSe	0.39	4.33	510.10	0.74	pro-MoSSe	TiBrCl	0.25	2.21	500.60	0.31
pro-BiTeI	AsBrSe	0.38	4.47	509.36	0.75	pro-MoSSe	WSeTe	0.25	1.76	511.69	0.26
pro-C	As_2	0.38	0.70	506.53	0.22	pro-BiTeI	ClSbTe	0.25	6.36	510.24	0.61
pro-BiTeI	AsBrS	0.38	4.94	509.48	0.79	pro-CH	Zn_2Se_2	0.25	1.78	504.54	0.26
pro-BiTeI	ISbTe	0.38	3.64	510.79	0.64	pro-CH	Cd_2Te_2	0.25	1.67	504.03	0.25
pro-MoSSe	ISbSe	0.38	3.31	511.51	0.61	pro-BiTeI	ClSbSe	0.25	5.98	511.09	0.58
pro-BiTeI	AsBrTe	0.37	4.76	509.70	0.75	pro-GeSe	GeTe	0.24	1.59	514.06	0.25
pro-MoS_2	ZrI_2	0.37	1.39	478.43	0.33	pro-$MnPSe_3$	$Zn_2P_2S_6$	0.24	1.35	509.92	0.21
pro-MoSSe	AsBrTe	0.37	3.72	512.22	0.65	pro-MoSSe	TiBrI	0.24	3.00	470.05	0.36
pro-MoSSe	BrSbTe	0.36	3.42	511.43	0.59	pro-BiTeI	BiBrSe	0.24	5.09	511.13	0.51
pro-MoS_2	$ZrBr_2$	0.36	1.21	499.69	0.29	**pro-MoS_2**	**$MoSe_2$**	**0.24**	**1.84**	**510.83**	**0.26**
pro-MoSSe	HfClI	0.36	1.12	507.76	0.28	pro-BiTeI	BiBrS	0.24	6.12	510.37	0.58
pro-MoS_2	$ZrCl_2$	0.35	1.13	508.95	0.28	pro-MoS_2	WO_2	0.24	0.93	506.07	0.16
pro-MoSSe	BrSbSe	0.35	4.10	510.23	0.65	pro-GeS_2	$ZnBr_2$	0.24	7.59	511.28	0.66
pro-MoSSe	ZrBrCl	0.35	1.21	504.96	0.28	**pro-MoS_2**	**MoS_2**	**0.23**	**4.54**	**507.31**	**0.46**
pro-GeS_2	$GeSe_2$	0.35	4.97	438.15	0.72	pro-MoSSe	BiClSe	0.23	4.87	514.31	0.48
pro-MoSSe	ZrBrI	0.34	1.32	495.50	0.30	pro-CdI_2	$PtSe_2$	0.23	13.85	508.10	0.97
pro-MoSSe	BrSSb	0.34	4.56	510.97	0.67	pro-MoSSe	BiClS	0.23	5.78	512.03	0.54
pro-CdI_2	SnS_2	0.33	4.59	514.58	0.67	pro-CdI_2	CdI_2	0.23	6.70	508.98	0.60
pro-CH	Pb2Te_2	0.32	2.76	507.98	0.47	pro-MoSSe	BiITe	0.23	5.83	507.56	0.55
pro-CH2Si	CH2Si	0.32	1.54	505.20	0.31	pro-MoS_2	MoO_2	0.23	0.95	505.08	0.16
pro-GeS_2	GeS_2	0.32	2.88	506.36	0.47	pro-CdI_2	$ZnBr_2$	0.23	7.39	509.92	0.65
pro-CdI_2	ZnI_2	0.32	4.95	510.13	0.69	pro-MoSSe	AsISe	0.23	1.74	495.92	0.24
pro-CdI_2	GeI_2	0.32	5.96	509.47	0.75	pro-BiTeI	BiBrTe	0.22	5.35	510.42	0.48
pro-BiTeI	AsClS	0.32	5.31	510.34	0.70	pro-MoSSe	AsITe	0.22	1.87	495.46	0.25
pro-MoS_2	**WSe_2**	**0.32**	**1.18**	**508.83**	**0.25**	pro-FeSe	Cs2F2	0.22	6.10	507.26	0.53
pro-BiTeI	AsClSe	0.31	5.29	509.73	0.69	pro-$MnPSe_3$	$Nb_2P_2S_6$	0.21	8.89	399.20	0.66
pro-MoSSe	ZrClI	0.31	1.34	506.95	0.28	pro-CdI_2	NiS_2	0.21	10.01	378.22	0.71
pro-BN	BN	0.31	1.66	507.95	0.31	pro-MoSSe	TiClI	0.21	3.87	496.25	0.37
pro-BiTeI	BrSSb	0.31	5.60	510.50	0.70	pro-MoSSe	MoSSe	0.21	5.65	506.89	0.48
pro-BiTeI	BiISe	0.30	4.91	510.85	0.63	pro-CdI_2	PdS_2	0.21	14.45	505.48	0.89

Table S6. Calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) for n-type carrier concentration of 2D isotropic materials at T=600 K.

n-type		T=600 K				n-type		T=600 K			
Prototype	Material	EFF_{max}	ρ	S	$S^2\sigma/\tau$	Prototype	Material	EFF_{max}	ρ	S	$S^2\sigma/\tau$
pro-C	As_2	0.95	2.11	506.50	1.10	pro-GaS	Al_2Se_2	0.45	2.92	507.47	0.64
pro-GeSe	GeTe	0.83	2.35	507.31	1.04	pro-MoS_2	WTe_2	0.45	0.91	509.10	0.30
pro-CdI_2	$PtTe_2$	0.82	4.50	506.54	1.58	pro-MoSSe	WSTe	0.44	5.32	509.76	0.95
pro-PbS	Pb_2Se_2	0.80	0.70	510.06	0.45	pro-Ti_2CO_2	Sc_2CF_2	0.44	2.61	507.09	0.60
pro-GeSe	SnTe	0.74	2.66	508.25	1.00	pro-MoSSe	ISbSe	0.44	2.37	509.65	0.56
pro-GeSe	GeSe	0.72	2.90	509.66	1.03	pro-GaSe	In_2S_2	0.44	0.31	508.16	0.14
pro-CH	Cd_2Se_2	0.71	0.39	507.22	0.27	pro-GaS	In_2S_2	0.44	0.31	509.24	0.14
pro-CH	Zn_2Te_2	0.71	0.11	501.16	0.12	pro-CdI_2	RuI_2	0.44	6.93	511.90	1.12
pro-CdI_2	$PdSe_2$	0.70	2.93	493.35	1.02	pro-MoSSe	ISSb	0.43	2.11	508.62	0.50
pro-CH	Cd_2Te_2	0.68	0.12	505.54	0.12	pro-MoS_2	WO_2	0.43	0.95	510.13	0.29
pro-CdI_2	$PtSe_2$	0.66	2.74	509.26	0.92	pro-Ti_2CO_2	Zr_2CO_2	0.42	3.44	509.11	0.68
pro-CdI_2	**$HfSe_2$**	**0.64**	**3.89**	**461.59**	**1.11**	pro-BiTeI	AsBrSe	0.42	0.26	510.65	0.12
pro-CH	Zn_2Se_2	0.63	0.18	507.32	0.14	pro-BiTeI	BiITe	0.42	0.25	509.52	0.12
pro-GaS	Al_2Te_2	0.63	2.84	507.31	0.89	pro-MoSSe	BiBrTe	0.42	3.72	501.93	0.71
pro-CdI_2	GeS_2	0.61	1.87	478.44	0.66	pro-MoSSe	BrSbSe	0.41	3.93	508.48	0.72
pro-GaS	Ga_2Se_2	0.60	0.21	506.75	0.15	pro-CdI_2	$ZnBr_2$	0.41	2.56	506.74	0.56
pro-CdI_2	NiS_2	0.59	9.88	470.96	1.94	pro-BN	BN	0.41	8.50	497.60	1.19
pro-BiTeI	HfSSe	0.59	2.70	506.06	0.81	pro-CdI_2	SrI_2	0.41	3.06	506.53	0.61
pro-GeSe	GeS	0.59	3.86	510.30	1.03	pro-GaS	Al_2S_2	0.41	2.99	507.88	0.59
pro-CdI_2	PdS_2	0.58	3.78	510.45	1.00	pro-CdI_2	CdI_2	0.41	1.92	508.25	0.44
pro-CdI_2	PtS_2	0.57	3.84	510.51	0.98	pro-MoS_2	$HfTe_2$	0.40	25.92	298.45	2.51
pro-GaS	Ga_2S_2	0.57	1.58	506.08	0.54	pro-BiTeI	BiClS	0.40	0.35	508.99	0.14
pro-CdI_2	$SnSe_2$	0.56	1.69	494.64	0.57	pro-MoSSe	BiISe	0.40	2.73	509.36	0.55
pro-CdI_2	HfS_2	0.54	2.79	508.55	0.76	pro-CdI_2	GeI_2	0.40	0.29	510.13	0.12
pro-CH	Zn_2S_2	0.54	0.30	506.26	0.17	pro-BiTeI	AsClS	0.39	0.32	508.59	0.13
pro-BiTeI	ClSbTe	0.54	0.18	509.51	0.12	pro-BiTeI	ISbTe	0.39	0.24	510.67	0.11
pro-CdI_2	**$ZrSe_2$**	**0.53**	**6.62**	**414.50**	**1.32**	pro-CdI_2	$MgBr_2$	0.39	0.41	507.60	0.15
pro-GeSe	PbTe	0.53	0.37	504.43	0.20	pro-MoSSe	BiClSe	0.38	6.42	510.59	0.94
pro-MoSSe	AsISe	0.53	2.20	506.25	0.63	pro-GeS_2	GeS_2	0.38	0.68	505.10	0.21
pro-BiTeI	BiClTe	0.53	0.20	507.82	0.13	pro-GaS	Ga_2O_2	0.38	0.41	506.33	0.15
pro-BiTeI	BiBrTe	0.52	0.21	508.06	0.13	pro-MoSSe	BiBrSe	0.38	4.78	509.81	0.77
pro-BiTeI	BrSbTe	0.52	0.20	508.21	0.13	pro-MoSSe	BrSSb	0.38	2.76	508.85	0.53
pro-CH	Cd_2S_2	0.51	0.25	507.37	0.15	pro-CdI_2	CaI_2	0.38	3.21	507.06	0.59
pro-BiTeI	ZrSSe	0.51	3.16	497.95	0.77	pro-BiTeI	BiBrS	0.38	0.36	508.56	0.14
pro-GeSe	SnSe	0.50	4.14	509.14	0.91	pro-MoSSe	ISbTe	0.38	2.02	504.50	0.43
pro-GaSe	Ga_2S_2	0.50	0.29	507.00	0.15	pro-MoSSe	AsITe	0.38	1.57	500.23	0.36
pro-BiTeI	AsClTe	0.50	0.20	508.95	0.12	pro-MoS_2	MoO_2	0.38	1.14	509.07	0.29
pro-Ti_2CO_2	Hf_2CO_2	0.50	2.70	509.09	0.68	pro-GeS_2	$GeSe_2$	0.38	2.15	376.07	0.44
pro-CdI_2	SnS_2	0.49	1.65	508.99	0.48	pro-CdI_2	GeO_2	0.38	0.43	508.44	0.15
pro-CdI_2	ZnI_2	0.49	1.59	508.73	0.47	pro-BiTeI	BrSSb	0.37	0.35	509.03	0.13
pro-Ti_2CO_2	Y_2CF_2	0.49	2.14	507.90	0.57	pro-GeSe	SnS	0.37	4.14	507.79	0.67
pro-CdI_2	MgI_2	0.49	1.66	508.88	0.48	pro-CdI_2	SnO_2	0.37	0.45	506.64	0.15
pro-MoS_2	**WS_2**	**0.48**	**1.12**	**508.30**	**0.37**	pro-MoSSe	BiITe	0.36	2.70	505.29	0.50
pro-BiTeI	ClSbSe	0.48	0.26	507.89	0.14	pro-GaSe	$Hg2I_2$	0.36	0.37	508.61	0.13
pro-MoS_2	**WSe_2**	**0.48**	**2.22**	**508.57**	**0.57**	pro-CH	Ag_2Cl_2	0.36	0.44	508.56	0.15
pro-MoSSe	WSSe	0.47	2.54	508.71	0.62	pro-CH	$Cu2I_2$	0.36	0.40	509.78	0.14
pro-BiTeI	BiClSe	0.47	0.27	508.14	0.14	pro-CdI_2	$PbBr_2$	0.35	0.43	508.75	0.14
pro-MoSSe	AsBrS	0.47	2.41	507.70	0.60	pro-BiTeI	AsBrS	0.35	0.32	509.90	0.12
pro-MoSSe	WSeTe	0.47	2.80	505.92	0.65	pro-MoSSe	BrSbTe	0.35	2.47	503.47	0.46
pro-CdI_2	ZrS_2	0.47	3.03	507.92	0.69	pro-GaSe	Al_2S_2	0.35	2.52	507.17	0.46
pro-BiTeI	AsClSe	0.46	0.25	509.06	0.13	pro-MoS_2	HfI_2	0.35	5.28	507.41	0.75
pro-BiTeI	AsBrTe	0.46	0.21	509.97	0.11	pro-MoSSe	BiBrS	0.35	3.31	509.05	0.55
pro-BiTeI	BiBrSe	0.45	0.28	509.40	0.14	pro-GaSe	Al_2Se_2	0.35	2.85	509.18	0.49
pro-BiTeI	BrSbSe	0.45	0.28	508.60	0.14	pro-CdI_2	$SrBr_2$	0.34	0.51	507.10	0.16

Table S7. Continued: Calculated maximum EFF ($10^{-19}\ W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) for n-type carrier concentration of 2D isotropic materials at T=600 K.

n-type		T=600 K				n-type		T=600 K			
Prototype	Material	EFF_{max}	ρ	S	$S^2\sigma/\tau$	Prototype	Material	EFF_{max}	ρ	S	$S^2\sigma/\tau$
pro-GeS_2	ZnI_2	0.34	0.45	508.87	0.14	pro-MoS_2	$MgCl_2$	0.32	0.51	508.83	0.15
pro-CH	In_2I_2	0.34	1.16	510.03	0.27	pro-CH	$Cu2Br_2$	0.32	0.50	508.74	0.14
pro-MoS_2	$HfBr_2$	0.34	5.60	508.93	0.75	pro-FeSe	$Cu2Br_2$	0.32	0.53	508.19	0.15
pro-MoS_2	**MoS_2**	**0.34**	**1.33**	**510.30**	**0.29**	pro-GeS_2	GeO_2	0.32	0.55	508.61	0.15
pro-MoS_2	$ZrTe_2$	0.33	23.27	338.22	1.95	pro-MoSSe	MoSTe	0.32	5.32	508.56	0.68
pro-MoSSe	AsBrTe	0.33	1.58	507.90	0.32	pro-GeS_2	$ZnBr_2$	0.31	0.51	507.86	0.14
pro-MoSSe	BiClS	0.33	4.28	509.47	0.62	pro-$MnPSe_3$	$Zn_2P_2S_6$	0.31	0.33	509.49	0.11
pro-MoSSe	HfBrI	0.33	5.44	510.14	0.72	pro-GeS_2	SnS_2	0.31	0.51	509.52	0.14
pro-CdI_2	$RuBr_2$	0.33	5.67	512.13	0.74	**pro-MoS_2**	**$MoSe_2$**	**0.31**	**2.28**	**509.04**	**0.38**
pro-CH	Ag_2I_2	0.33	0.47	508.34	0.14	pro-CdI_2	$ZnCl_2$	0.31	0.76	505.16	0.18
pro-CdI_2	$CaBr_2$	0.33	3.96	508.34	0.58	pro-MoSSe	HfClI	0.31	5.71	509.95	0.70
pro-MoSSe	MoSSe	0.33	2.33	507.46	0.40	pro-MoS_2	$HfCl_2$	0.31	5.72	511.01	0.70
pro-CdI_2	$BaBr_2$	0.33	1.55	508.57	0.31	pro-MoS_2	ZrI_2	0.31	5.89	504.80	0.70
pro-MoSSe	HfBrCl	0.33	5.62	510.76	0.72	pro-MoSSe	MoSeTe	0.30	3.56	507.49	0.50
pro-BiTeI	BiISe	0.32	0.33	512.09	0.11	pro-MoSSe	HfSeTe	0.30	46.49	256.98	2.68

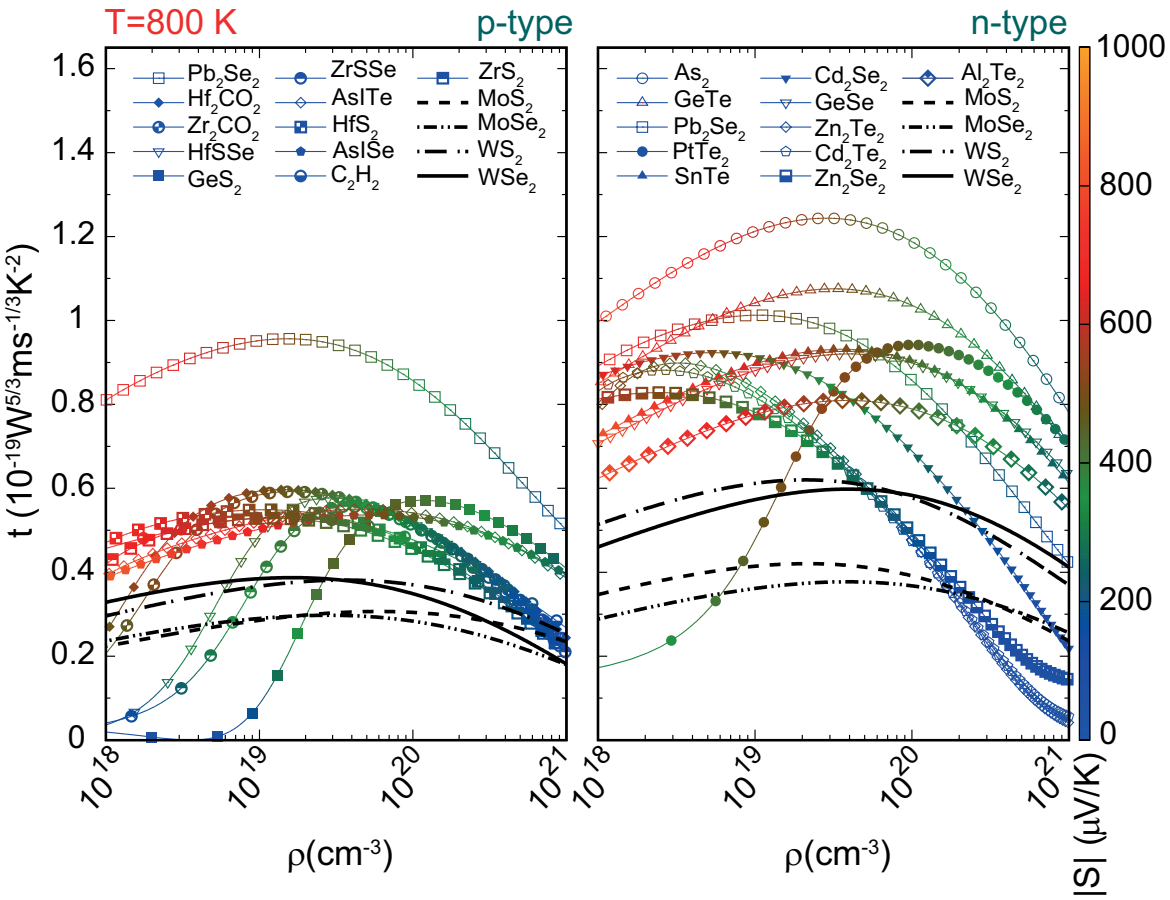


Figure S8. (Color online) Calculated EFF of selected 2D isotropic materials as a function of charge carrier concentration for p-type and n-type carriers at T=800 K. The corresponding Seebeck coefficient at the same carrier concentration is indicated by color.

Table S8. Calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) for p-type carrier concentration of 2D isotropic materials at T=800 K.

p-type		T=800 K				p-type		T=800 K			
Prototype	Material	EFF$_{max}$	ρ	S	S$^2\sigma/\tau$	Prototype	Material	EFF$_{max}$	ρ	S	S$^2\sigma/\tau$
pro-PbS	Pb_2Se_2	0.96	1.53	509.56	0.76	pro-BiTel	BrSSb	0.37	6.77	511.89	0.80
pro-Ti_2CO_2	Hf_2CO_2	0.60	1.46	480.10	0.46	pro-GeS_2	ZnI_2	0.37	6.53	510.85	0.77
pro-Ti_2CO_2	Zr_2CO_2	0.59	1.60	467.76	0.48	pro-BiTel	BiITe	0.37	4.93	511.59	0.64
pro-BiTel	HfSSe	0.58	2.87	396.81	0.69	pro-BiTel	BiISe	0.37	5.86	511.27	0.72
pro-CdI_2	GeS_2	0.57	11.58	418.93	1.77	pro-BiTel	BrSbSe	0.37	5.88	510.70	0.72
pro-BiTel	ZrSSe	0.56	3.85	366.92	0.81	pro-BiTel	AsClTe	0.37	7.19	511.51	0.82
pro-BiTel	AsITe	0.55	4.63	510.79	0.91	pro-BiTel	BrSbTe	0.37	6.01	510.33	0.72
pro-CdI_2	HfS_2	0.55	1.08	506.62	0.35	pro-CdI_2	SnS_2	0.36	6.09	515.48	0.74
pro-BiTel	AsISe	0.54	5.42	510.85	0.98	pro-MoSSe	ISSb	0.36	6.67	509.81	0.77
pro-CH	C_2H_2	0.53	1.52	506.16	0.42	pro-MoSSe	WSSe	0.35	3.90	510.82	0.52
pro-CdI_2	ZrS_2	0.53	1.19	506.24	0.36	pro-GeS_2	SnS_2	0.35	5.00	507.89	0.61
pro-CdI_2	$HfSe_2$	0.52	7.52	295.29	1.16	pro-MoSSe	BiBrTe	0.35	5.82	510.76	0.68
pro-MoS_2	$HfCl_2$	0.51	1.87	474.80	0.46	pro-MoSSe	BiBrSe	0.35	5.13	514.13	0.61
pro-MoSSe	ISbTe	0.49	3.66	512.39	0.71	pro-BiTel	BiIS	0.34	7.51	512.55	0.79
pro-MoS_2	$HfBr_2$	0.49	3.20	420.83	0.63	pro-CdI_2	PtS_2	0.34	16.98	509.00	1.34
pro-MoS_2	HfI_2	0.49	3.98	387.03	0.73	pro-MoS_2	WTe_2	0.34	1.76	497.87	0.29
pro-MoSSe	HfBrCl	0.49	2.42	452.91	0.53	pro-MoSSe	BiBrS	0.34	6.10	512.31	0.67
pro-C	As_2	0.49	1.08	508.52	0.31	pro-CH	Zn_2Se_2	0.32	2.25	507.08	0.33
pro-BiTel	AsIS	0.48	6.90	511.35	1.03	pro-CH	Cd_2Te_2	0.32	2.42	495.09	0.35
pro-BiTel	AsBrSe	0.48	5.41	509.57	0.87	pro-CdI_2	$PtSe_2$	0.32	19.08	504.80	1.35
pro-BiTel	ISSb	0.48	6.54	511.08	0.99	pro-MoS_2	WO_2	0.32	1.21	506.90	0.21
pro-BiTel	ISbSe	0.47	5.21	510.91	0.85	pro-MoS_2	$TiCl_2$	0.31	5.28	453.06	0.56
pro-BiTel	AsBrS	0.47	6.06	509.51	0.93	pro-CH	In_2I_2	0.31	4.88	497.93	0.53
pro-CdI_2	$ZrSe_2$	0.47	11.73	252.46	1.37	pro-Ti_2CO_2	Ti_2CO_2	0.31	31.54	141.73	1.57
pro-MoSSe	HfBrI	0.47	3.31	419.93	0.62	pro-CdI_2	$PtTe_2$	0.31	14.64	373.75	1.08
pro-BiTel	ISbTe	0.47	4.44	509.79	0.75	pro-MoS_2	MoS_2	0.31	5.95	507.98	0.60
pro-BiTel	AsBrTe	0.46	5.77	509.43	0.88	pro-BiTel	ClSbTe	0.30	7.59	511.21	0.69
pro-MoSSe	AsBrS	0.46	4.82	513.53	0.78	pro-BiTel	ClSbSe	0.30	7.23	511.21	0.66
pro-CdI_2	$SnSe_2$	0.45	10.98	437.16	1.36	pro-MoS_2	$MoSe_2$	0.30	2.82	510.50	0.35
pro-MoSSe	ISbSe	0.44	4.38	512.69	0.71	pro-MoSSe	BiITe	0.30	7.59	507.70	0.70
pro-MoS_2	$ZrCl_2$	0.44	2.19	474.86	0.45	pro-GeSe	GeTe	0.30	3.41	514.64	0.41
pro-MoSSe	HfClI	0.44	2.51	460.21	0.48	pro-MoS_2	MoO_2	0.30	2.01	461.03	0.28
pro-MoSSe	AsBrTe	0.44	4.95	512.45	0.77	pro-$MnPSe_3$	$Zn_2P_2S_6$	0.30	1.84	509.96	0.26
pro-MoS_2	$ZrBr_2$	0.43	3.69	423.06	0.61	pro-MoSSe	WSeTe	0.30	2.93	511.40	0.36
pro-MoSSe	ZrBrCl	0.43	2.76	455.97	0.50	pro-BiTel	BiBrSe	0.29	6.06	511.41	0.58
pro-MoSSe	BrSbTe	0.43	4.30	512.47	0.67	pro-MoS_2	$TiBr_2$	0.29	8.48	400.49	0.73
pro-CH_2Si	CH_2Si	0.43	2.01	506.43	0.41	pro-MoSSe	TiBrCl	0.29	7.11	431.70	0.64
pro-MoSSe	BrSbSe	0.43	4.92	512.71	0.73	pro-BiTel	BiBrS	0.29	7.14	512.90	0.64
pro-CH	Pb_2Te_2	0.42	3.33	507.98	0.57	pro-MoSSe	AsITe	0.28	5.81	425.50	0.56
pro-MoS_2	ZrI_2	0.42	5.21	383.17	0.75	pro-$ScPSe_3$	$Sc_2P_2Se_6$	0.28	12.80	341.54	0.94
pro-GeS_2	GeS_2	0.42	3.87	507.79	0.61	pro-GeS_2	$ZnBr_2$	0.28	8.78	511.02	0.73
pro-GeS_2	$GeSe_2$	0.41	16.56	354.81	1.55	pro-CdI_2	PdS_2	0.28	18.68	505.99	1.17
pro-BN	BN	0.41	2.30	506.18	0.42	pro-FeSe	Cs2F2	0.28	8.13	508.26	0.68
pro-MoSSe	ZrBrI	0.41	4.32	412.81	0.64	pro-MoSSe	AsISe	0.28	5.45	419.89	0.52
pro-MoSSe	BrSSb	0.41	5.63	511.80	0.77	pro-CdI_2	CdI_2	0.28	8.28	510.52	0.69
pro-CdI_2	ZnI_2	0.40	6.61	509.93	0.86	pro-MoSSe	MoSSe	0.27	7.28	507.75	0.61
pro-BiTel	AsClS	0.39	6.47	510.40	0.81	pro-BiTel	BiBrTe	0.27	6.59	510.89	0.57
pro-CdI_2	GeI_2	0.39	7.20	510.95	0.87	pro-Ti_2CO_2	Y_2CF_2	0.27	14.42	497.94	0.95
pro-CH	Zn_2Te_2	0.39	2.56	484.06	0.44	pro-CdI_2	$ZnBr_2$	0.27	9.23	511.53	0.74
pro-BiTel	AsClSe	0.39	6.41	509.84	0.80	pro-MoS_2	SrI_2	0.27	11.97	505.91	0.83
pro-MoS_2	WSe_2	0.39	1.66	510.34	0.32	pro-MoSSe	BiClS	0.27	6.77	513.65	0.56
pro-MoSSe	ZrClI	0.38	3.28	452.58	0.51	pro-MoS_2	TiI_2	0.27	15.38	338.40	0.98
pro-CH	Ag_2Cl_2	0.38	3.98	504.52	0.58	pro-MoSSe	BiClSe	0.26	5.99	514.44	0.52
pro-MoS_2	WS_2	0.38	3.63	510.60	0.53	pro-MoSSe	TiBrI	0.26	12.69	376.92	0.86

Table S9. Calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) for n-type carrier concentration of 2D isotropic materials at T=800 K.

n-type		T=800 K				n-type		T=800 K			
Prototype	Material	EFF_{max}	ρ	S	$S^2\sigma/\tau$	Prototype	Material	EFF_{max}	ρ	S	$S^2\sigma/\tau$
pro-C	As_2	1.24	2.84	507.80	1.45	pro-MoS_2	WTe_2	0.57	1.64	501.87	0.46
pro-GeSe	GeTe	1.08	3.19	508.41	1.37	pro-GaSe	In_2S_2	0.57	0.41	509.15	0.18
pro-PbS	Pb_2Se_2	1.01	1.05	510.21	0.62	pro-BiTel	BrSbSe	0.56	0.41	498.38	0.18
pro-CdI_2	$PtTe_2$	0.94	10.22	455.44	2.62	pro-GaS	Al_2Se_2	0.56	3.96	508.43	0.82
pro-GeSe	SnTe	0.93	3.61	509.52	1.28	pro-GaS	In_2S_2	0.56	0.42	508.51	0.18
pro-CH	Cd_2Se_2	0.92	0.53	508.48	0.36	pro-GeS_2	GeS_2	0.56	1.54	500.70	0.44
pro-GeSe	GeSe	0.92	3.95	509.89	1.34	pro-MoSSe	ISbSe	0.55	3.29	510.38	0.71
pro-CH	Zn_2Te_2	0.90	0.33	440.13	0.26	pro-MoS_2	WO_2	0.55	1.30	509.07	0.38
pro-CH	Cd_2Te_2	0.88	0.27	469.67	0.22	pro-MoSSe	ISSb	0.55	2.81	508.59	0.64
pro-CH	Zn_2Se_2	0.83	0.24	508.26	0.19	pro-BiTel	AsBrTe	0.54	0.30	511.82	0.14
pro-GaS	Al_2Te_2	0.81	3.87	509.26	1.17	pro-Ti_2CO_2	Zr_2CO_2	0.54	5.16	498.13	0.93
pro-CdI_2	$PtSe_2$	0.80	3.94	511.82	1.18	pro-MoSSe	BiBrTe	0.53	5.60	506.64	0.99
pro-CdI_2	$PdSe_2$	0.80	9.63	421.19	2.15	pro-CdI_2	SrI_2	0.53	4.03	507.18	0.80
pro-GaS	Ga_2Se_2	0.78	0.33	507.27	0.22	pro-MoSSe	WSTe	0.53	6.85	513.47	1.11
pro-CdI_2	$HfSe_2$	0.75	12.08	380.66	2.29	pro-CdI_2	$ZnBr_2$	0.53	3.32	508.60	0.72
pro-GaS	Ga_2S_2	0.75	2.93	508.87	0.89	pro-GaS	Al_2S_2	0.52	4.08	509.57	0.77
pro-BiTel	HfSSe	0.74	5.65	461.88	1.38	pro-CdI_2	CdI_2	0.51	2.52	509.57	0.56
pro-GeSe	GeS	0.74	5.02	510.53	1.27	pro-BiTel	BiClS	0.51	0.47	508.86	0.18
pro-CdI_2	GeS_2	0.74	6.56	387.88	1.50	pro-CdI_2	RuI_2	0.51	9.90	504.94	1.38
pro-CH	Zn_2S_2	0.73	0.45	505.70	0.25	pro-BiTel	AsBrSe	0.51	0.36	507.65	0.15
pro-GeSe	PbTe	0.72	0.90	505.36	0.40	pro-MoSSe	BrSbSe	0.50	5.28	510.51	0.89
pro-CdI_2	HfS_2	0.70	3.70	508.31	0.99	pro-BiTel	BiITe	0.50	0.33	512.63	0.14
pro-CdI_2	PdS_2	0.69	5.57	510.95	1.27	pro-CdI_2	$MgBr_2$	0.50	0.55	507.77	0.20
pro-CdI_2	$SnSe_2$	0.69	5.30	414.21	1.23	pro-GeS_2	$GeSe_2$	0.50	10.41	310.97	1.33
pro-CdI_2	PtS_2	0.68	5.53	512.38	1.25	pro-GaS	Ga_2O_2	0.50	0.54	508.45	0.19
pro-BiTel	ClSbTe	0.67	0.26	509.41	0.16	pro-MoSSe	ISbTe	0.50	3.29	505.47	0.65
pro-CH	Cd_2S_2	0.66	0.35	507.63	0.20	pro-CdI_2	CaI_2	0.49	4.16	508.35	0.75
pro-GaSe	Ga_2S_2	0.66	0.46	507.87	0.23	pro-CdI_2	GeO_2	0.49	0.57	508.93	0.20
pro-BiTel	BiClTe	0.66	0.26	510.62	0.16	pro-BiTel	AsClS	0.49	0.42	510.70	0.16
pro-MoSSe	AsISe	0.65	4.68	473.19	1.07	pro-MoSSe	AsITe	0.49	4.41	449.91	0.77
pro-BiTel	BiBrTe	0.65	0.27	510.60	0.16	pro-MoSSe	BiISe	0.49	3.75	510.68	0.69
pro-BiTel	BrSbTe	0.64	0.27	507.94	0.16	pro-CdI_2	SnO_2	0.48	0.60	508.19	0.20
pro-CdI_2	NiS_2	0.64	31.36	387.10	3.74	pro-MoS_2	MoO_2	0.48	2.00	484.08	0.44
pro-CdI_2	SnS_2	0.64	2.21	507.76	0.63	pro-CdI_2	GeI_2	0.48	0.39	511.34	0.15
pro-Ti_2CO_2	Hf_2CO_2	0.64	3.92	500.64	0.92	pro-BiTel	BiBrS	0.48	0.47	510.25	0.17
pro-Ti_2CO_2	Y_2CF_2	0.63	2.96	504.48	0.77	pro-MoSSe	BrSSb	0.48	3.66	510.44	0.66
pro-CdI_2	MgI_2	0.63	2.20	509.27	0.62	pro-MoSSe	BrSbTe	0.47	4.18	505.73	0.72
pro-CdI_2	ZnI_2	0.63	2.09	509.05	0.60	pro-GeSe	SnS	0.47	5.25	508.86	0.82
pro-BiTel	ZrSSe	0.62	8.11	435.86	1.47	pro-BiTel	BrSSb	0.47	0.47	508.90	0.17
pro-GeSe	SnSe	0.62	5.25	510.19	1.10	pro-MoSSe	BiBrSe	0.46	6.30	510.71	0.93
pro-MoS_2	WS_2	0.62	2.12	507.88	0.60	pro-MoSSe	BiITe	0.46	4.22	508.15	0.71
pro-BiTel	ClSbSe	0.61	0.36	506.41	0.18	pro-CH	Ag_2Cl_2	0.46	0.58	508.74	0.19
pro-BiTel	AsClTe	0.61	0.29	511.59	0.16	pro-MoSSe	BiClSe	0.46	7.78	512.03	1.06
pro-CdI_2	$ZrSe_2$	0.61	20.67	334.90	2.62	pro-GaSe	Al_2S_2	0.46	3.35	508.05	0.60
pro-BiTel	BiClSe	0.60	0.36	508.70	0.18	pro-CdI_2	$SrBr_2$	0.45	0.77	508.08	0.22
pro-CdI_2	ZrS_2	0.60	4.07	507.82	0.90	pro-CdI_2	$PbBr_2$	0.45	0.57	508.80	0.18
pro-MoS_2	WSe_2	0.60	3.94	509.11	0.87	pro-CH	Cu_2I_2	0.45	0.54	509.74	0.17
pro-MoSSe	AsBrS	0.60	3.30	509.99	0.78	pro-BiTel	ISbTe	0.45	0.40	497.41	0.14
pro-MoSSe	WSSe	0.59	4.39	510.31	0.92	pro-GaSe	Al_2Se_2	0.45	3.85	508.56	0.64
pro-BiTel	AsClSe	0.58	0.33	510.40	0.16	pro-GeS_2	ZnI_2	0.44	0.69	508.25	0.20
pro-MoSSe	WSeTe	0.58	4.42	509.78	0.91	pro-GaSe	Hg_2I_2	0.44	0.51	509.31	0.17
pro-BN	BN	0.58	11.68	500.86	1.72	pro-MoSSe	AsBrTe	0.43	2.50	506.96	0.46
pro-Ti_2CO_2	Sc2CF2	0.57	3.91	496.00	0.84	pro-MoSSe	BiBrS	0.43	4.42	509.86	0.68
pro-BiTel	BiBrSe	0.57	0.37	510.05	0.17	pro-CdI_2	$CaBr_2$	0.42	5.25	508.29	0.75

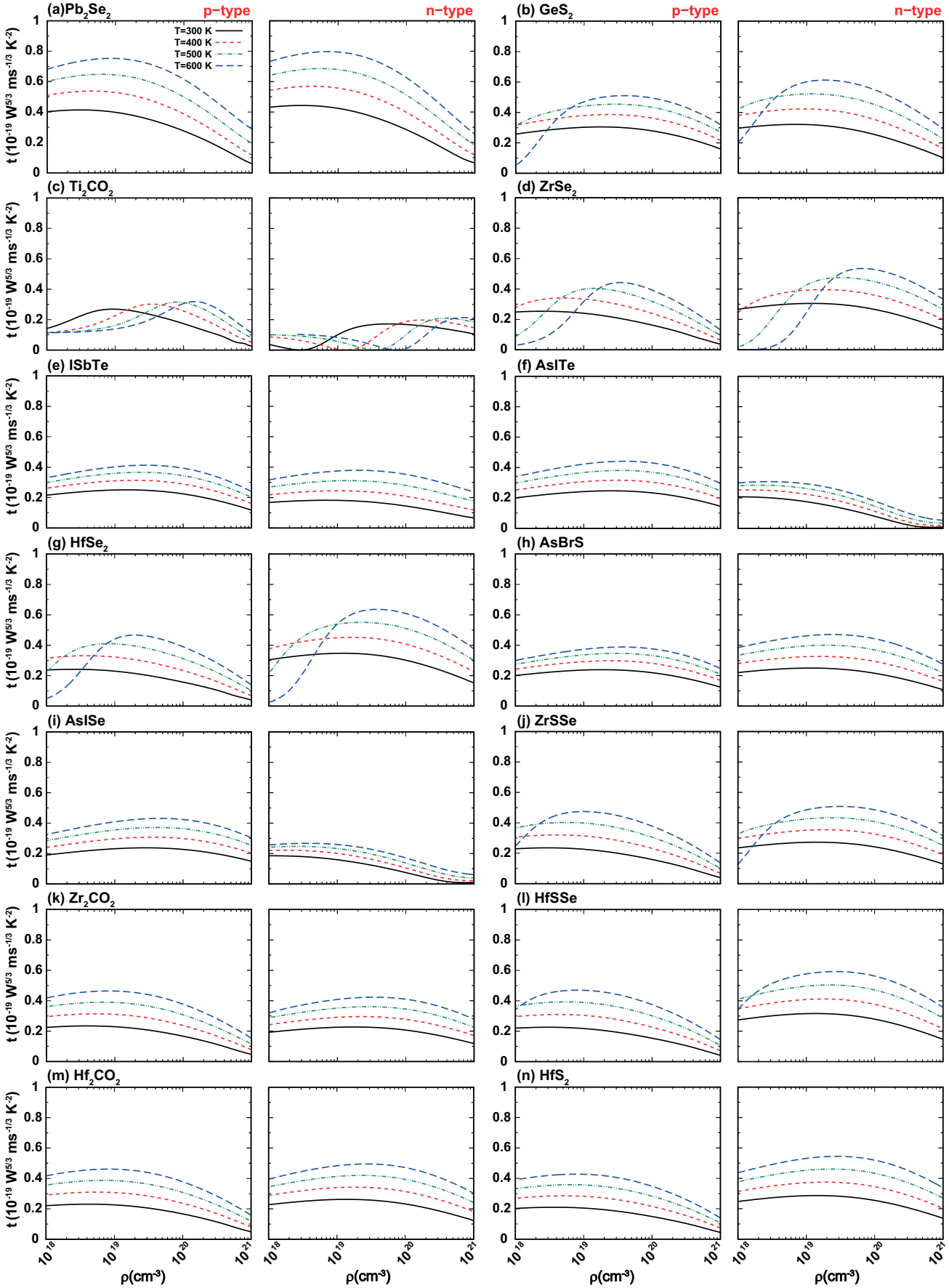


Figure S9. (Color online)Calculated EFF as a function of charge carrier concentration in temperature range of 300-600 K.

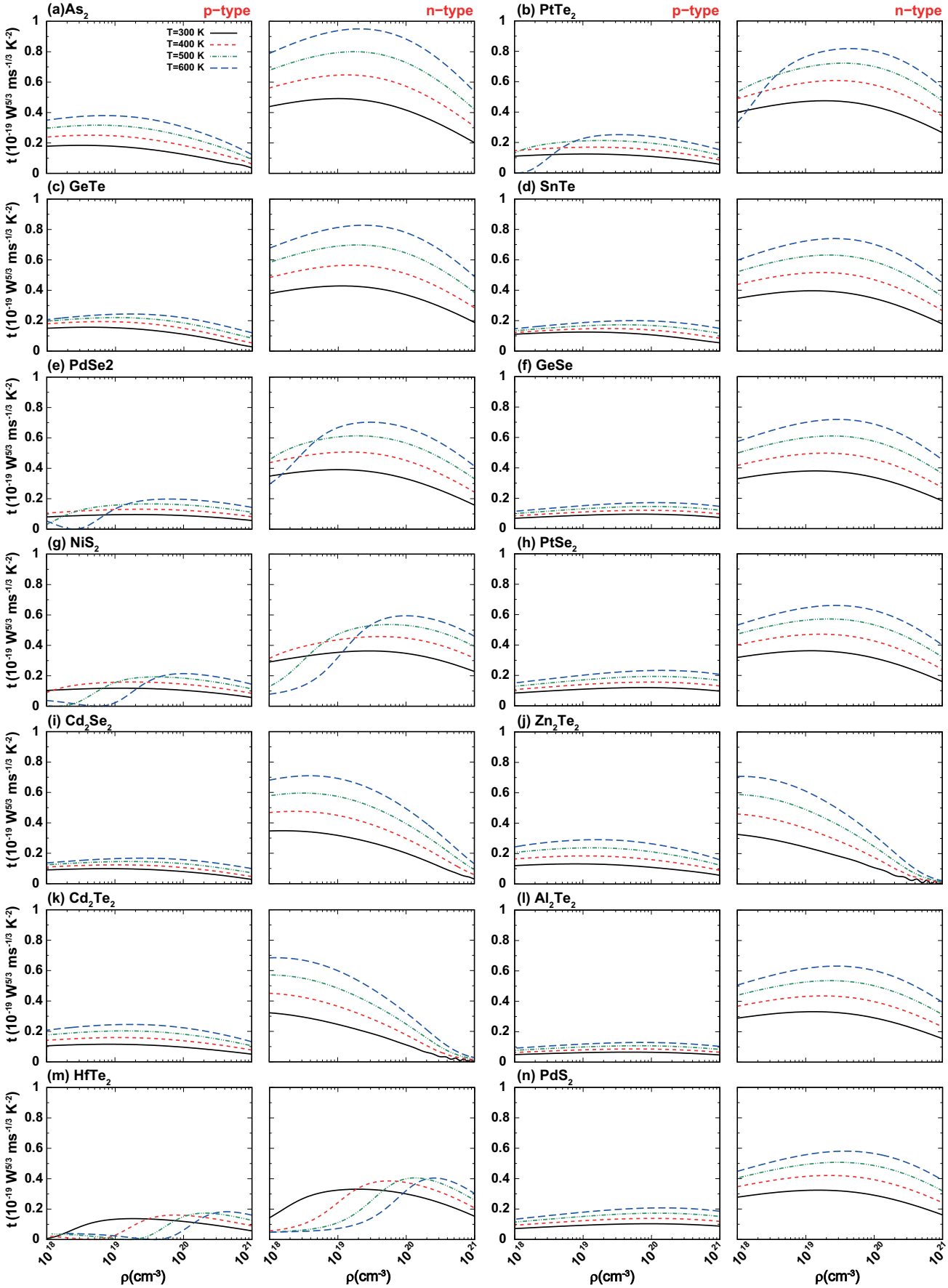


Figure S10. (Color online)Calculated EFF as a function of charge carrier concentration in temperature range of 300-600 K.

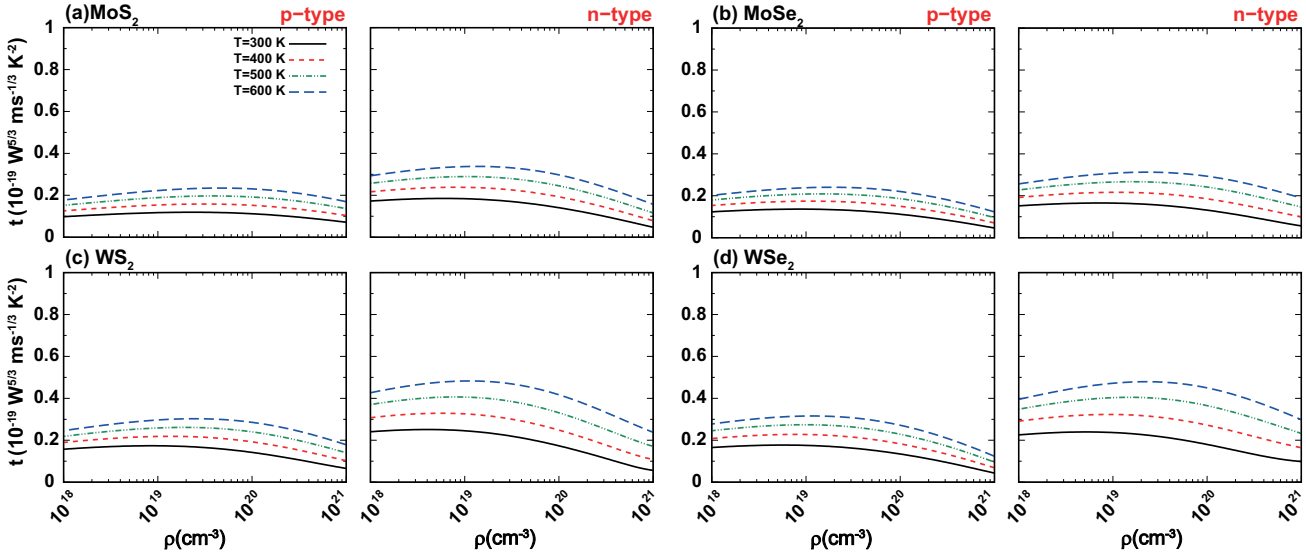


Figure S11. (Color online)Calculated EFF as a function of charge carrier concentration in temperature range of 300-600 K.

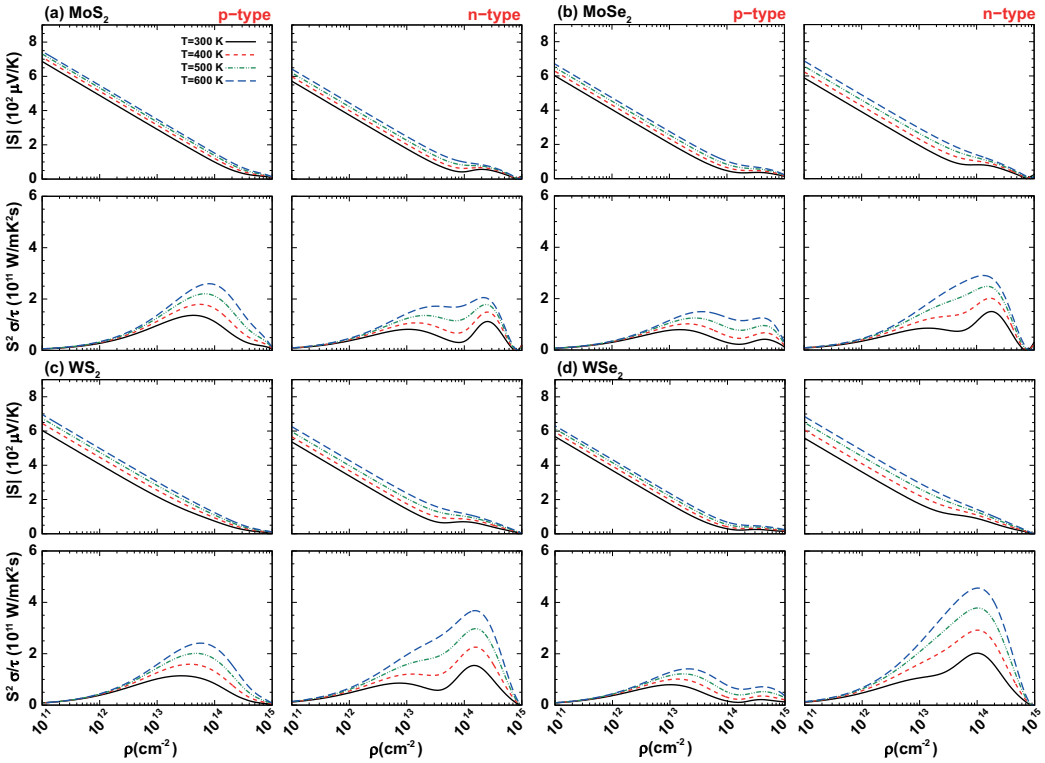


Figure S12. (Color online) Calculated Seebeck coefficient and power factor of MX_2 (M=Mo,W; X=S, Se) materials.

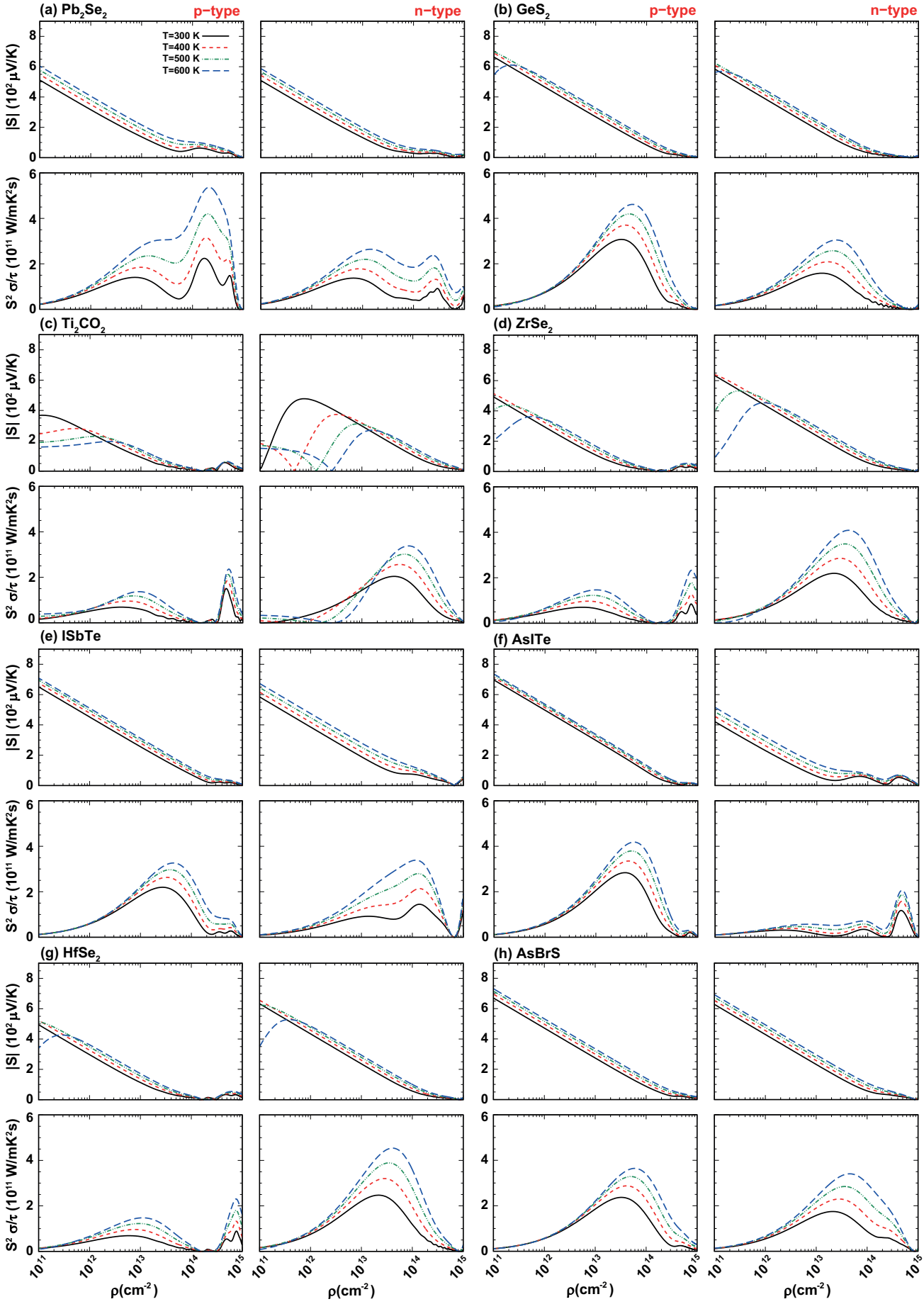


Figure S13. Calculated Seebeck coefficient and power factor of selected 2D materials as a function of charge carrier concentration at different temperatures.

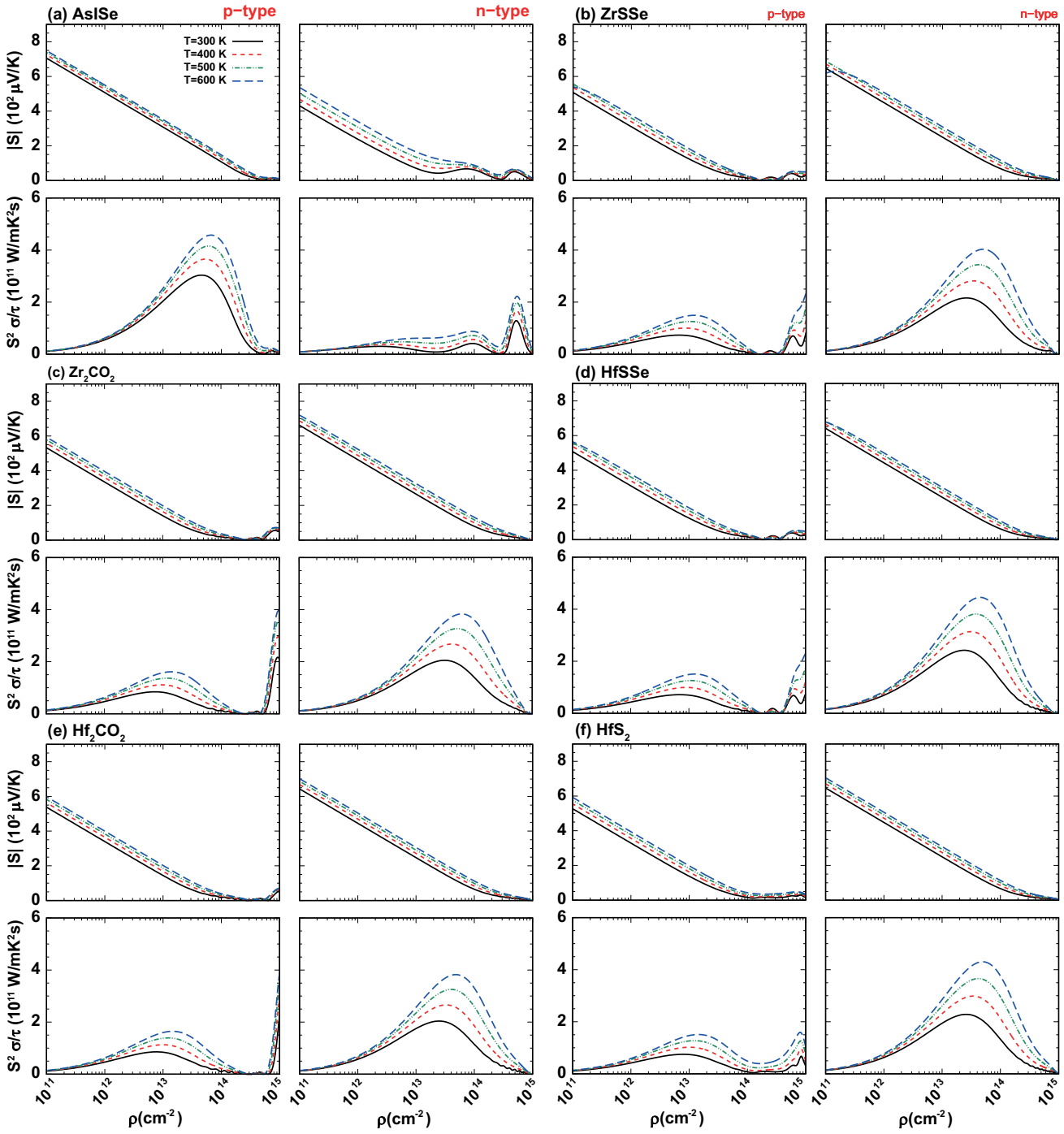


Figure S14. Calculated Seebeck coefficient and power factor of selected 2D materials as a function of charge carrier concentration at different temperatures.

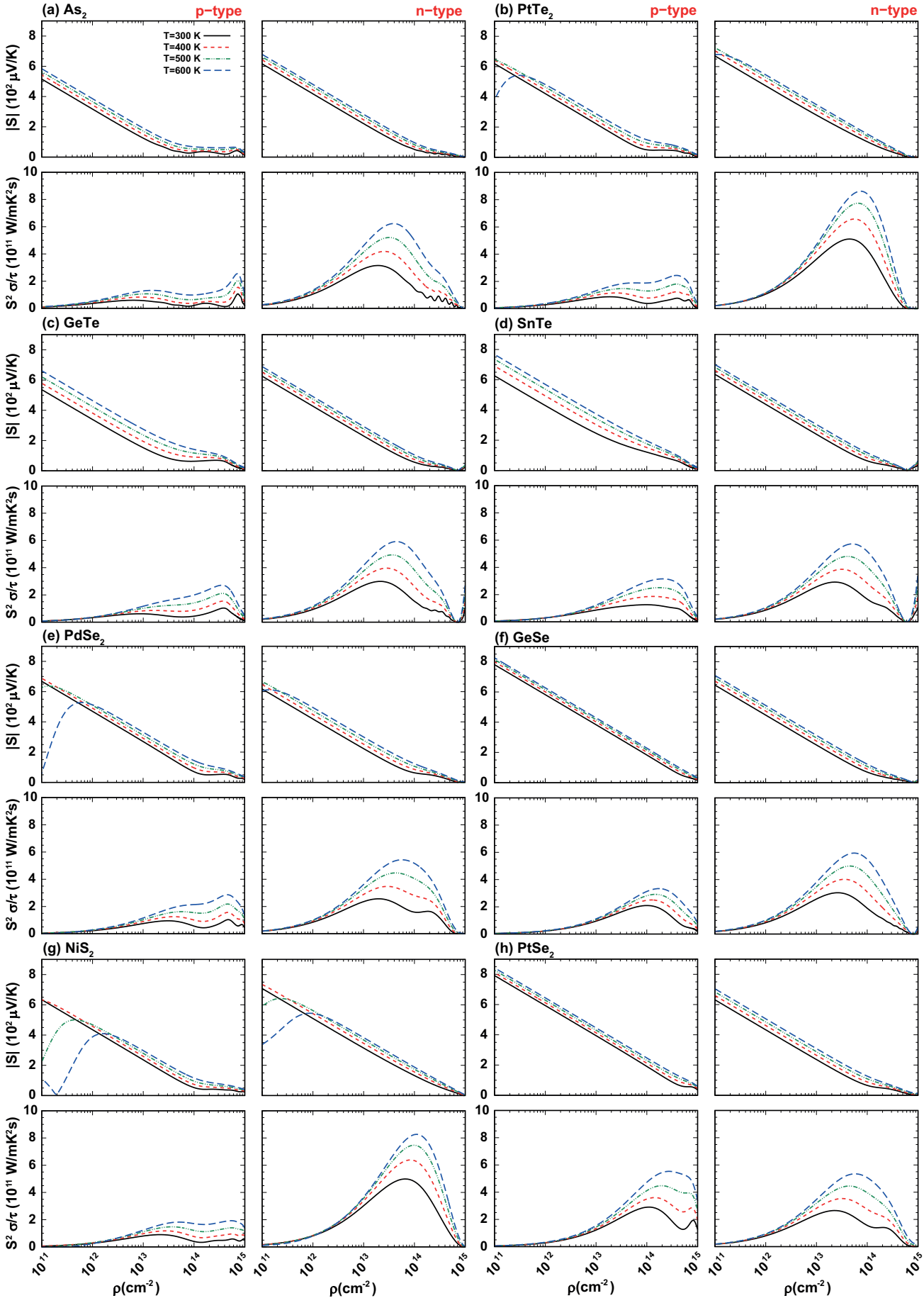


Figure S15. Calculated Seebeck coefficient and power factor of selected 2D materials as a function of charge carrier concentration at different temperatures.

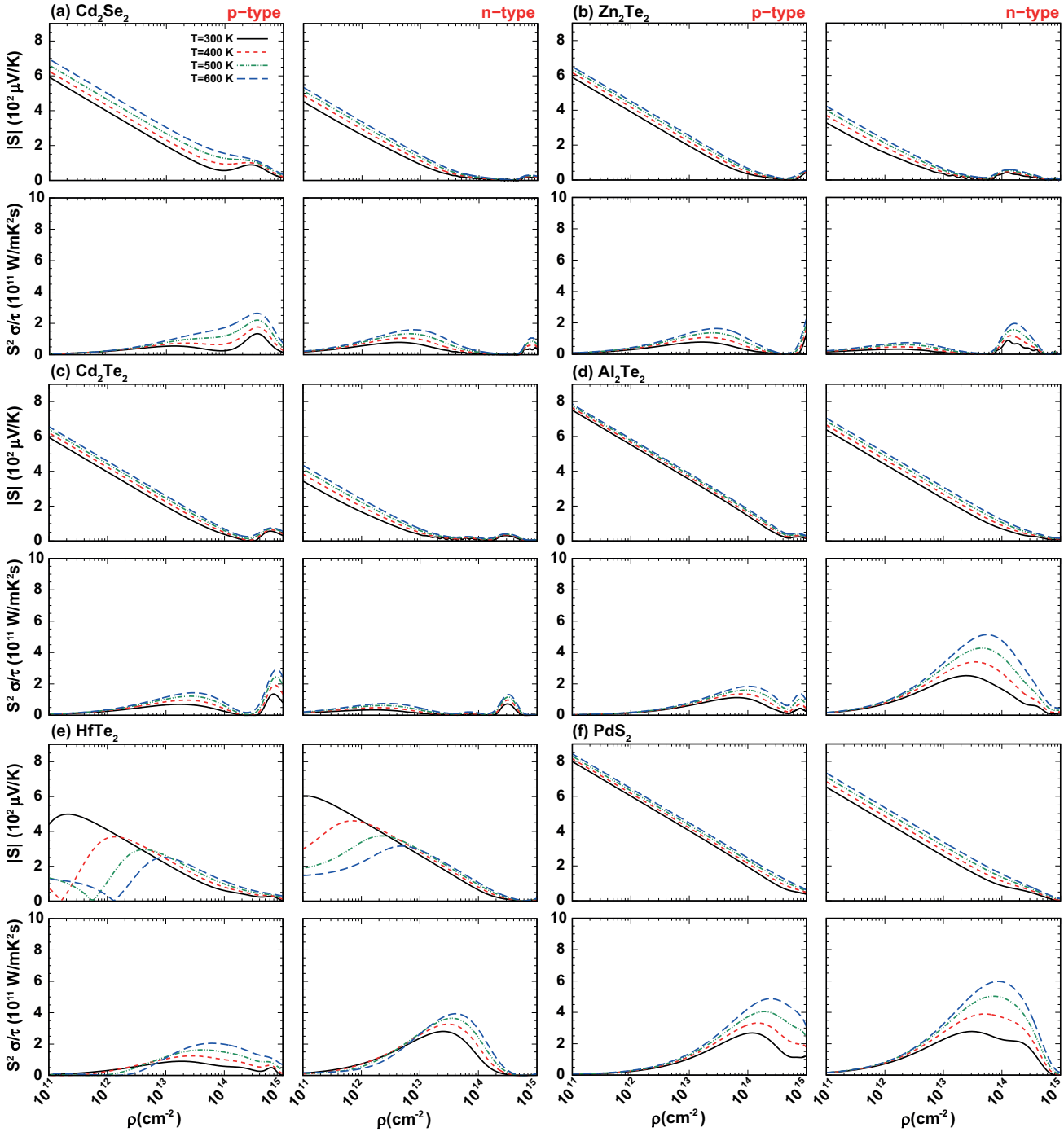


Figure S16. Calculated Seebeck coefficient and power factor of selected 2D materials as a function of charge carrier concentration at different temperatures.

Table S10. Calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) through x-direction for p-type and n-type 2D anisotropic materials at T=300 K.

p-type		T=300 K				n-type		T=300 K			
Prototype	Material	t_x^p(max)	ρ	S	$S^2\sigma/\tau$	Prototype	Material	t_x^n(max)	ρ	S	$S^2\sigma/\tau$
pro-FeOCl	$Ir_2Cl_2O_2$	0.54	0.85	393.28	0.56	pro-WTe_2	Hf_2Cl_4	0.56	1.24	504.47	0.72
pro-AuSe	Au_2S_2	0.34	0.70	506.47	0.31	pro-WTe_2	Zr_2Cl_4	0.56	2.50	507.65	1.13
pro-WTe_2	Os_2O_4	0.27	5.18	497.14	0.94	pro-WTe_2	Hf_2Br_4	0.52	1.49	509.27	0.75
pro-AuSe	Ag_2S_2	0.27	1.51	511.55	0.40	pro-WTe_2	Zr_2Br_4	0.45	2.55	506.75	0.93
pro-FeOCl	$Al_2Br_2O_2$	0.22	1.36	503.67	0.32	pro-AuSe	Ag_2Te_2	0.42	1.24	508.36	0.54
pro-WTe_2	Hf_2Br_4	0.22	2.82	502.25	0.50	pro-AuSe	Au_2Te_2	0.39	1.04	506.23	0.45
pro-WTe_2	Os_2S_4	0.21	1.44	505.78	0.31	pro-FeOCl	$Ir_2Cl_2O_2$	0.38	3.26	445.67	0.91
pro-PdS_2	Pt_2Te_4	0.21	1.08	512.30	0.25	pro-AuSe	Ag_2Se_2	0.34	1.35	506.54	0.47
pro-WTe_2	Ru_2Te_4	0.20	1.84	508.70	0.35	pro-AuSe	Au_2Se_2	0.34	1.25	506.42	0.43
pro-WTe_2	Os_2Te_4	0.20	0.68	506.97	0.18	pro-AuSe	Au_2S_2	0.32	1.91	504.44	0.54
pro-PdS_2	Pd_2Te_4	0.20	1.51	511.86	0.29	pro-AuSe	Ag_2S_2	0.31	1.57	507.79	0.46
pro-AuSe	Au_2O_2	0.19	11.16	221.55	1.00	pro-WTe_2	Mo_2S_4	0.30	39.28	194.42	3.44
pro-FeOCl	$Ga_2Br_2O_2$	0.19	1.72	505.42	0.32	pro-AuSe	Cu_2S_2	0.27	1.14	507.63	0.33
pro-WTe_2	Os_2Se_4	0.19	0.96	508.61	0.21	pro-$CrWS_4$	$Mo_2W_2S_8$	0.20	0.52	507.89	0.14
pro-WTe_2	Ru_2S_4	0.19	2.44	504.60	0.39	pro-CrW_3S_8	MoW_3S_8	0.20	0.44	509.85	0.13
pro-CrW_3S_8	MoW_3Se_8	0.16	0.58	510.74	0.13	pro-FeOCl	$Sc_2I_2S_2$	0.19	3.37	508.34	0.47
pro-WTe_2	Hf_2Cl_4	0.16	1.35	504.16	0.22	pro-$CrWS_4$	$Mo_2W_2Se_8$	0.19	0.66	510.04	0.16
pro-WTe_2	Ru_2Se_4	0.16	1.22	505.55	0.20	pro-WTe_2	Ti_2Cl_4	0.18	4.74	461.98	0.57
pro-PdS_2	Pt_2Se_4	0.15	0.84	510.11	0.15	pro-CrW_3S_8	MoW_3Se_8	0.18	0.57	511.47	0.14
pro-$CrWS_4$	$Mo_2W_2Se_8$	0.15	0.63	511.86	0.12	pro-CrW_3S_8	Mo_3WS_8	0.17	0.53	508.31	0.12
pro-WTe_2	Zr_2Cl_4	0.15	1.31	506.73	0.20	pro-TiS_3	Ti_2O_6	0.16	4.50	507.89	0.49
pro-CrW_3S_8	Mo_3WSe_8	0.14	0.69	510.92	0.12	pro-WTe_2	Os_2Se_4	0.16	1.45	509.07	0.23
pro-PdS_2	Ni_2Te_4	0.13	1.87	511.08	0.24	pro-CrW_3S_8	Mo_3WSe_8	0.15	0.62	510.32	0.12
pro-CrW_3S_8	CrW_3Se_8	0.13	0.64	510.19	0.11	pro-AuSe	Ag_2O_2	0.14	16.91	242.39	0.98
pro-WTe_2	Zr_2Br_4	0.13	1.27	510.02	0.17	pro-FeOCl	$Sc_2Br_2S_2$	0.13	2.51	508.62	0.28
pro-$CrWS_4$	$Cr_2W_2Se_8$	0.12	0.83	511.13	0.12	pro-WTe_2	Ru_2S_4	0.12	0.92	503.00	0.13
pro-CrW_3S_8	CrW_3S_8	0.11	0.88	514.45	0.12	pro-P	P_4	0.12	233.75	114.06	2.09
pro-CrW_3S_8	MoW_3S_8	0.11	0.83	513.89	0.11	pro-WTe_2	Ru_2Te_4	0.12	3.15	506.59	0.28
pro-PdS_2	Pd_2Se_4	0.11	1.23	512.06	0.15	pro-PdS_2	Pt_2Te_4	0.11	2.68	500.83	0.23
pro-FeOCl	$Sc_2Br_2S_2$	0.11	2.11	515.84	0.21	pro-FeOCl	$Al_2Br_2Se_2$	0.11	0.97	508.41	0.11
pro-WTe_2	Fe_2S_4	0.11	7.09	509.81	0.45	pro-AuSe	Au_2O_2	0.10	29.42	236.75	0.99
pro-$CrWS_4$	$Mo_2W_2S_8$	0.11	1.19	511.58	0.14	pro-PdS_2	Pd_2Te_4	0.10	3.04	511.31	0.24
pro-CrW_3S_8	$CrMo_3Se_8$	0.10	0.82	512.77	0.10	pro-WTe_2	Os_2Te_4	0.10	2.03	511.80	0.18
pro-$CrWS_4$	$Cr_2Mo_2Se_8$	0.10	1.00	510.53	0.12	pro-WTe_2	Fe_2Te_4	0.10	5.14	505.19	0.32
pro-AuSe	Ag_2Te_2	0.10	2.47	493.80	0.21	pro-FeOCl	$Sc_2I_2Se_2$	0.10	4.18	501.45	0.28
pro-WTe_2	Fe2Se_4	0.10	5.58	511.14	0.36	pro-PdS_2	Pt_2S_4	0.10	3.02	509.77	0.22

Table S11. Calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) through x-direction for p-type and n-type 2D anisotropic materials at T=600 K.

p-type		T=600 K				n-type		T=600 K			
Prototype	Material	t_x^p(max)	ρ	S_{xx}	$S_{xx}^2\sigma_{xx}/\tau$	Prototype	Material	t_x^n(max)	ρ	S_{xx}	$S_{xx}^2\sigma_{xx}/\tau$
pro-AuSe	Au_2S_2	0.59	1.88	512.31	0.64	pro-WTe_2	Hf_2Cl_4	1.06	2.65	507.32	1.43
pro-WTe_2	Os_2S_4	0.44	4.45	486.83	0.86	pro-WTe_2	Hf_2Br_4	0.92	3.05	507.53	1.37
pro-FeOCl	$Al_2Br_2O_2$	0.44	2.75	506.56	0.62	pro-WTe_2	Zr_2Cl_4	0.90	6.35	455.50	2.19
pro-AuSe	Ag_2S_2	0.44	3.43	511.52	0.72	pro-AuSe	Ag_2Te_2	0.81	3.90	473.98	1.42
pro-WTe_2	Hf_2Br_4	0.43	6.07	503.62	1.02	pro-AuSe	Au_2Te_2	0.79	2.27	507.65	0.96
pro-WTe_2	Os_2Se_4	0.38	2.91	490.69	0.55	pro-WTe_2	Zr_2Br_4	0.75	6.72	452.47	1.88
pro-WTe_2	Os_2Te_4	0.37	2.29	488.26	0.46	pro-AuSe	Au_2Se_2	0.68	2.86	506.02	0.96
pro-WTe_2	Ru_2S_4	0.37	7.15	503.52	0.99	pro-AuSe	Ag_2Se_2	0.67	3.06	505.33	1.00
pro-WTe_2	Hf_2Cl_4	0.36	4.93	496.29	0.76	pro-AuSe	Au_2S_2	0.62	3.75	508.65	1.06
pro-FeOCl	$Ga_2Br_2O_2$	0.34	4.02	509.38	0.62	pro-AuSe	Ag_2S_2	0.61	3.48	507.21	0.98
pro-PdS_2	Pt_2Te_4	0.34	2.30	511.94	0.42	pro-AuSe	Cu_2S_2	0.52	4.38	459.81	0.99
pro-WTe_2	Ru_2Te_4	0.32	7.19	478.51	0.87	pro-FeOCl	$Hf_2Br_2N_2$	0.38	0.42	507.30	0.15
pro-WTe_2	Ru_2Se_4	0.32	4.52	502.41	0.63	pro-FeOCl	$Hf_2Cl_2N_2$	0.38	0.49	508.27	0.16
pro-FeOCl	$Hf_2Cl_2N_2$	0.31	0.49	507.42	0.14	pro-$CrWS_4$	$Mo_2W_2S_8$	0.33	1.21	512.96	0.26
pro-PdS_2	Pd_2Te_4	0.29	2.56	514.81	0.38	pro-FeOCl	$Sc_2I_2S_2$	0.32	7.30	511.58	0.85
pro-FeOCl	$Hf_2Br_2N_2$	0.26	0.55	506.47	0.13	pro-CrW_3S_8	MoW_3S_8	0.31	1.07	513.82	0.23
pro-PdS_2	Pt_2Se_4	0.26	1.94	511.73	0.29	pro-FeOCl	$Ga_2Br_2O_2$	0.30	0.45	508.68	0.13
pro-CrW_3S_8	MoW_3Se_8	0.26	1.13	511.74	0.20	pro-$CrWS_4$	$Mo_2W_2Se_8$	0.30	1.83	513.09	0.32
pro-AuSe	Ag_2Te_2	0.26	8.88	428.91	0.78	pro-TiS_3	Ti_2O_6	0.29	8.33	509.18	0.86
pro-AuSe	Ag_2Se_2	0.25	6.85	486.74	0.65	pro-CrW_3S_8	MoW_3Se_8	0.28	1.83	514.24	0.29
pro-AuSe	Au_2Te_2	0.24	3.61	489.66	0.41	pro-FeOCl	$Al_2Br_2O_2$	0.26	0.52	506.71	0.12
pro-WTe_2	Zr_2Cl_4	0.24	10.86	377.77	0.83	pro-WTe_2	Os_2Se_4	0.26	3.54	489.53	0.42
pro-$CrWS_4$	$Mo_2W_2Se_8$	0.24	1.28	511.53	0.20	pro-CrW_3S_8	Mo_3WS_8	0.26	1.05	514.37	0.19
pro-AuSe	Au_2Se_2	0.23	4.71	489.83	0.47	pro-FeOCl	$Sc_2Br_2S_2$	0.26	7.20	509.14	0.68
pro-CrW_3S_8	Mo_3WSe_8	0.22	1.37	513.52	0.19	pro-WTe_2	Os_2S_4	0.25	3.43	444.28	0.40
pro-WTe_2	Zr_2Br_4	0.22	12.38	383.01	0.82	pro-CrW_3S_8	Mo_3WSe_8	0.23	1.80	514.47	0.24
pro-CrW_3S_8	CrW_3Se_8	0.19	1.21	514.44	0.16	pro-WTe_2	Ru_2S_4	0.23	3.44	486.08	0.36
pro-$CrWS_4$	$Mo_2W_2S_8$	0.18	3.17	511.22	0.27	pro-FeOCl	$Sc_2I_2Se_2$	0.23	9.25	502.03	0.71
pro-WTe_2	Fe_2S_4	0.18	21.39	463.12	0.98	pro-FeOCl	$Al_2Br_2Se_2$	0.22	2.27	505.83	0.27
pro-CrW_3S_8	CrW_3S_8	0.17	2.79	513.07	0.25	pro-WTe_2	Ti_2Cl_4	0.22	63.70	274.72	2.45
pro-PdS_2	Ni_2Te_4	0.17	2.71	513.47	0.24	pro-WTe_2	Ru_2Te_4	0.21	12.30	477.41	0.80
pro-AuSe	Cu_2S_2	0.17	11.47	410.04	0.61	pro-FeOCl	$Sc_2Cl_2Se_2$	0.21	6.78	500.95	0.53
pro-CrW_3S_8	MoW_3S_8	0.17	2.51	512.68	0.23	pro-FeOCl	$Sc_2Br_2Se_2$	0.20	8.00	503.58	0.57
pro-$CrWS_4$	$Cr_2W_2Se_8$	0.17	1.68	509.69	0.17	pro-FeOCl	$Al_2I_2Se_2$	0.20	1.49	500.22	0.18
pro-PdS_2	Pd_2Se_4	0.16	2.76	513.80	0.23	pro-PdS_2	Pt_2Te_4	0.19	5.03	509.54	0.40
pro-$CrWS_4$	$Cr_2W_2S_8$	0.16	3.92	511.64	0.28	pro-FeOCl	$Ga_2I_2S_2$	0.19	1.04	503.92	0.14
pro-WTe_2	Fe2Se_4	0.16	33.03	415.06	1.16	pro-PdS_2	Pd_2S_4	0.18	2.17	508.48	0.21
pro-CrW_3S_8	$CrMo_3Se_8$	0.15	1.61	514.79	0.15	pro-WTe_2	Fe_2Te_4	0.17	73.27	338.16	2.05
pro-FeOCl	$Sc_2Br_2S_2$	0.15	4.76	515.44	0.30	pro-FeOCl	$Al_2Cl_2S_2$	0.16	1.34	496.97	0.13
pro-$CrWS_4$	$Cr_2Mo_2Se_8$	0.14	1.93	510.93	0.16	pro-WTe_2	Os_2Te_4	0.16	6.90	495.36	0.40
pro-CrW_3S_8	Mo_3WS_8	0.14	3.85	509.52	0.25	pro-PdS_2	Pd_2Te_4	0.15	4.88	514.22	0.31
pro-WTe_2	Ti_2O_4	0.13	25.61	468.66	0.81	pro-PdS_2	Ni_2Te_4	0.14	6.74	509.94	0.36
pro-PdS_2	Pt_2S_4	0.13	2.73	513.39	0.18	pro-PdS_2	Ni_2S_4	0.14	2.26	501.48	0.17
pro-CrW_3S_8	Cr_3WSe_8	0.13	2.28	501.46	0.16	pro-PdS_2	Pt_2S_4	0.14	5.86	513.33	0.32
pro-WTe_2	Fe_2Te_4	0.12	79.29	323.39	1.62	pro-PdS_2	Pt_2Se_4	0.14	3.31	509.01	0.21
pro-CrW_3S_8	CrW_3Te_8	0.11	1.75	479.69	0.12	pro-WTe_2	Fe2Se_4	0.12	43.40	408.95	1.04
pro-CrW_3S_8	Cr_3MoSe_8	0.11	2.33	501.51	0.13	pro-WTe_2	Os_2O_4	0.12	0.32	273.92	0.53
pro-$CrWS_4$	$Cr_2W_2Te_8$	0.10	3.92	418.85	0.19	pro-WTe_2	Ru_2Se_4	0.12	12.45	503.78	0.45

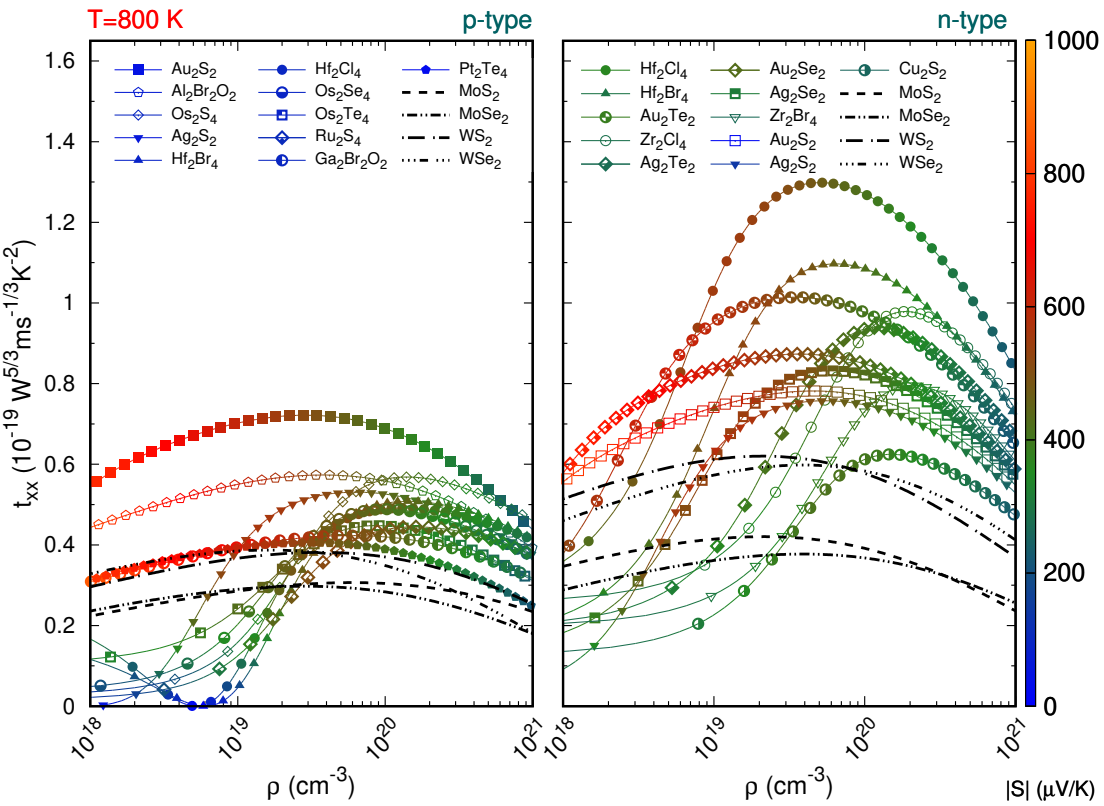


Figure S17. (Color online) Calculated EFF of selected 2D anisotropic materials as a function of charge carrier concentration through x-direction for *p*- type and *n*-type carriers at T=800 K. The corresponding Seebeck coefficient at the same carrier concentration is indicated by color.

Table S12. Calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) through x-direction for p-type and n-type 2D anisotropic materials at T=800 K.

p-type		T=800 K				n-type		T=800 K			
Prototype	Material	t_x^p(max)	ρ	S	$S^2\sigma/\tau$	Prototype	Material	t_x^n(max)	ρ	S	$S^2\sigma/\tau$
pro-AuSe	Au_2S_2	0.72	2.90	511.07	0.87	pro-WTe_2	Hf_2Cl4	1.30	5.00	470.26	2.23
pro-FeOCl	$Al_2Br_2O_2$	0.57	3.77	508.41	0.82	pro-WTe_2	Hf_2Br4	1.10	6.49	455.14	2.25
pro-WTe_2	Os_2S_4	0.57	13.91	420.51	1.94	pro-AuSe	Au_2Te_2	1.01	3.49	494.29	1.37
pro-AuSe	Ag_2S_2	0.53	6.35	481.20	1.08	pro-WTe_2	Zr2Cl4	0.98	18.92	365.61	4.14
pro-WTe_2	Hf_2Br4	0.51	14.52	445.89	1.79	pro-AuSe	Ag_2Te_2	0.94	12.02	391.58	2.92
pro-WTe_2	Hf_2Cl4	0.49	12.78	448.84	1.58	pro-AuSe	Au_2Se_2	0.87	3.71	506.79	1.22
pro-WTe_2	Os_2Se_4	0.49	10.03	421.03	1.34	pro-AuSe	Ag_2Se_2	0.83	6.04	466.28	1.62
pro-WTe_2	Os_2Te_4	0.45	8.67	416.32	1.13	pro-WTe_2	Zr2Br4	0.80	20.75	358.60	3.57
pro-WTe_2	Ru_2S_4	0.44	16.15	455.02	1.68	pro-AuSe	Au_2S_2	0.78	4.57	508.96	1.26
pro-FeOCl	$Ga_2Br_2O_2$	0.42	5.84	511.30	0.81	pro-AuSe	Ag_2S_2	0.76	5.42	487.75	1.37
pro-FeOCl	Hf_2Cl_2N2	0.42	0.67	506.77	0.19	pro-AuSe	Cu_2S_2	0.62	15.07	376.48	2.24
pro-PdS_2	Pt_2Te_4	0.41	3.15	511.73	0.52	pro-FeOCl	$Ir_2Cl_2O_2$	0.61	93.10	225.76	6.65
pro-WTe_2	Ru_2Se_4	0.40	12.32	452.58	1.26	pro-FeOCl	Hf_2Br_2N2	0.49	0.56	509.06	0.19
pro-WTe_2	Os_2O_4	0.38	87.57	279.67	4.55	pro-FeOCl	Hf_2Cl_2N2	0.49	0.66	508.53	0.22
pro-AuSe	Ag_2Se_2	0.38	15.06	439.94	1.34	pro-FeOCl	$Ga_2Br_2O_2$	0.40	0.62	506.71	0.17
pro-AuSe	Au_2Te_2	0.37	6.52	459.88	0.75	pro-FeOCl	$Sc_2I_2S_2$	0.39	9.19	512.62	1.00
pro-AuSe	Au_2Se_2	0.36	6.78	486.56	0.76	pro-$CrWS_4$	$Mo_2W_2S_8$	0.39	1.96	512.88	0.35
pro-FeOCl	$Hf_2Br_2N_2$	0.35	0.77	506.75	0.18	pro-P	P_4	0.37	145.50	206.90	4.01
pro-AuSe	Ag_2Te_2	0.35	32.35	335.45	2.00	pro-TiS_3	Ti_2O_6	0.36	10.16	511.37	1.00
pro-WTe_2	Ru_2Te_4	0.35	26.51	387.61	1.84	pro-CrW_3S_8	MoW_3S_8	0.36	1.87	514.06	0.32
pro-PdS_2	Pd_2Te_4	0.32	3.26	513.30	0.42	pro-$CrWS_4$	$Mo_2W_2Se_8$	0.35	2.91	514.21	0.41
pro-PdS_2	Pt_2Se_4	0.32	2.89	510.95	0.38	pro-FeOCl	$Al_2Br_2O_2$	0.34	0.69	507.09	0.15
pro-CrW_3S_8	MoW_3Se_8	0.30	1.52	514.09	0.23	pro-CrW_3S_8	MoW_3Se_8	0.32	3.24	513.47	0.41
pro-$CrWS_4$	$Mo_2W_2Se_8$	0.27	1.74	513.31	0.24	pro-FeOCl	$Sc_2Br_2S_2$	0.32	9.29	509.82	0.84
pro-AuSe	Cu_2S_2	0.25	46.02	319.76	1.75	pro-FeOCl	$Sc_2I_2Se_2$	0.31	11.74	503.70	0.93
pro-WTe_2	Zr2Cl4	0.25	44.32	283.94	1.76	pro-FeOCl	$Al_2Br_2Se_2$	0.30	3.30	504.05	0.39
pro-CrW_3S_8	Mo_3WSe_8	0.25	1.93	514.32	0.23	pro-CrW_3S_8	Mo_3WS_8	0.29	1.70	515.21	0.24
pro-WTe_2	Zr2Br4	0.24	51.68	295.86	1.87	pro-WTe_2	Os_2S_4	0.29	13.91	348.53	0.97
pro-FeOCl	$Sc_2Br_2Se_2$	0.24	0.78	506.84	0.12	pro-FeOCl	$Sc_2Cl_2Se_2$	0.29	8.76	503.04	0.71
pro-$CrWS_4$	$Mo_2W_2S_8$	0.23	4.55	510.65	0.37	pro-FeOCl	$Al_2I_2Se_2$	0.28	2.67	501.51	0.32
pro-FeOCl	$Sc_2Cl_2Se_2$	0.22	0.63	507.29	0.10	pro-FeOCl	$Sc_2Br_2Se_2$	0.27	10.59	503.70	0.77
pro-FeOCl	$Al_2I_2Se_2$	0.22	0.81	508.83	0.11	pro-WTe_2	Os_2Se_4	0.27	13.13	394.47	0.88
pro-CrW_3S_8	MoW_3S_8	0.22	4.08	510.04	0.33	pro-FeOCl	$Ga_2I_2S_2$	0.27	2.18	495.36	0.26
pro-CrW_3S_8	CrW_3S_8	0.22	4.34	511.66	0.34	pro-CrW_3S_8	Mo_3WSe_8	0.26	3.12	514.72	0.32
pro-CrW_3S_8	CrW_3Se_8	0.21	1.89	504.53	0.19	pro-FeOCl	$Al_2I_2S_2$	0.26	0.63	506.43	0.11
pro-FeOCl	$Sc_2I_2Se_2$	0.21	0.84	505.99	0.11	pro-WTe_2	Ru_2S_4	0.25	14.12	393.81	0.84
pro-FeOCl	$Al_2Br_2S_2$	0.21	0.82	509.51	0.11	pro-WTe_2	Ru_2Te_4	0.25	44.25	386.26	1.77
pro-FeOCl	$Al_2Br_2Se_2$	0.20	0.67	508.80	0.09	pro-PdS_2	Pt_2Te_4	0.24	6.44	510.00	0.49
pro-FeOCl	$Al_2Cl_2S_2$	0.20	0.79	508.95	0.10	pro-WTe_2	Mo_2S_4	0.24	158.41	121.40	3.98
pro-$CrWS_4$	$Cr_2W_2S_8$	0.19	6.15	502.11	0.39	pro-FeOCl	$Al_2Cl_2S_2$	0.24	2.59	495.36	0.26
pro-PdS_2	Pd_2Se_4	0.19	4.01	513.77	0.28	pro-PdS_2	Pd_2S_4	0.23	3.07	505.06	0.28
pro-CrW_3S_8	Mo_3WS_8	0.19	5.77	507.71	0.36	pro-FeOCl	$Al_2Br_2S_2$	0.21	0.91	505.05	0.12
pro-WTe_2	Ti_2O_4	0.19	22.28	491.63	0.87	pro-WTe_2	Os_2Te_4	0.18	24.84	414.84	0.91
pro-WTe_2	Fe_2S_4	0.18	68.36	366.76	1.80	pro-PdS_2	Pt_2Se_4	0.17	5.00	511.05	0.29
pro-$CrWS_4$	$Cr_2W_2Se_8$	0.18	4.85	443.36	0.30	pro-PdS_2	Ni_2Te_4	0.17	11.09	473.60	0.49
pro-PdS_2	Ni_2Te_4	0.17	6.30	455.49	0.35	pro-PdS_2	Pd_2Te_4	0.17	5.73	512.88	0.31
pro-FeOCl	$Sc_2Br_2S_2$	0.17	6.50	515.66	0.35	pro-PdS_2	Ni_2S_4	0.16	6.55	428.41	0.33
pro-PdS_2	Pt_2S_4	0.17	4.59	510.44	0.27	pro-PdS_2	Pt_2S_4	0.16	7.21	516.13	0.34
pro-CrW_3S_8	$CrMo_3Se_8$	0.16	2.58	502.33	0.18	pro-WTe_2	Ru_2Se_4	0.14	34.20	439.33	0.87
pro-WTe_2	Fe_2Se_4	0.15	112.43	316.26	2.05	pro-$CrWS_4$	$Cr_2W_2S_8$	0.13	7.64	499.44	0.30
pro-$CrWS_4$	$Cr_2Mo_2Se_8$	0.14	5.12	450.05	0.25	pro-WTe_2	Fe_2Se_4	0.13	151.15	317.61	2.14
pro-CrW_3S_8	Cr_3WSe_8	0.13	7.48	428.69	0.30	pro-WTe_2	Os_2O_4	0.13	0.66	218.43	0.89
pro-TiS_3	Ti_2O_6	0.13	17.45	503.86	0.51	pro-PdS_2	Pd_2Se_4	0.12	5.51	511.60	0.22
pro-TiS_3	Hf_2O_6	0.11	15.52	501.63	0.42	pro-$CrWS_4$	$Cr_2W_2Se_8$	0.12	10.97	459.48	0.35

Table S13. Calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) through y-direction for p-type and n-type 2D anisotropic materials at T=300 K.

p-type		T=300 K				n-type		T=300 K			
Prototype	Material	t_y^p(max)	ρ	S_{yy}	$S_{yy}^2\sigma_{yy}/\tau$	Prototype	Material	t_y^n(max)	ρ	S_{yy}	$S_{yy}^2\sigma_{yy}/\tau$
pro-FeOCl	$Ga_2I_2S_2$	0.56	0.98	507.93	0.64	pro-P	P_4	0.45	0.25	509.69	0.20
pro-FeOCl	$Al_2I_2S_2$	0.56	1.09	504.75	0.69	pro-FeOCl	$Al_2I_2Se_2$	0.40	0.28	506.25	0.19
pro-P	P_4	0.55	0.45	509.03	0.37	pro-FeOCl	$Al_2Cl_2S_2$	0.37	0.31	506.45	0.18
pro-FeOCl	$Al_2Br_2Se_2$	0.31	0.25	506.16	0.14	pro-FeOCl	$Al_2Br_2S_2$	0.36	0.26	507.74	0.16
pro-FeOCl	$Sc_2I_2S_2$	0.27	0.30	506.56	0.14	pro-FeOCl	$Al_2I_2S_2$	0.34	0.23	507.89	0.14
pro-FeOCl	$Al_2I_2Se_2$	0.26	0.24	506.30	0.12	pro-TiS_3	Hf_2O_6	0.34	2.13	506.14	0.62
pro-FeOCl	$Al_2Cl_2S_2$	0.26	0.29	509.17	0.13	pro-FeOCl	$Ga_2I_2S_2$	0.33	0.26	509.79	0.15
pro-FeOCl	$Al_2Br_2S_2$	0.23	0.30	506.14	0.12	pro-TiS_3	Zr_2O_6	0.27	2.11	504.73	0.49
pro-CrW_3S_8	MoW_3Se_8	0.17	0.64	508.74	0.14	pro-PdS_2	Ni_2Se_4	0.26	3.74	506.93	0.70
pro-CrW_3S_8	MoW_3S_8	0.16	1.23	508.49	0.21	pro-PdS_2	Pd_2Te_4	0.25	2.90	512.25	0.56
pro-$CrWS_4$	$Mo_2W_2Se_8$	0.15	0.71	508.14	0.14	pro-WTe_2	Os_2O_4	0.25	1.03	429.47	0.29
pro-CrW_3S_8	CrW_3Te_8	0.15	0.76	510.43	0.15	pro-PdS_2	Pd_2Se_4	0.23	2.66	506.87	0.49
pro-CrW_3S_8	CrW_3Se_8	0.15	0.75	509.96	0.14	pro-PdS_2	Ni_2Te_4	0.22	3.02	513.08	0.52
pro-CrW_3S_8	CrW_3S_8	0.15	1.18	511.95	0.19	pro-PdS_2	Pt_2Te_4	0.22	1.37	514.72	0.30
pro-CrW_3S_8	Mo_3WSe_8	0.15	0.80	506.67	0.14	pro-CrW_3S_8	MoW_3S_8	0.22	0.51	506.44	0.15
pro-$CrWS_4$	$Mo_2W_2S_8$	0.14	1.55	512.43	0.22	pro-PdS_2	Pd_2S_4	0.21	1.00	508.97	0.24
pro-PdS_2	Pt_2S_4	0.14	1.85	508.73	0.24	pro-PdS_2	Ni_2S_4	0.21	1.13	507.67	0.25
pro-WTe_2	Os_2Te_4	0.13	0.60	509.69	0.11	pro-$CrWS_4$	$Mo_2W_2S_8$	0.20	0.55	507.64	0.15
pro-WTe_2	Ti_2O_4	0.13	2.04	509.47	0.23	pro-PdS_2	Pt_2Se_4	0.20	0.95	509.22	0.22
pro-AuSe	Au_2Te_2	0.12	0.91	510.58	0.13	pro-CrW_3S_8	MoW_3Se_8	0.20	0.73	506.47	0.18
pro-CrW_3S_8	$CrMo_3Se_8$	0.12	1.02	507.16	0.14	pro-FeOCl	$Al_2Br_2Se_2$	0.19	0.81	510.36	0.18
pro-$CrWS_4$	$Cr_2W_2Se_8$	0.12	0.95	508.42	0.14	pro-$CrWS_4$	$Mo_2W_2Se_8$	0.19	0.75	509.75	0.17
pro-$CrWS_4$	$Cr_2W_2S_8$	0.12	1.69	509.63	0.20	pro-CrW_3S_8	Mo_3WS_8	0.18	0.60	506.75	0.14
pro-CrW_3S_8	Mo_3WS_8	0.12	2.05	509.13	0.22	pro-CrW_3S_8	CrW_3Te_8	0.17	0.69	511.59	0.15
pro-$CrWS_4$	$Cr_2W_2Te_8$	0.12	0.96	511.26	0.13	pro-CrW_3S_8	Mo_3WSe_8	0.17	0.74	507.58	0.15
pro-AuSe	Au_2Se_2	0.12	1.29	506.27	0.16	pro-PdS_2	Pt_2S_4	0.17	3.77	509.36	0.45
pro-PdS_2	Pd_2Te_4	0.11	4.45	484.16	0.35	pro-CrW_3S_8	CrW_3S_8	0.14	0.82	512.18	0.13
pro-CrW_3S_8	Cr_3WSe_8	0.11	1.16	508.10	0.14	pro-CrW_3S_8	CrW_3Se_8	0.13	0.80	513.02	0.13
pro-$CrWS_4$	$Cr_2Mo_2Se_8$	0.11	1.18	506.91	0.14	pro-CrW_3S_8	$CrMo_3Se_8$	0.13	0.95	510.81	0.14
pro-CrW_3S_8	Cr_3WTe_8	0.11	1.08	510.02	0.13	pro-CrW_3S_8	Cr_3WTe_8	0.12	0.96	512.79	0.13
pro-CrW_3S_8	Cr_3MoSe_8	0.10	1.26	508.21	0.14	pro-CrW_3S_8	Cr_3WSe_8	0.12	1.13	513.66	0.14
pro-PdS_2	Pt_2Se_4	0.10	1.22	502.26	0.13	pro-CrW_3S_8	Cr_3MoSe_8	0.12	1.20	510.05	0.15
pro-WTe_2	Ru_2Se_4	0.10	0.90	509.58	0.11	pro-$CrWS_4$	$Cr_2W_2Te_8$	0.11	1.09	512.05	0.14
pro-$CrWS_4$	Cr_2Mo_2Te8	0.10	1.26	509.45	0.13	pro-WTe_2	Ru_2Te_4	0.11	1.94	515.72	0.19

Table S14. Calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) through y-direction for p-type and n-type 2D anisotropic materials at T=600 K.

p-type		T=600 K				n-type		T=600 K			
Prototype	Material	t_y^p(max)	ρ	S_{yy}	$S_{yy}^2\sigma_{yy}/\tau$	Prototype	Material	t_y^n(max)	ρ	S_{yy}	$S_{yy}^2\sigma_{yy}/\tau$
pro-FeOCl	$Ga_2I_2S_2$	1.05	1.87	507.51	1.14	pro-P	P_4	0.84	0.59	507.53	0.41
pro-FeOCl	$Al_2I_2S_2$	1.02	1.92	510.33	1.13	pro-FeOCl	$Al_2I_2Se_2$	0.73	0.94	510.11	0.49
pro-P	P_4	0.97	0.77	510.19	0.59	pro-FeOCl	$Al_2Cl_2S_2$	0.69	0.80	507.31	0.42
pro-FeOCl	$Al_2Br_2Se_2$	0.59	0.48	509.77	0.26	pro-TiS_3	Hf_2O_6	0.69	4.80	506.52	1.39
pro-FeOCl	$Sc_2I_2S_2$	0.51	0.64	507.40	0.27	pro-FeOCl	$Al_2Br_2S_2$	0.69	0.53	506.37	0.32
pro-FeOCl	$Al_2Cl_2S_2$	0.50	0.60	506.79	0.25	pro-FeOCl	$Al_2I_2S_2$	0.66	0.45	506.80	0.27
pro-FeOCl	$Al_2I_2Se_2$	0.46	0.47	509.64	0.20	pro-FeOCl	$Ga_2I_2S_2$	0.63	0.83	505.07	0.39
pro-FeOCl	$Al_2Br_2S_2$	0.43	0.57	508.04	0.21	pro-TiS_3	Zr_2O_6	0.55	4.91	505.57	1.12
pro-FeOCl	$Sc_2I_2Se_2$	0.43	0.45	509.42	0.18	pro-FeOCl	$Al_2Br_2Se_2$	0.42	2.48	503.80	0.54
pro-FeOCl	$Ga_2Br_2O_2$	0.40	27.41	439.78	2.53	pro-PdS_2	Pd_2Se_4	0.41	4.26	510.70	0.76
pro-FeOCl	$Sc_2Cl_2Se_2$	0.39	0.48	507.60	0.17	pro-PdS_2	Ni_2Se_4	0.40	5.35	514.23	0.86
pro-FeOCl	$Sc_2Br_2Se_2$	0.37	0.47	508.59	0.16	pro-FeOCl	$Al_2Br_2O_2$	0.39	0.50	507.72	0.17
pro-FeOCl	$Hf_2Br_2N_2$	0.35	0.47	508.12	0.15	pro-CrW_3S_8	MoW_3S_8	0.39	1.33	511.01	0.33
pro-FeOCl	$Hf_2Cl_2N_2$	0.34	0.44	507.89	0.14	pro-FeOCl	$Ga_2Br_2O_2$	0.39	0.42	508.70	0.16
pro-CrW_3S_8	MoW_3Se_8	0.29	1.33	509.64	0.25	pro-PdS_2	Pd_2S_4	0.38	1.90	509.97	0.42
pro-CrW_3S_8	MoW_3S_8	0.28	3.06	511.16	0.42	pro-PdS_2	Ni_2S_4	0.38	2.39	501.18	0.48
pro-$CrWS_4$	$Mo_2W_2Se_8$	0.27	1.49	510.30	0.25	pro-$CrWS_4$	$Mo_2W_2S_8$	0.38	1.47	508.64	0.34
pro-$CrWS_4$	$Mo_2W_2S_8$	0.26	3.72	508.74	0.45	pro-CrW_3S_8	MoW_3Se_8	0.35	2.17	511.22	0.42
pro-CrW_3S_8	CrW_3Se_8	0.26	1.54	511.25	0.25	pro-PdS_2	Pd_2Te_4	0.35	4.76	514.95	0.70
pro-CrW_3S_8	Mo_3WSe_8	0.26	1.65	510.94	0.26	pro-$CrWS_4$	$Mo_2W_2Se_8$	0.34	2.13	511.07	0.39
pro-CrW_3S_8	CrW_3S_8	0.25	3.31	510.96	0.40	pro-PdS_2	Ni_2Te_4	0.33	5.64	512.37	0.74
pro-PdS_2	Pt_2S_4	0.25	3.52	509.36	0.41	pro-CrW_3S_8	Mo_3WS_8	0.33	1.31	511.05	0.27
pro-AuSe	Au_2Se_2	0.24	2.55	506.54	0.33	pro-FeOCl	$Hf_2Br_2N_2$	0.32	0.39	509.05	0.12
pro-PdS_2	Pt_2Te_4	0.24	5.08	497.01	0.51	pro-PdS_2	Pt_2Te_4	0.32	3.42	514.29	0.52
pro-PdS_2	Pd_2Te_4	0.24	4.95	503.77	0.50	pro-PdS_2	Pt_2Se_4	0.30	2.20	514.20	0.36
pro-AuSe	Au_2Te_2	0.23	1.66	508.68	0.23	pro-CrW_3S_8	Mo_3WSe_8	0.29	2.16	510.66	0.35
pro-CrW_3S_8	Mo_3WS_8	0.23	4.23	506.73	0.43	pro-PdS_2	Pt_2S_4	0.26	6.20	513.86	0.62
pro-CrW_3S_8	CrW_3Te_8	0.23	1.91	478.75	0.25	pro-FeOCl	$Hf_2Cl_2N_2$	0.25	0.44	509.91	0.10
pro-PdS_2	Pt_2Se_4	0.22	2.83	504.83	0.31	pro-WTe_2	Os_2O_4	0.23	13.74	245.27	1.14
pro-$CrWS_4$	$Cr_2W_2S_8$	0.21	4.33	510.95	0.41	pro-CrW_3S_8	CrW_3Te_8	0.23	1.63	473.66	0.22
pro-$CrWS_4$	$Cr_2W_2Se_8$	0.21	2.23	507.33	0.26	pro-FeOCl	$Sc_2Br_2Se_2$	0.20	7.11	505.67	0.53
pro-CrW_3S_8	$CrMo_3Se_8$	0.21	2.19	509.99	0.26	pro-WTe_2	Ti_2O_4	0.18	3.07	509.97	0.26
pro-WTe_2	Ti_2O_4	0.20	5.09	513.17	0.43	pro-CrW_3S_8	CrW_3S_8	0.18	1.41	516.51	0.16
pro-$CrWS_4$	$Cr_2Mo_2Se_8$	0.19	2.84	508.28	0.27	pro-WTe_2	Os_2Te_4	0.17	7.12	502.48	0.45
pro-CrW_3S_8	Cr_3WSe_8	0.18	2.98	497.41	0.27	pro-CrW_3S_8	$CrMo_3Se_8$	0.17	1.45	514.70	0.15
pro-WTe_2	Os_2Te_4	0.18	1.78	471.25	0.19	pro-FeOCl	$Sc_2I_2Se_2$	0.16	7.60	505.53	0.45
pro-$CrWS_4$	$Cr_2W_2Te_8$	0.18	4.59	440.93	0.36	pro-WTe_2	Os_2S_4	0.16	2.57	461.98	0.22
pro-WTe_2	Os_2O_4	0.18	0.23	295.68	0.79	pro-CrW_3S_8	Cr_3MoSe_8	0.16	2.37	494.91	0.20
pro-AuSe	Cu_2S_2	0.18	4.74	437.41	0.36	pro-WTe_2	Ru_2Te_4	0.16	8.42	481.59	0.46
pro-PdS_2	Pd_2Se_4	0.18	4.31	508.57	0.34	pro-CrW_3S_8	CrW_3Se_8	0.16	1.31	517.63	0.13
pro-CrW_3S_8	Cr_3MoSe_8	0.17	3.21	499.13	0.27	pro-CrW_3S_8	Cr_3WSe_8	0.16	2.46	489.96	0.20
pro-PdS_2	Ni_2Te_4	0.17	4.75	508.73	0.34	pro-FeOCl	$Sc_2Cl_2Se_2$	0.15	6.00	504.28	0.35
pro-PdS_2	Pd_2S_4	0.16	4.92	509.44	0.33	pro-$CrWS_4$	$Cr_2W_2Te_8$	0.14	5.40	432.87	0.30
pro-WTe_2	Os_2Se_4	0.16	1.96	492.87	0.18	pro-CrW_3S_8	Cr_3WTe_8	0.14	7.43	369.69	0.37
pro-$CrWS_4$	Cr_2Mo_2Te8	0.15	5.18	455.65	0.32	pro-$CrWS_4$	Cr_2Mo_2Te8	0.13	5.39	448.27	0.28
pro-PdS_2	Ni_2S_4	0.14	5.98	492.41	0.34	pro-WTe_2	Ru_2S_4	0.12	2.55	495.59	0.16
pro-PdS_2	Ni_2Se_4	0.14	6.66	507.34	0.36	pro-AuSe	Cu_2S_2	0.11	6.02	411.61	0.26
pro-TiS_3	Zr_2O_6	0.14	6.60	510.64	0.36	pro-$CrWS_4$	$Cr_2Mo_2Se_8$	0.10	3.54	513.41	0.17
pro-AuSe	Ag_2Se_2	0.14	3.13	505.89	0.22	pro-AuSe	Au_2Te_2	0.10	1.74	510.06	0.10
pro-CrW_3S_8	Cr_3WTe_8	0.14	8.41	379.32	0.40	pro-AuSe	Au_2Se_2	0.10	2.07	511.70	0.11

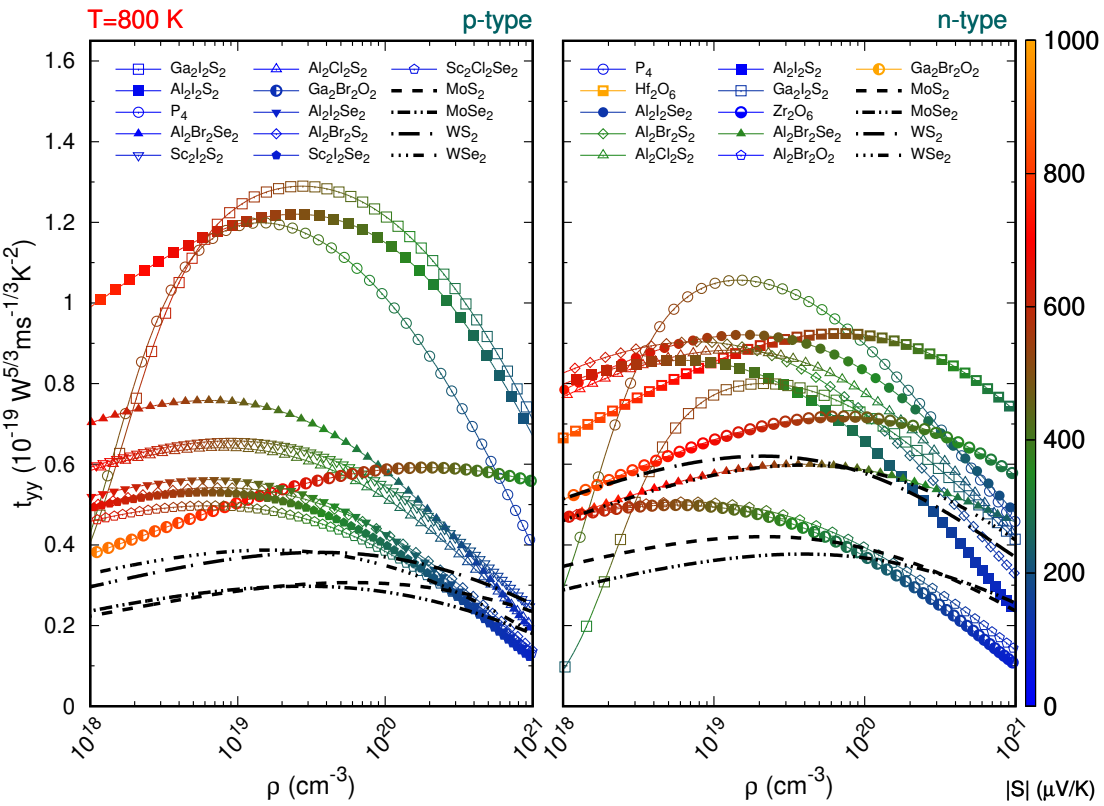


Figure S18. (Color online) Calculated EFF of selected 2D anisotropic materials as a function of charge carrier concentration through y-direction for *p*- type and *n*-type carriers at T=800 K. The corresponding Seebeck coefficient at the same carrier concentration is indicated by color.

Table S15. Calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) through y-direction for p-type and n-type 2D anisotropic materials at T=800 K.

p-type		T=800 K				n-type		T=800 K			
Prototype	Material	t_y^p(max)	ρ	S	$S^2\sigma/\tau$	Prototype	Material	t_y^n(max)	ρ	S	$S^2\sigma/\tau$
pro-FeOCl	$Ga_2I_2S_2$	1.29	2.76	495.38	1.50	pro-P	P_4	1.06	1.46	466.51	0.79
pro-FeOCl	$Al_2I_2S_2$	1.22	2.49	511.42	1.33	pro-TiS_3	Hf_2O_6	0.92	6.67	506.56	1.91
pro-P	P_4	1.20	1.44	474.32	0.90	pro-FeOCl	$Al_2I_2Se_2$	0.92	1.62	510.64	0.74
pro-FeOCl	$Al_2Br_2Se_2$	0.76	0.64	509.19	0.33	pro-FeOCl	$Al_2Br_2S_2$	0.90	0.75	508.38	0.44
pro-FeOCl	$Sc_2I_2S_2$	0.66	0.90	508.96	0.36	pro-FeOCl	$Al_2Cl_2S_2$	0.88	1.33	509.13	0.62
pro-FeOCl	$Al_2Cl_2S_2$	0.64	0.79	507.78	0.32	pro-FeOCl	$Al_2I_2S_2$	0.86	0.60	506.89	0.36
pro-FeOCl	$Ga_2Br_2O_2$	0.59	19.12	481.54	2.48	pro-FeOCl	$Ga_2I_2S_2$	0.80	2.13	470.02	0.77
pro-FeOCl	$Al_2I_2Se_2$	0.56	0.65	510.99	0.25	pro-TiS_3	Zr_2O_6	0.72	7.10	507.59	1.55
pro-FeOCl	$Al_2Br_2S_2$	0.54	0.75	509.68	0.26	pro-FeOCl	$Al_2Br_2Se_2$	0.60	3.87	500.57	0.86
pro-FeOCl	$Sc_2I_2Se_2$	0.53	0.62	510.25	0.23	pro-FeOCl	$Al_2Br_2O_2$	0.51	0.65	509.05	0.22
pro-FeOCl	$Sc_2Cl_2Se_2$	0.50	0.64	508.18	0.22	pro-FeOCl	$Ga_2Br_2O_2$	0.50	0.56	509.20	0.20
pro-FeOCl	$Sc_2Br_2Se_2$	0.46	0.63	509.64	0.20	pro-PdS_2	Pd_2S_4	0.47	2.51	507.04	0.51
pro-FeOCl	$Hf_2Br_2N_2$	0.44	0.60	510.66	0.18	pro-PdS_2	Pd_2Se4	0.47	4.90	512.56	0.79
pro-FeOCl	$Hf_2Cl_2N_2$	0.43	0.57	509.98	0.17	pro-CrW_3S_8	MoW_3S_8	0.46	2.05	513.38	0.43
pro-CrW_3S_8	MoW_3Se_8	0.36	1.89	511.26	0.32	pro-$CrWS_4$	$Mo_2W_2S_8$	0.45	2.21	510.71	0.45
pro-CrW_3S_8	MoW_3S_8	0.35	4.32	509.80	0.55	pro-PdS_2	Ni_2S_4	0.45	6.28	435.94	0.89
pro-$CrWS_4$	$Mo_2W_2S_8$	0.34	5.01	508.81	0.58	pro-PdS_2	Ni_2Se4	0.44	7.53	497.73	0.99
pro-$CrWS_4$	$Mo_2W_2Se_8$	0.33	2.14	511.80	0.33	pro-FeOCl	$Hf_2Br_2N_2$	0.41	0.52	509.23	0.15
pro-AuSe	Au_2Se_2	0.33	3.58	503.73	0.46	pro-CrW_3S_8	MoW_3Se_8	0.40	3.19	513.52	0.50
pro-PdS_2	Pt_2Te_4	0.32	5.51	502.91	0.60	pro-PdS_2	Pd_2Te_4	0.40	5.94	513.04	0.76
pro-CrW_3S_8	CrW_3S_8	0.32	4.76	509.84	0.53	pro-PdS_2	Ni_2Te_4	0.39	9.15	487.70	1.01
pro-CrW_3S_8	CrW_3Se_8	0.31	2.44	504.13	0.33	pro-$CrWS_4$	$Mo_2W_2Se_8$	0.39	3.11	512.90	0.48
pro-CrW_3S_8	Mo_3WSe_8	0.31	2.47	510.35	0.34	pro-CrW_3S_8	Mo_3WS_8	0.38	2.01	511.93	0.36
pro-PdS_2	Pt_2S_4	0.30	4.40	511.61	0.48	pro-PdS_2	Pt_2Te_4	0.37	4.57	514.13	0.60
pro-CrW_3S_8	Mo_3WS_8	0.30	5.50	507.70	0.55	pro-PdS_2	Pt_2Se4	0.33	3.19	515.81	0.42
pro-AuSe	Au_2Te_2	0.30	2.73	486.36	0.34	pro-CrW_3S_8	Mo_3WSe_8	0.33	3.29	513.75	0.42
pro-PdS_2	Pd_2Te_4	0.29	5.07	508.78	0.51	pro-FeOCl	$Hf_2Cl_2N_2$	0.32	0.58	510.45	0.13
pro-PdS_2	Pt_2Se4	0.29	4.08	505.08	0.44	pro-PdS_2	Pt_2S_4	0.28	6.92	515.66	0.59
pro-$CrWS_4$	$Cr_2W_2S_8$	0.27	6.39	504.66	0.55	pro-FeOCl	$Sc_2Br_2Se_2$	0.26	8.77	507.23	0.66
pro-CrW_3S_8	$CrMo_3Se_8$	0.26	3.54	502.70	0.35	pro-FeOCl	$Sc_2I_2Se_2$	0.21	10.01	506.82	0.59
pro-$CrWS_4$	$Cr_2W_2Se_8$	0.25	5.39	464.19	0.46	pro-WTe_2	Ti_2O_4	0.21	4.97	511.69	0.37
pro-WTe_2	Ti_2O_4	0.23	7.30	513.54	0.52	pro-FeOCl	$Sc_2Cl_2Se_2$	0.21	8.42	503.46	0.50
pro-CrW_3S_8	CrW_3Te_8	0.23	6.84	385.59	0.49	pro-CrW_3S_8	CrW_3Te_8	0.20	6.43	365.62	0.40
pro-PdS_2	Pd_2Se4	0.22	5.59	509.13	0.41	pro-WTe_2	$Os2Te_4$	0.19	18.32	433.89	0.77
pro-$CrWS_4$	$Cr_2Mo_2Se_8$	0.22	6.32	471.54	0.45	pro-WTe_2	$Os2S_4$	0.19	9.09	377.13	0.48
pro-CrW_3S_8	Cr_3WSe_8	0.21	9.95	424.83	0.57	pro-WTe_2	$Os2O_4$	0.18	26.10	198.27	1.34
pro-AuSe	Cu_2S_2	0.21	16.60	351.72	0.80	pro-WTe_2	Ru_2Te_4	0.17	31.39	395.07	1.01
pro-PdS_2	Pd_2S_4	0.21	6.30	504.54	0.42	pro-CrW_3S_8	CrW_3S_8	0.17	1.90	516.64	0.15
pro-PdS_2	Ni_2Te_4	0.19	10.38	454.15	0.55	pro-CrW_3S_8	$CrMo_3Se_8$	0.16	2.52	485.80	0.18
pro-CrW_3S_8	Cr_3MoSe_8	0.19	10.48	427.44	0.55	pro-CrW_3S_8	Cr_3MoSe_8	0.15	8.93	395.10	0.38
pro-AuSe	Au_2S_2	0.19	8.03	489.41	0.45	pro-CrW_3S_8	CrW_3Se_8	0.15	2.33	491.69	0.15
pro-PdS_2	Ni_2S_4	0.18	16.35	418.76	0.68	pro-FeOCl	$Sc_2I_2S_2$	0.15	0.00	993.70	0.00
pro-$CrWS_4$	$Cr_2W_2Te_8$	0.18	17.37	347.83	0.71	pro-CrW_3S_8	Cr_3WSe_8	0.14	9.40	388.65	0.38
pro-PdS_2	Ni_2Se4	0.18	11.82	468.70	0.54	pro-WTe_2	Ru_2S_4	0.13	9.73	417.11	0.35
pro-AuSe	Ag_2Se_2	0.17	6.08	466.53	0.34	pro-$CrWS_4$	$Cr_2W_2Te_8$	0.12	21.40	326.02	0.55
pro-FeOCl	$Sc_2Br_2S_2$	0.17	13.31	504.10	0.57	pro-AuSe	Au_2Se_2	0.12	2.92	505.05	0.14
pro-TiS_3	Zr_2O_6	0.17	7.88	513.27	0.39	pro-AuSe	Au_2Te_2	0.12	3.89	457.21	0.17
pro-WTe_2	$Os2Se4$	0.16	6.63	404.69	0.35	pro-AuSe	Au_2S_2	0.12	4.11	510.31	0.18
pro-WTe_2	$Os2Te_4$	0.16	8.27	362.21	0.40	pro-$CrWS_4$	$Cr_2Mo_2Te_8$	0.12	21.38	342.84	0.52
pro-WTe_2	$Os2O_4$	0.16	0.45	230.73	1.10	pro-AuSe	Cu_2S_2	0.11	22.20	314.49	0.50
pro-TiS_3	Hf_2O_6	0.16	8.27	513.03	0.38	pro-$CrWS_4$	$Cr_2Mo_2Se_8$	0.11	8.80	447.30	0.27
pro-$CrWS_4$	$Cr_2Mo_2Te_8$	0.15	19.34	360.94	0.63	pro-CrW_3S_8	Cr_3WTe_8	0.10	27.69	272.51	0.56
pro-WTe_2	Zr_2Cl4	0.14	11.35	392.17	0.44	pro-$CrWS_4$	$Cr_2W_2S_8$	0.10	6.45	488.35	0.20
pro-WTe_2	Hf_2Cl4	0.13	4.19	477.64	0.19	pro-$CrWS_4$	$Cr_2W_2Se_8$	0.10	10.23	435.76	0.27

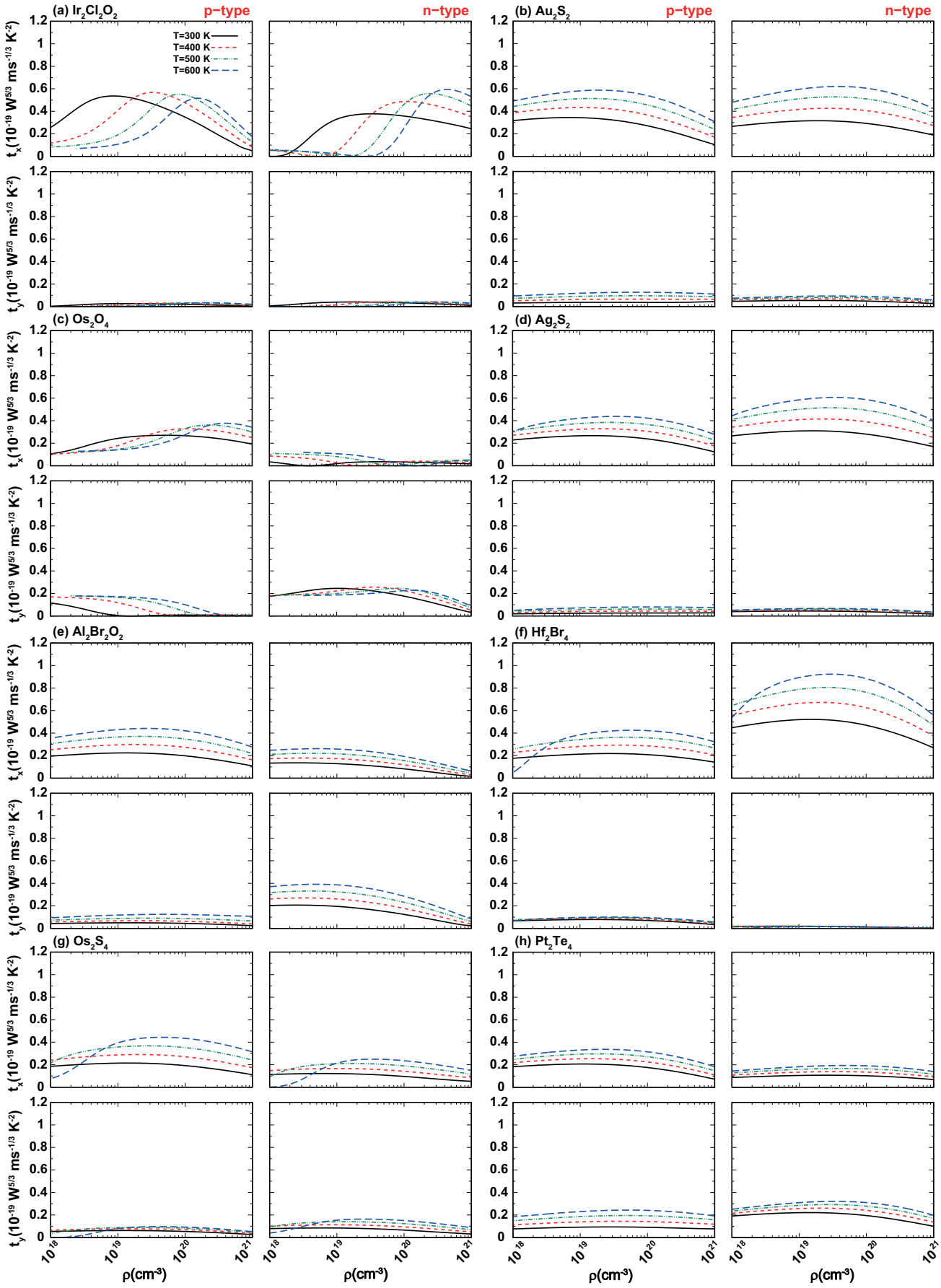


Figure S19. (Color online) Calculated EFF as a function of charge carrier concentration through x- and y-directions within different temperatures from 300 K to 600 K.

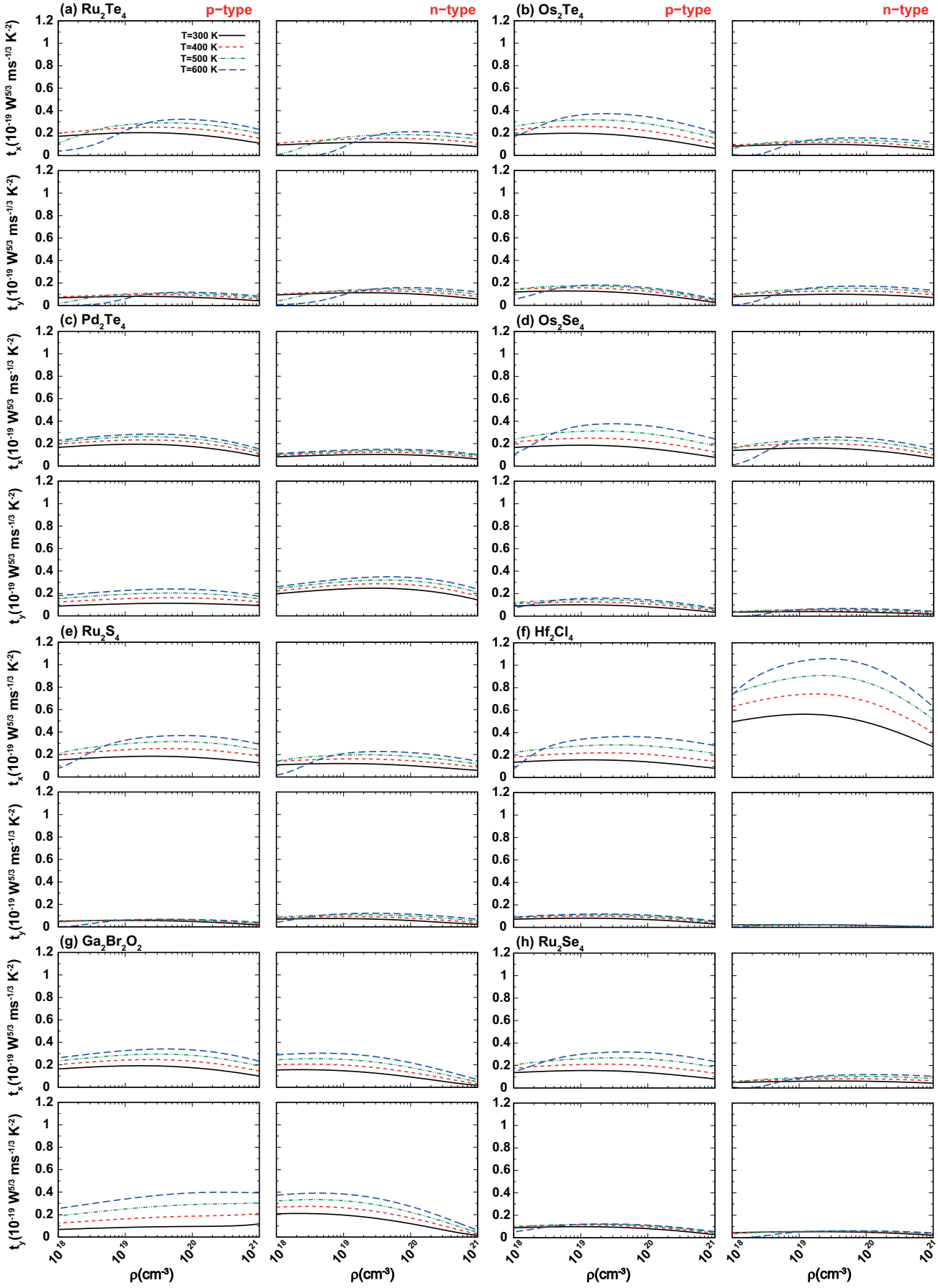


Figure S20. (Color online) Calculated EFF as a function of charge carrier concentration through x- and y-directions within different temperatures from 300 K to 600 K.

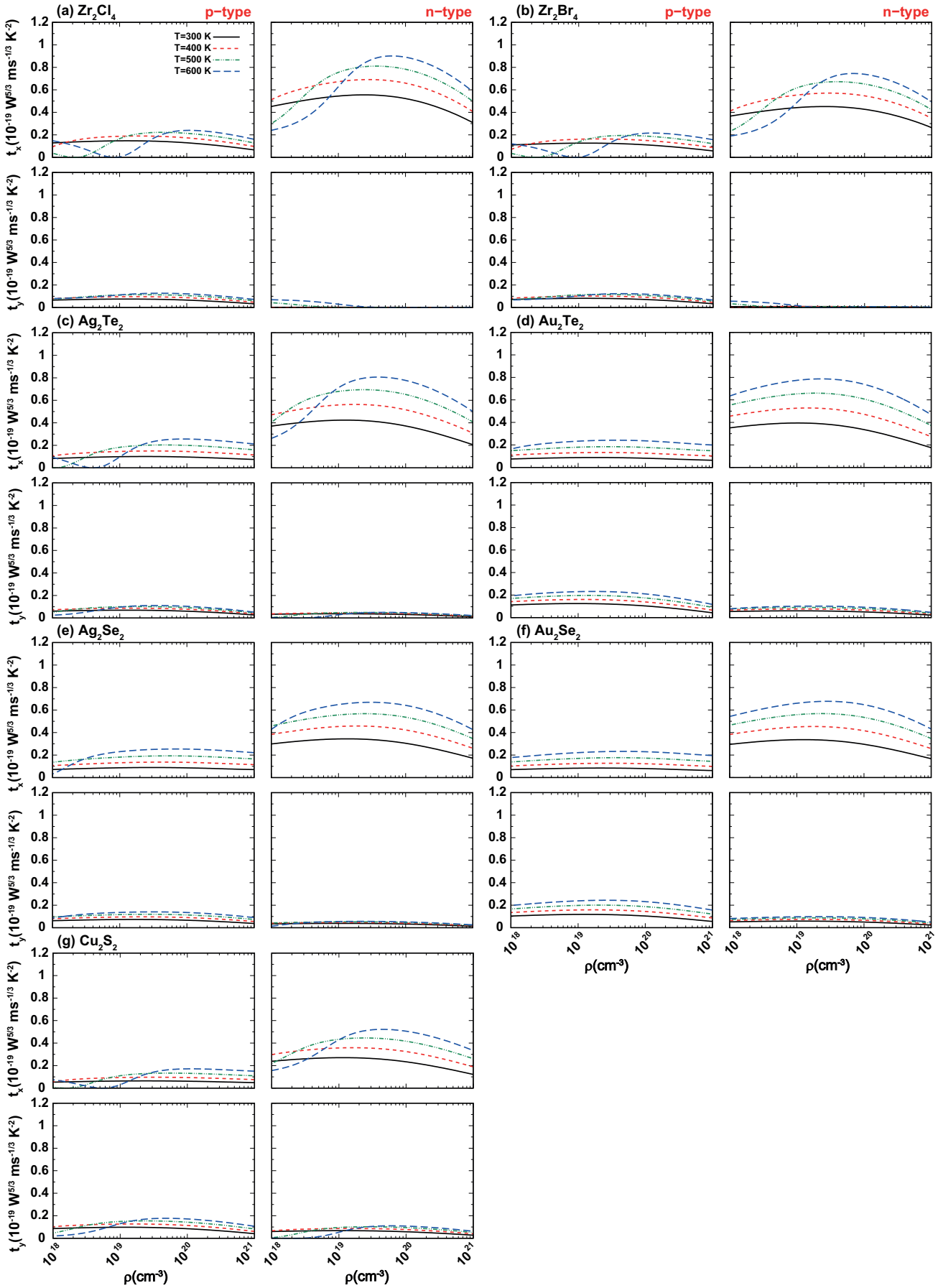


Figure S21. (Color online) Calculated EFF as a function of charge carrier concentration through x- and y-directions within different temperatures from 300 K to 600 K.

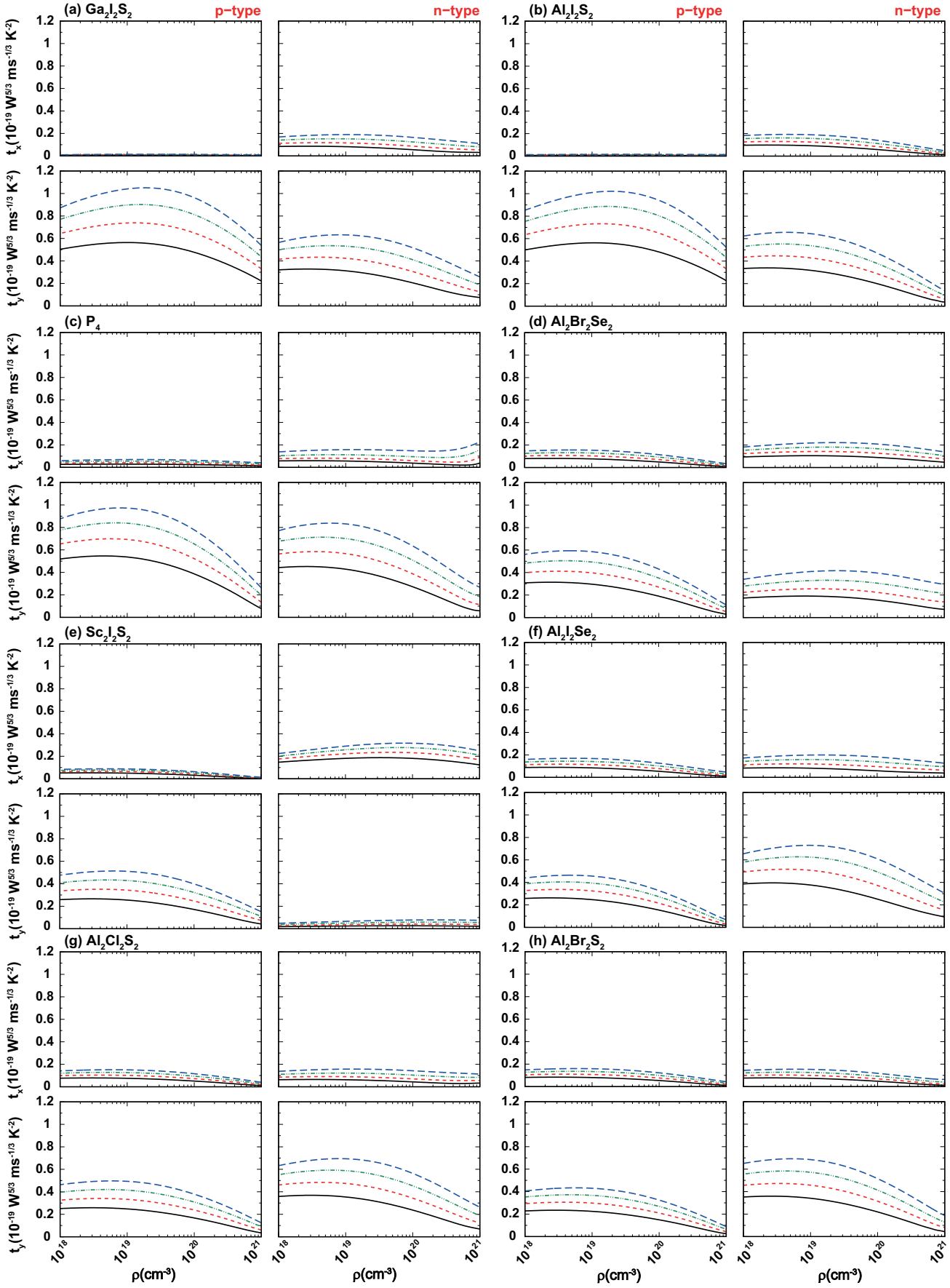


Figure S22. (Color online) Calculated EFF as a function of charge carrier concentration through x- and y-directions within different temperatures from 300 K to 600 K.

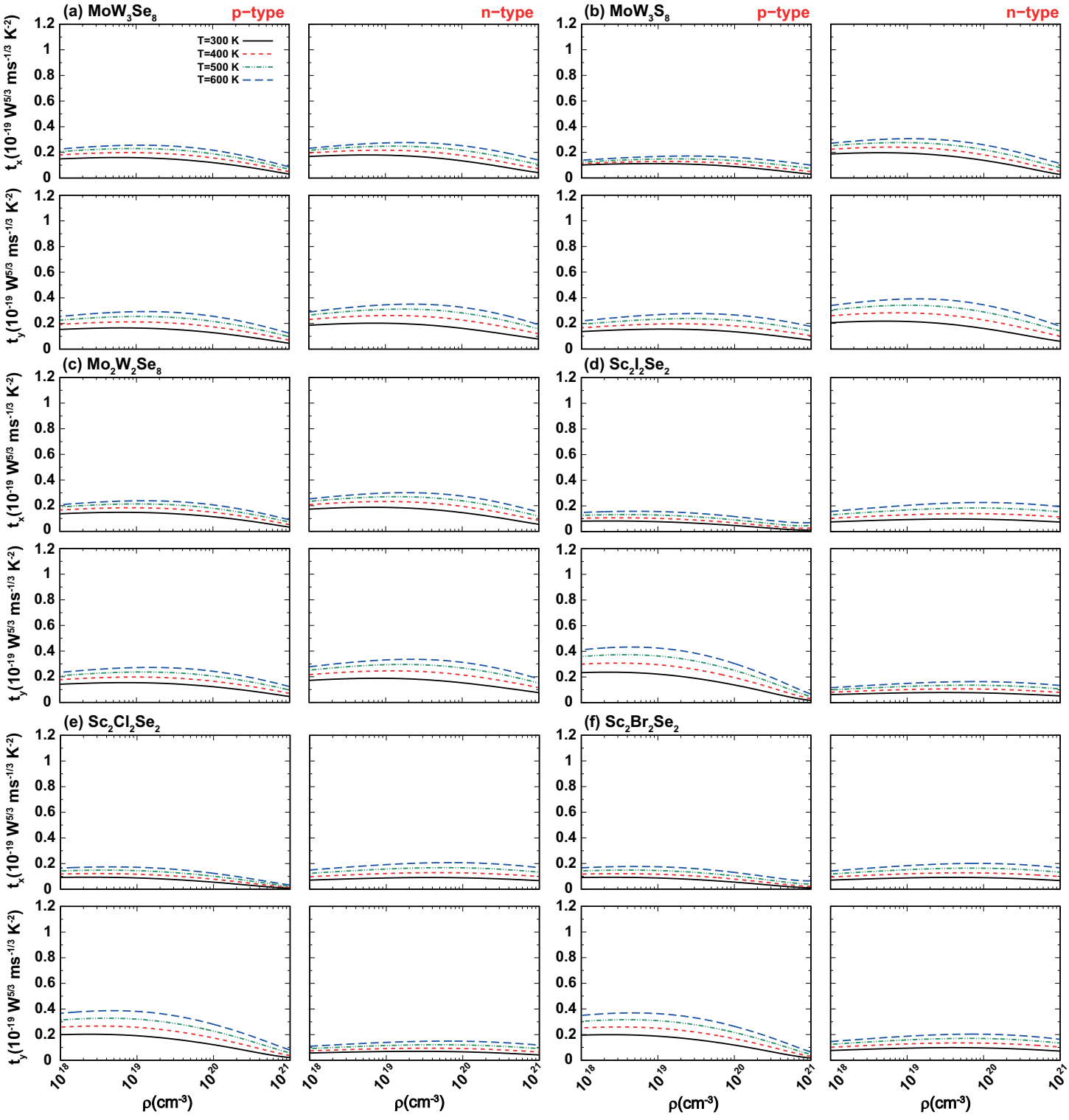


Figure S23. (Color online) Calculated EFF as a function of charge carrier concentration through x- and y-directions within different temperatures from 300 K to 600 K.

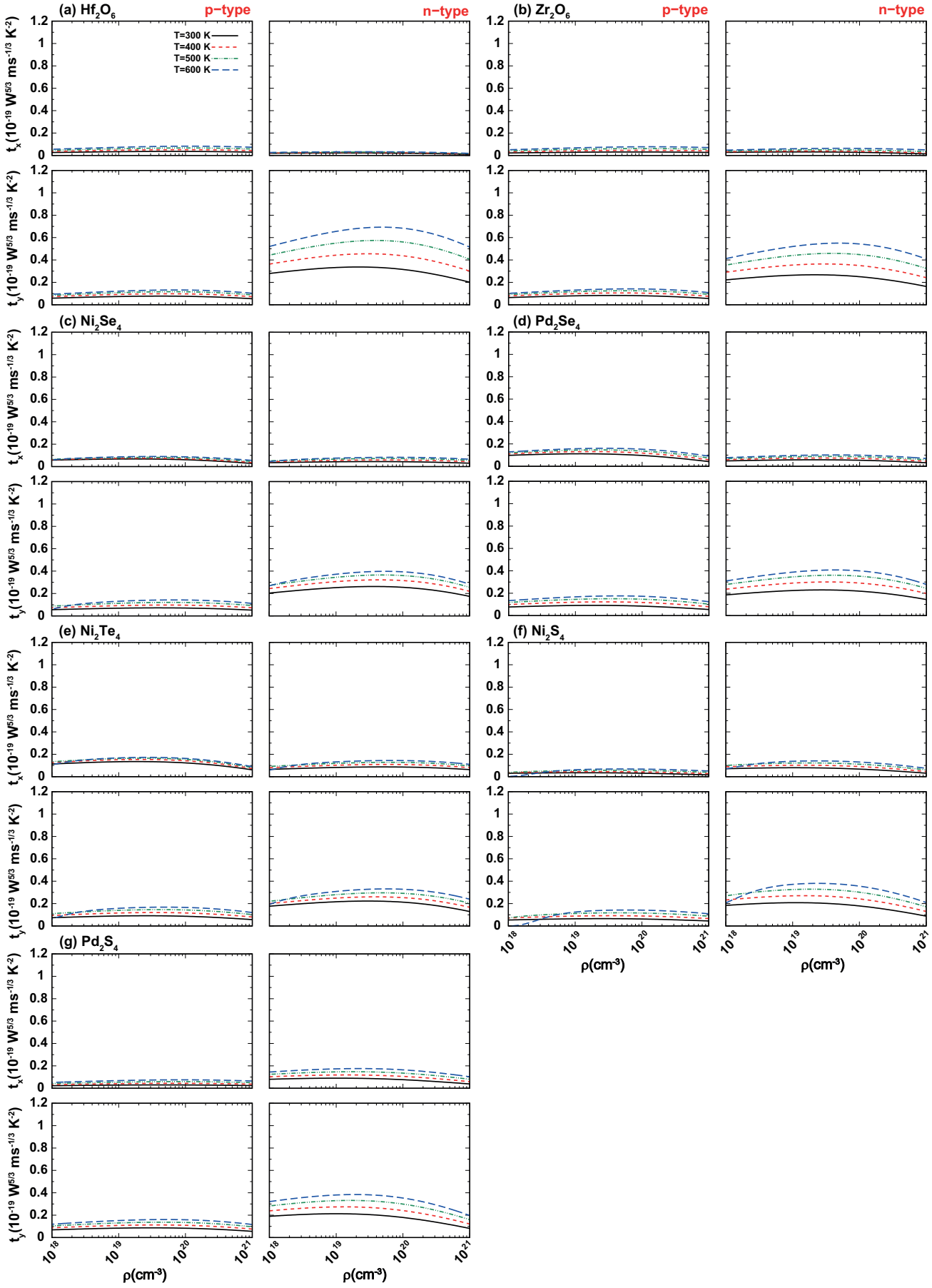


Figure S24. (Color online) Calculated EFF as a function of charge carrier concentration through x- and y-directions within different temperatures from 300 K to 600 K.

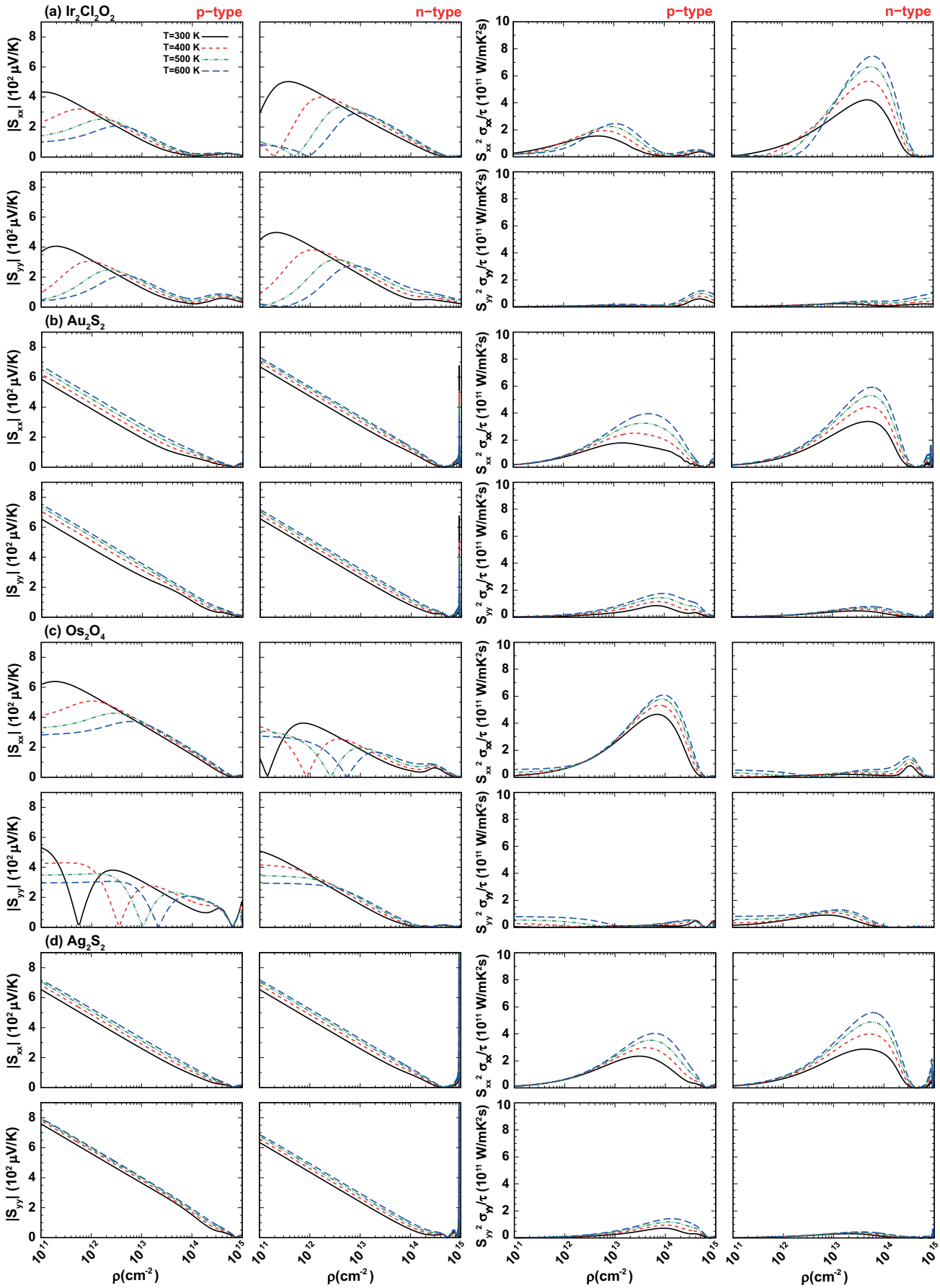


Figure S25. Calculated Seebeck coefficient and power factor of selected 2D anisotropic materials as a function of charge carrier concentration in temperature range of 300-600 K.

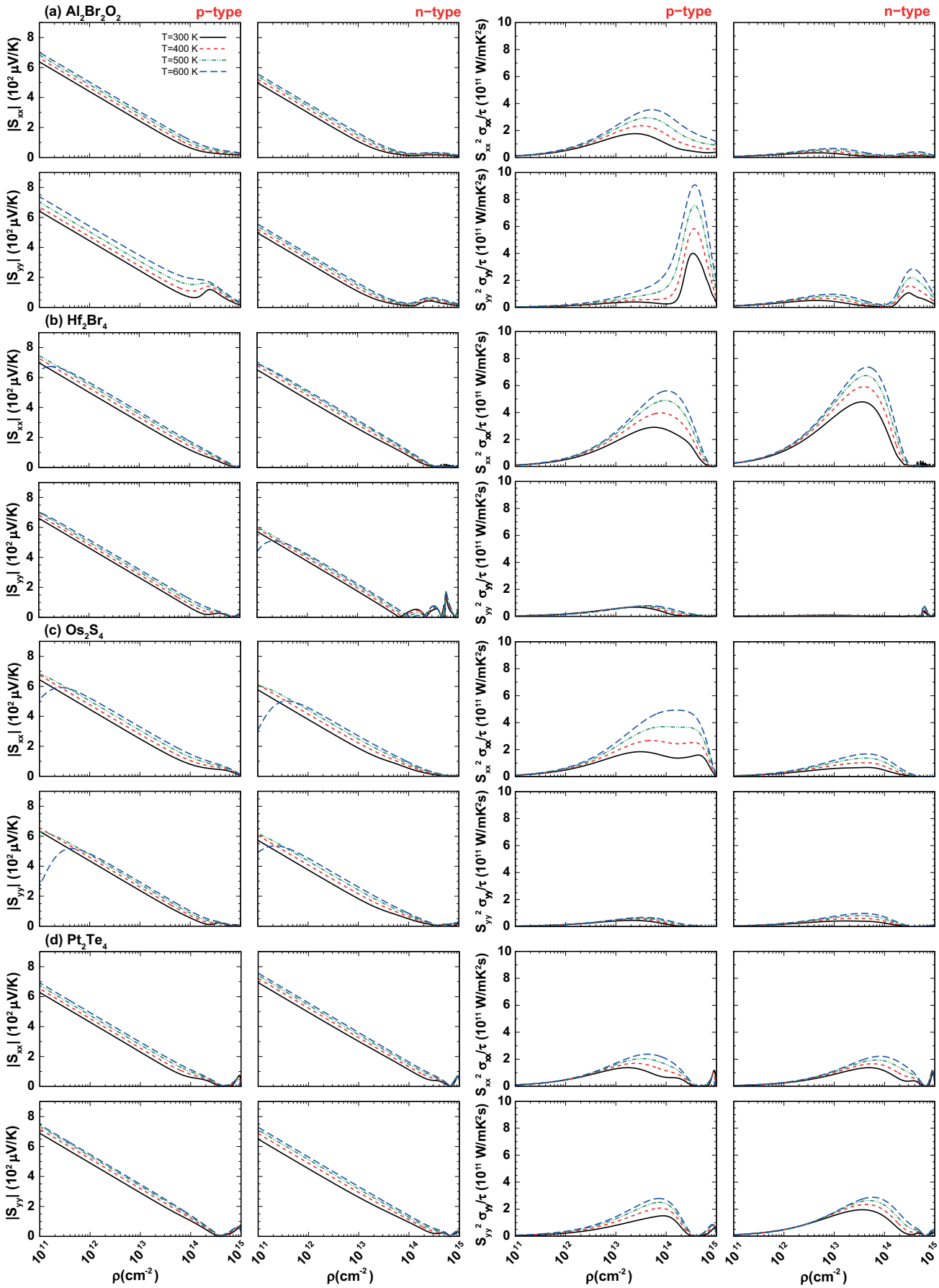


Figure S26. Calculated Seebeck coefficient and power factor of selected 2D anisotropic materials as a function of charge carrier concentration in temperature range of 300-600 K.

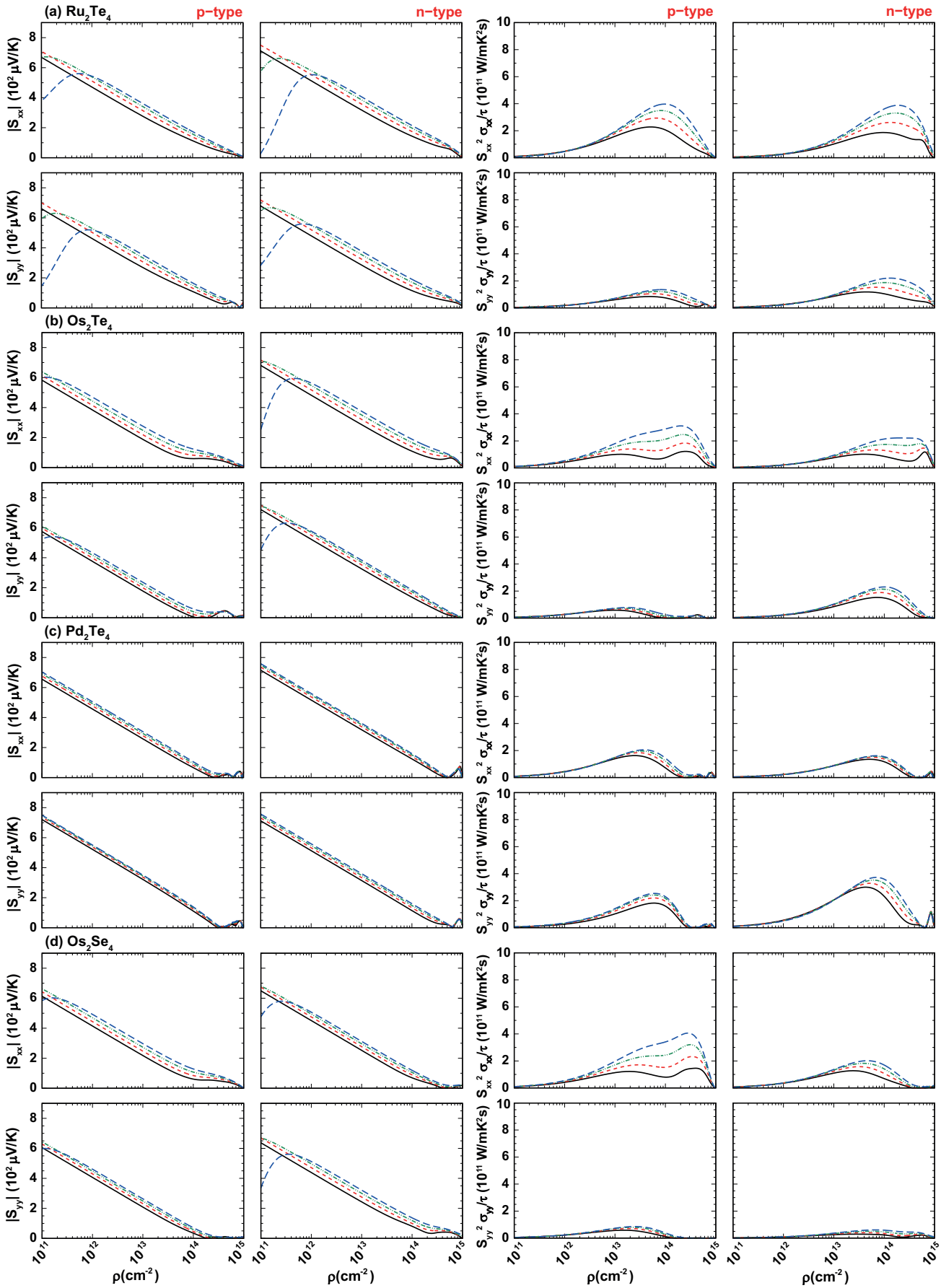


Figure S27. Calculated Seebeck coefficient and power factor of selected 2D anisotropic materials as a function of charge carrier concentration in temperature range of 300-600 K.

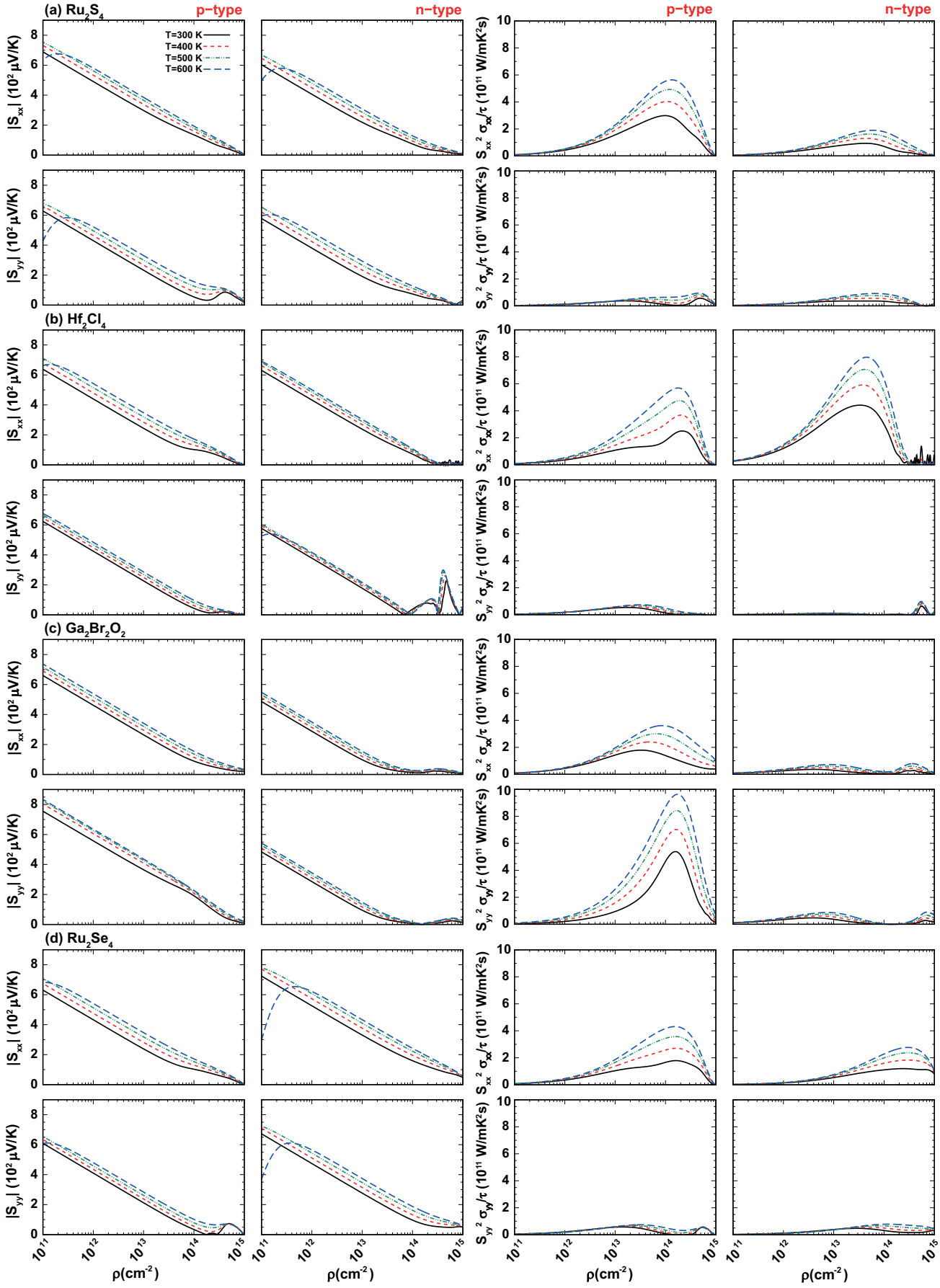


Figure S28. Calculated Seebeck coefficient and power factor of selected 2D anisotropic materials as a function of charge carrier concentration in temperature range of 300-600 K.

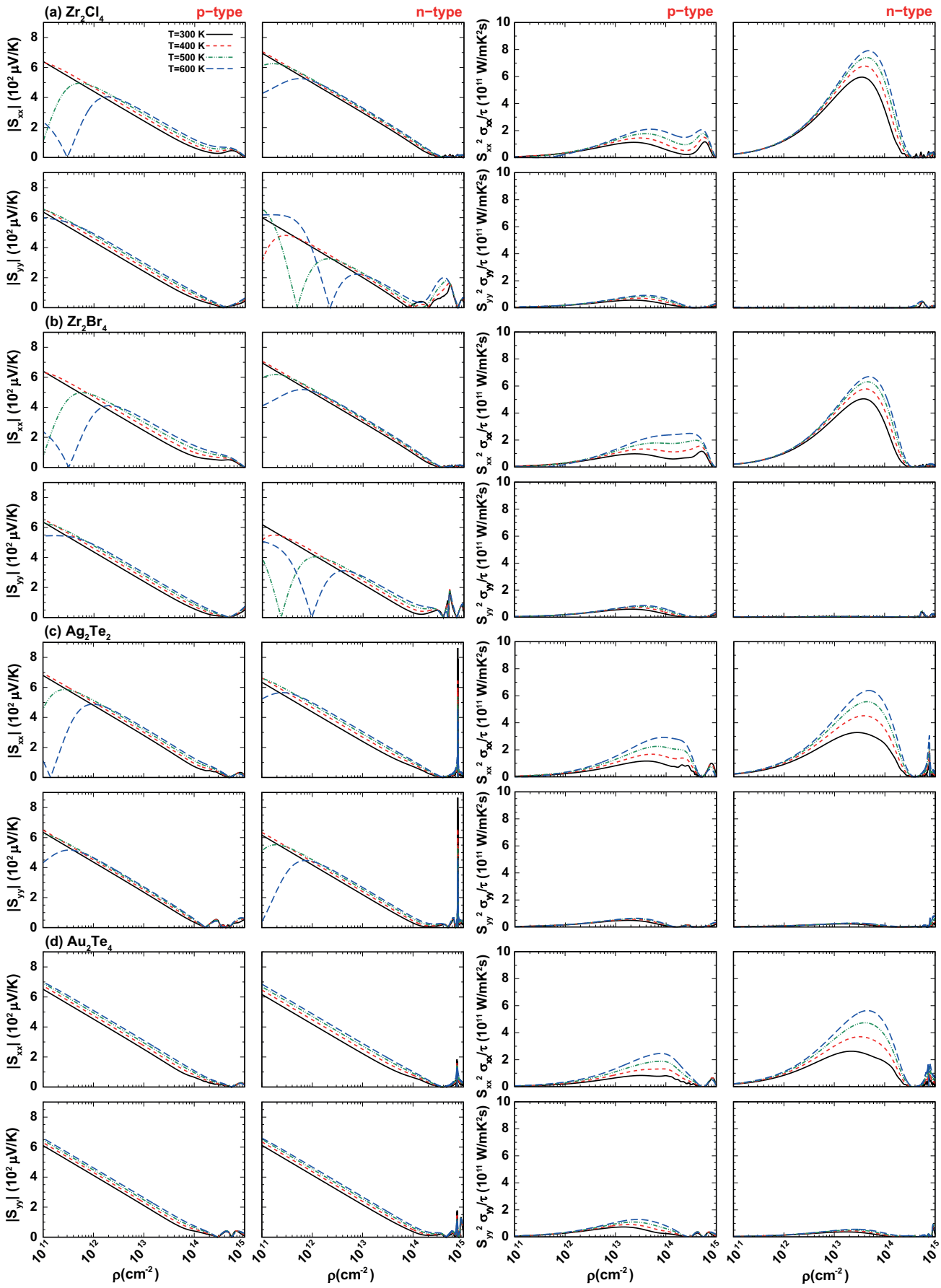


Figure S29. Calculated Seebeck coefficient and power factor of selected 2D anisotropic materials as a function of charge carrier concentration in temperature range of 300-600 K.

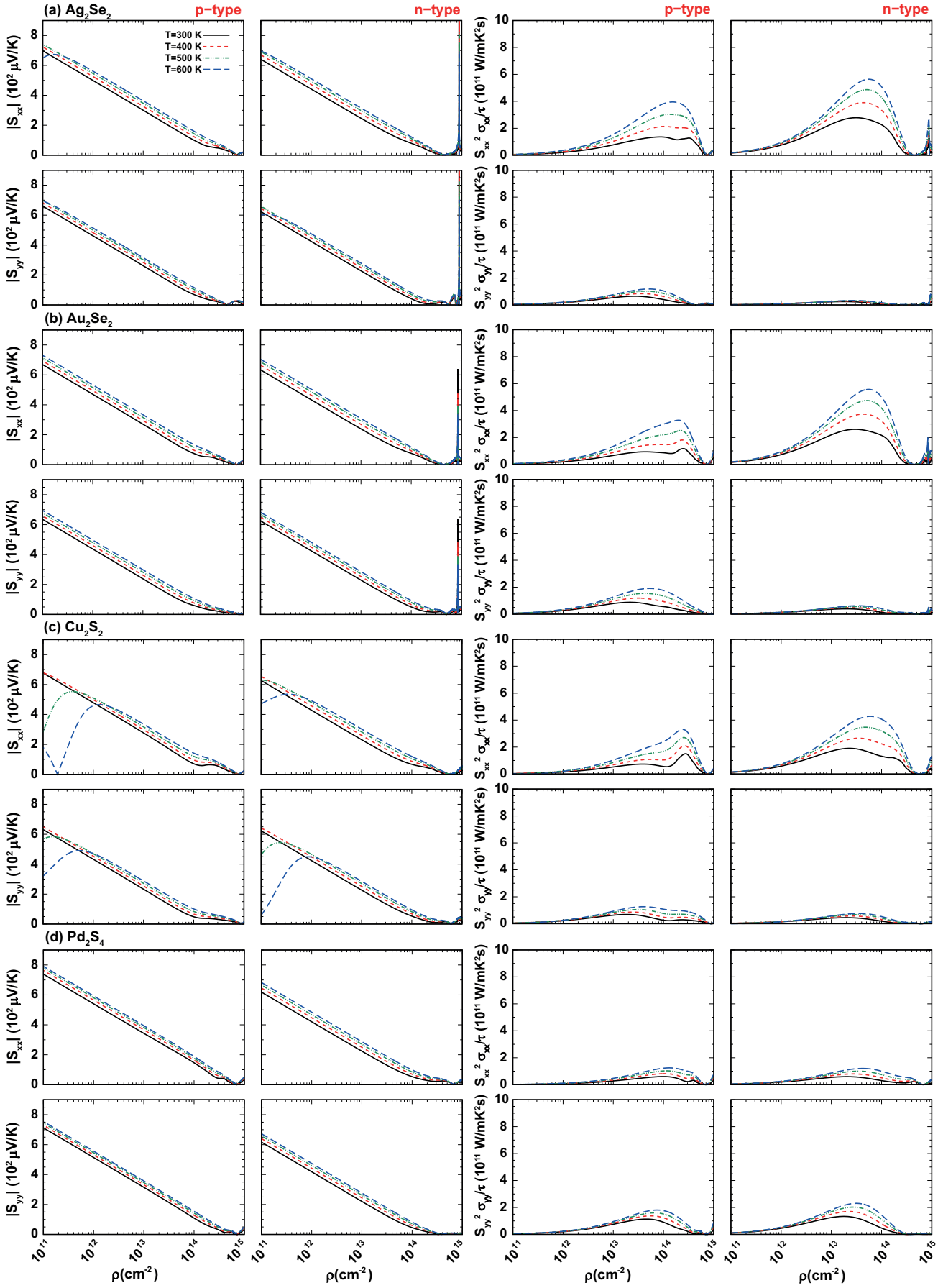


Figure S30. Calculated Seebeck coefficient and power factor of selected 2D anisotropic materials as a function of charge carrier concentration in temperature range of 300-600 K.

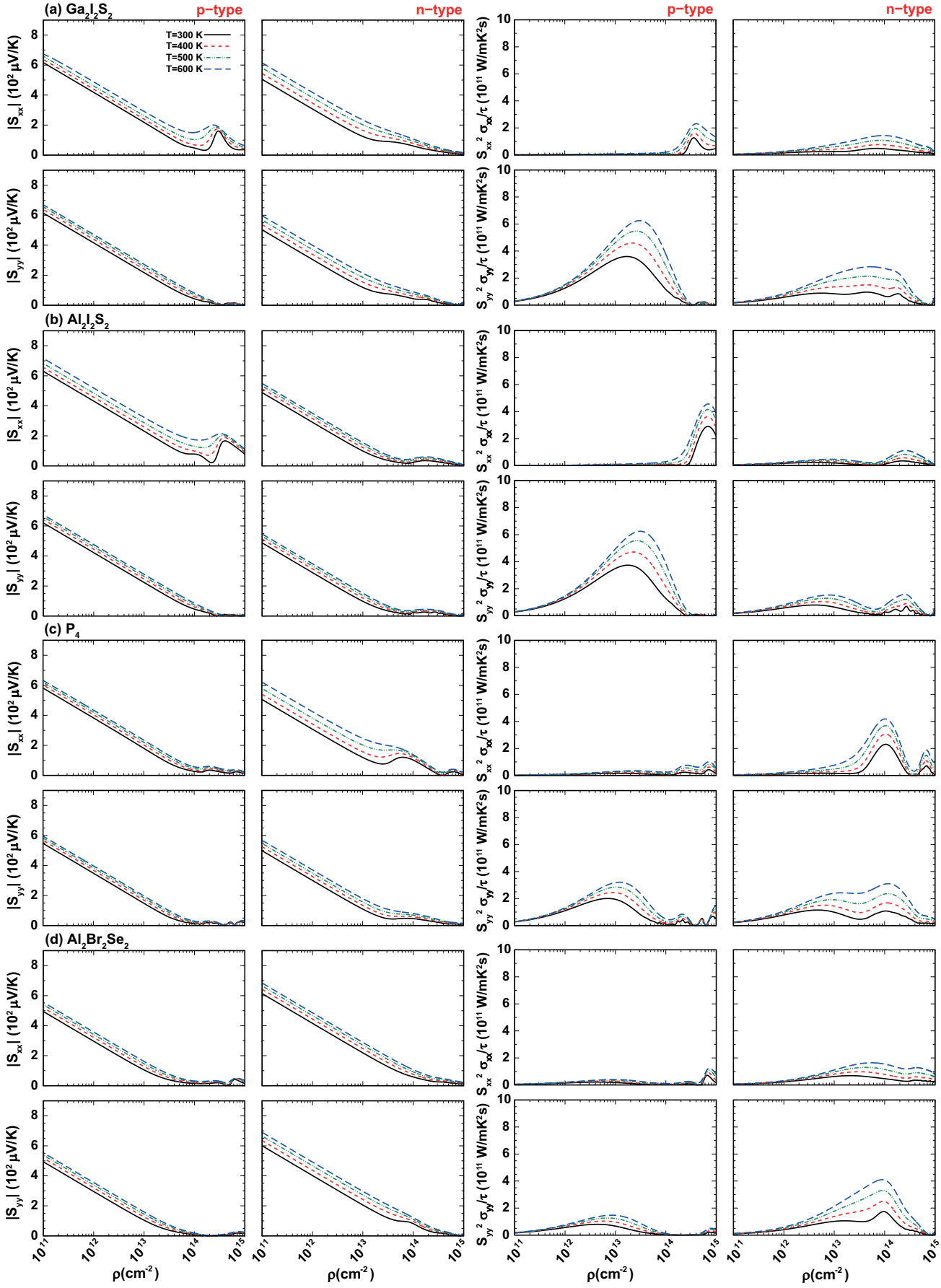


Figure S31. Calculated Seebeck coefficient and power factor of selected 2D anisotropic materials as a function of charge carrier concentration in temperature range of 300-600 K.

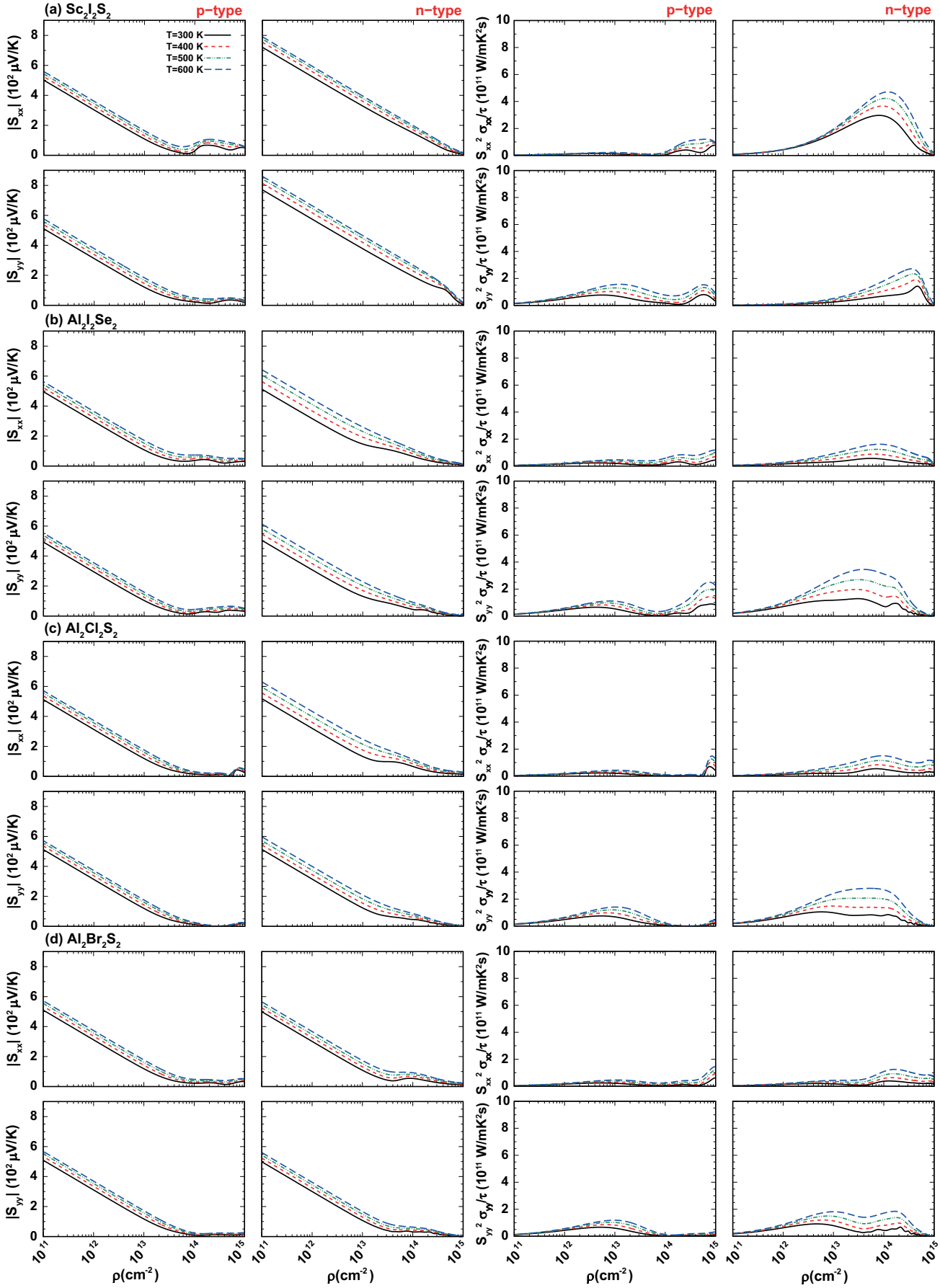


Figure S32. Calculated Seebeck coefficient and power factor of selected 2D anisotropic materials as a function of charge carrier concentration in temperature range of 300-600 K.

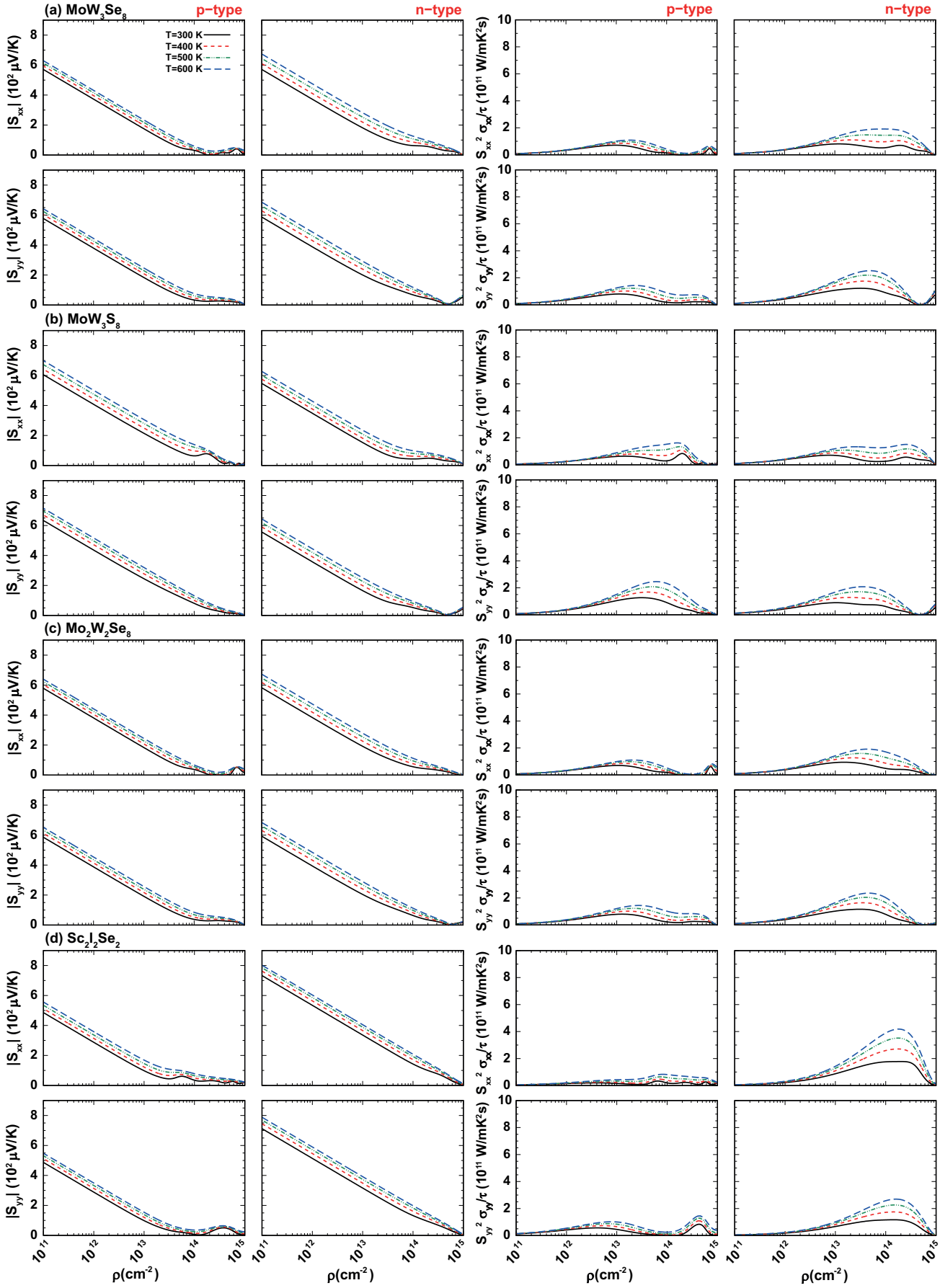


Figure S33. Calculated Seebeck coefficient and power factor of selected 2D anisotropic materials as a function of charge carrier concentration in temperature range of 300-600 K.

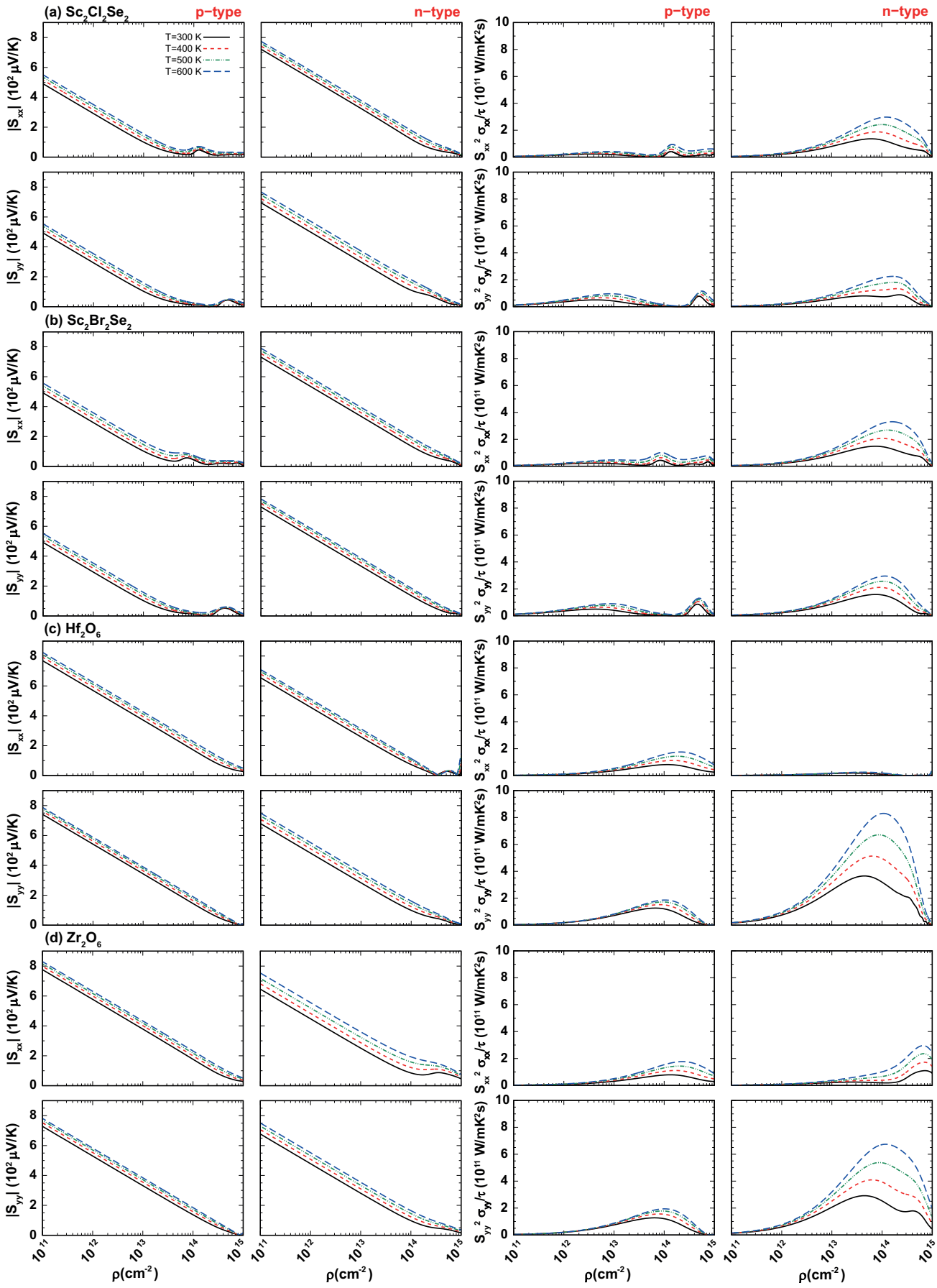


Figure S34. Calculated Seebeck coefficient and power factor of selected 2D anisotropic materials as a function of charge carrier concentration in temperature range of 300-600 K.

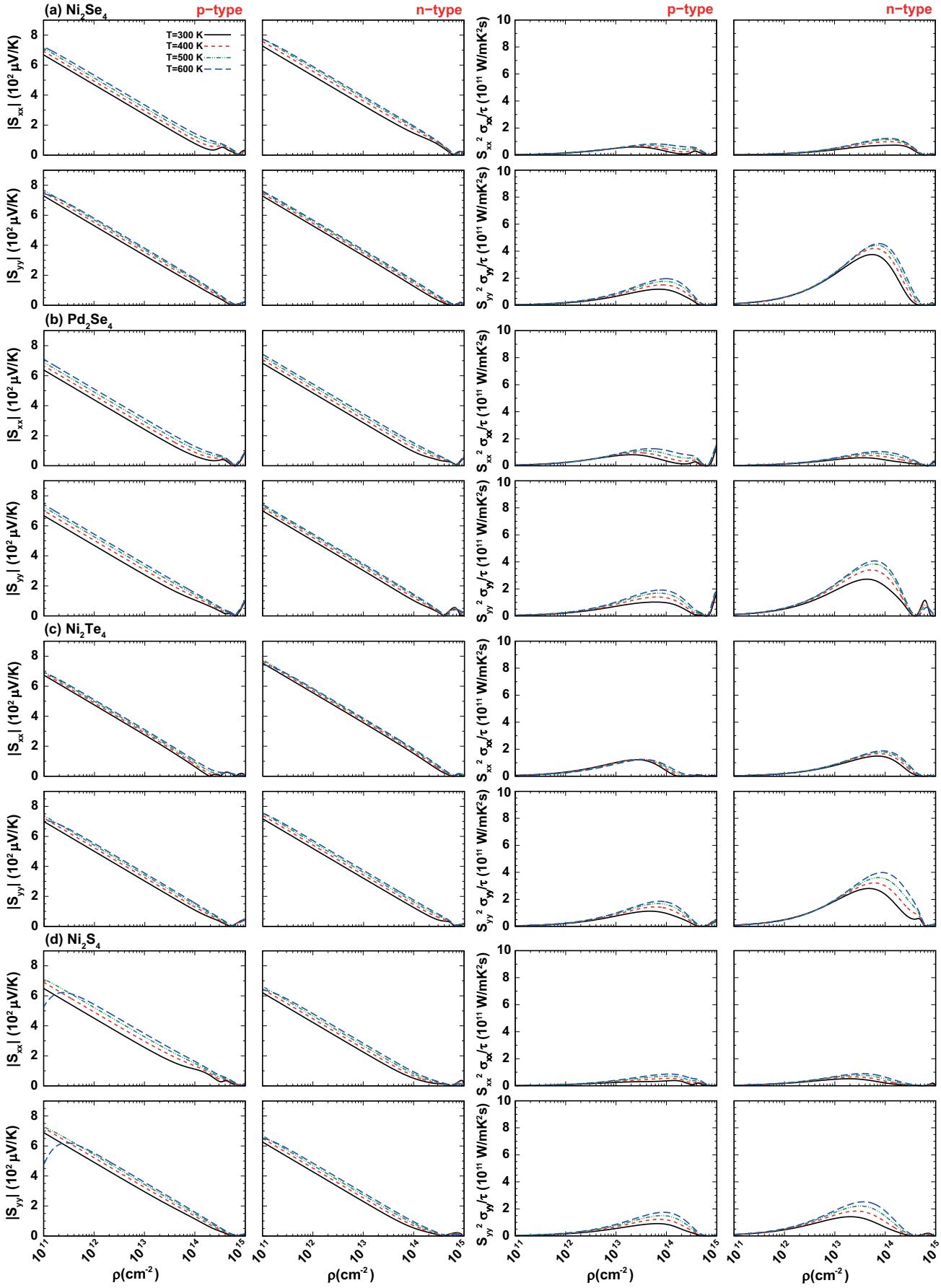


Figure S35. Calculated Seebeck coefficient and power factor of selected 2D anisotropic materials as a function of charge carrier concentration in temperature range of 300-600 K.

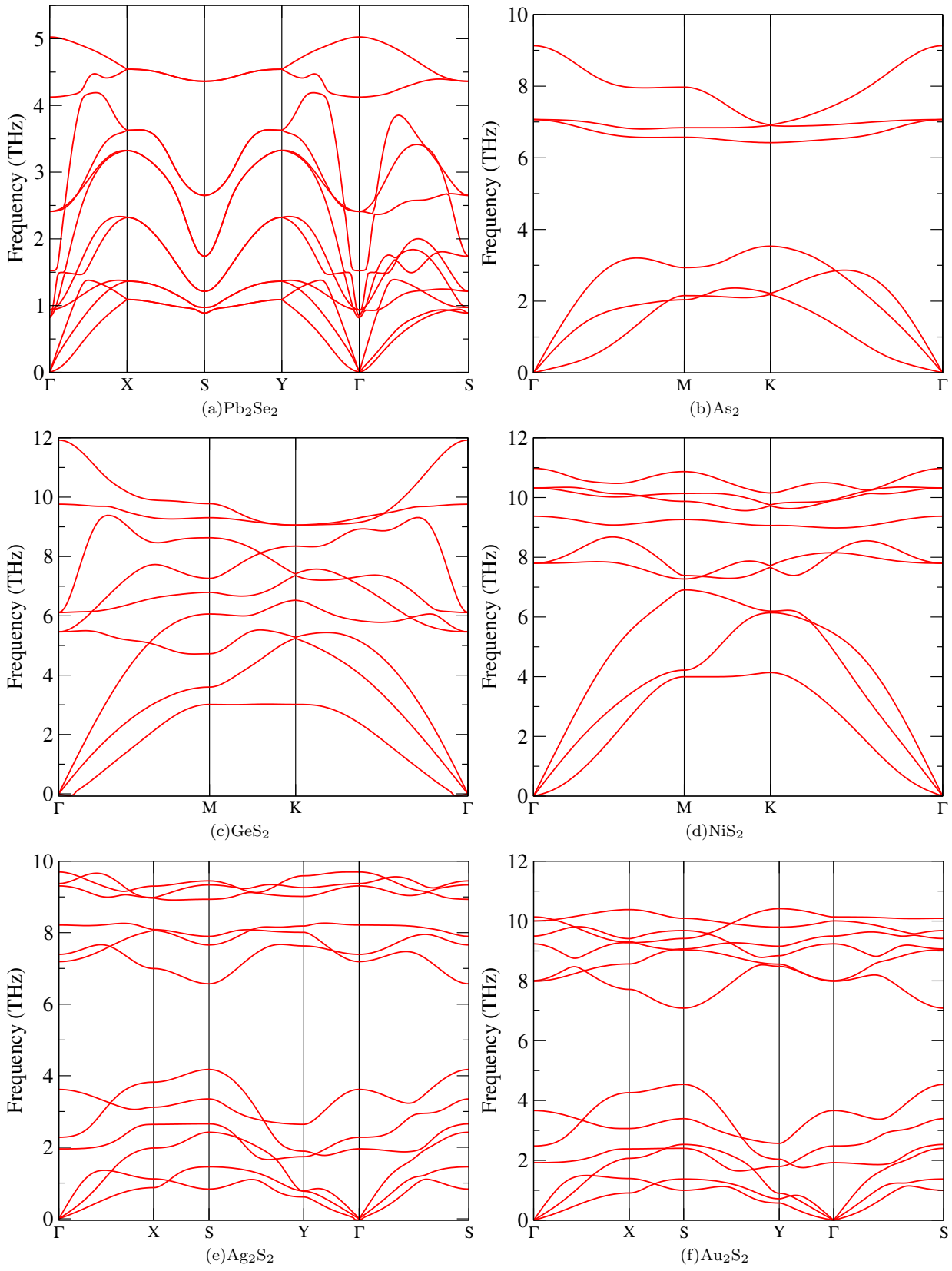


Figure S36. Phonon dispersion curves of (a) Pb_2Se_2, (b)As_2, (c)GeS_2, (d)NiS_2, (e)Ag_2S_2, and (f)Au_2S_2.

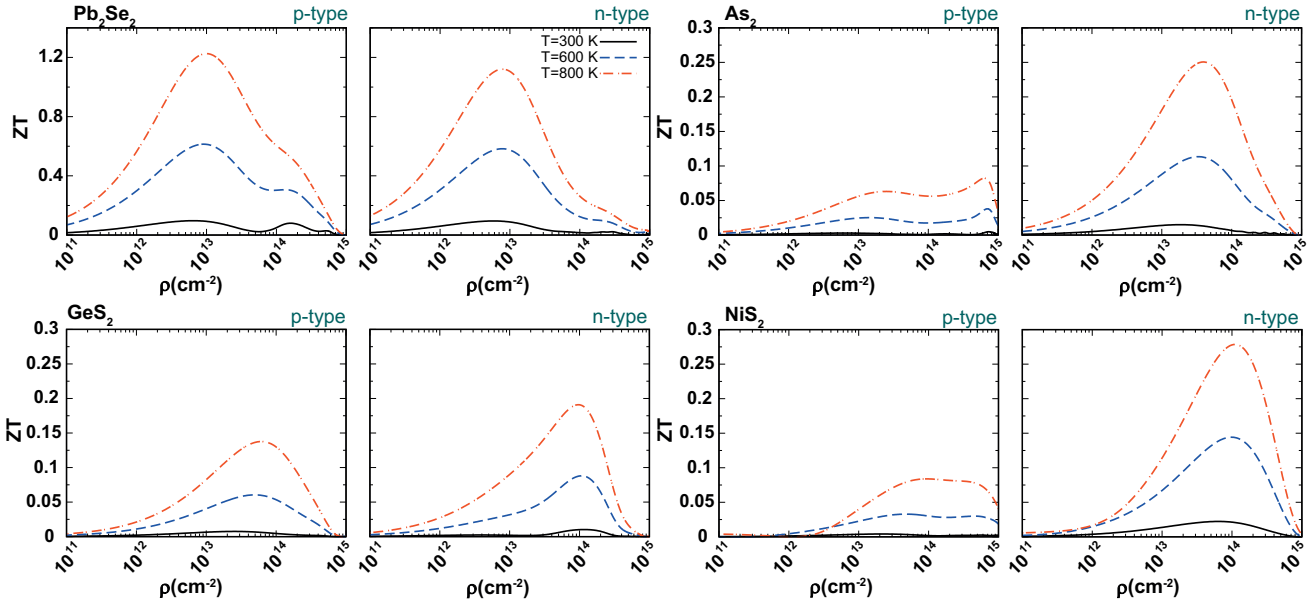
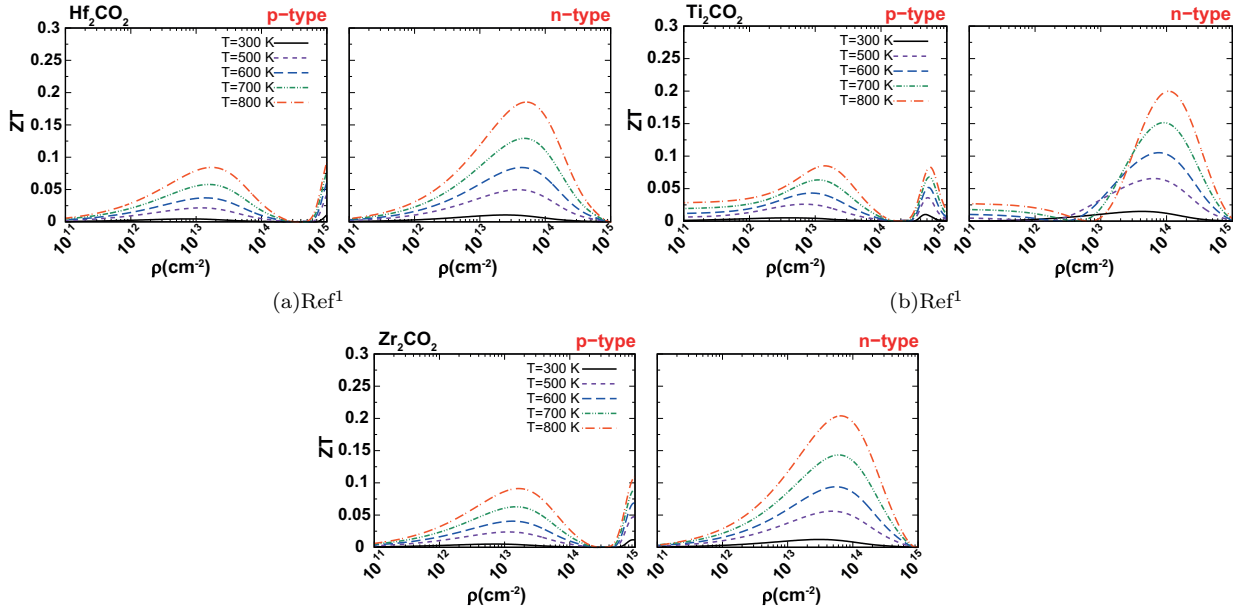


Figure S37. The estimated figure of merit as a function of carrier density using constant relaxation time approximation with $\tau = 10$ fs for p-type and n-type carrier concentration of Pb_2Se_2, As_2, GeS_2, and NiS_2.



(a)Ref[1] (b)Ref[1]

(c)Ref[1]

Figure S38. The estimation of TE figure of merit as a function of carrier density using constant relaxation time approximation with $\tau = 10$ fs for p-type and n-type carrier concentration of Hf_2CO_2, Ti_2CO_2, and Zr_2CO_2. The lattice thermal conductivity values have been provided from literature as cited in captions.

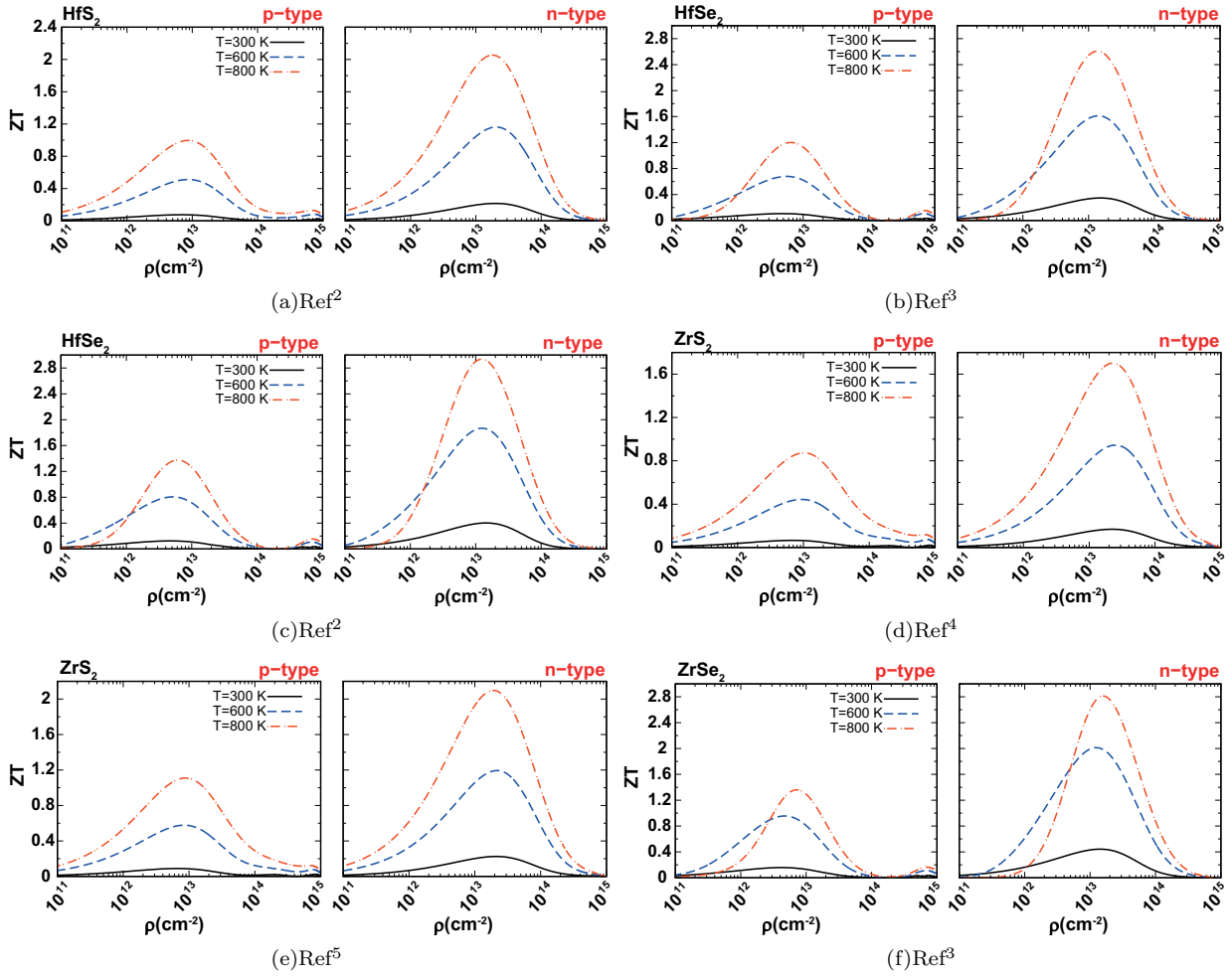


Figure S39. The estimated figure of merit as a function of carrier density using constant relaxation time approximation with τ = 10 fs for p-type and n-type carrier concentration of HfX_2 and ZrX_2 (X=S, Se). The lattice thermal conductivity values have been provided from literature as cited in captions.

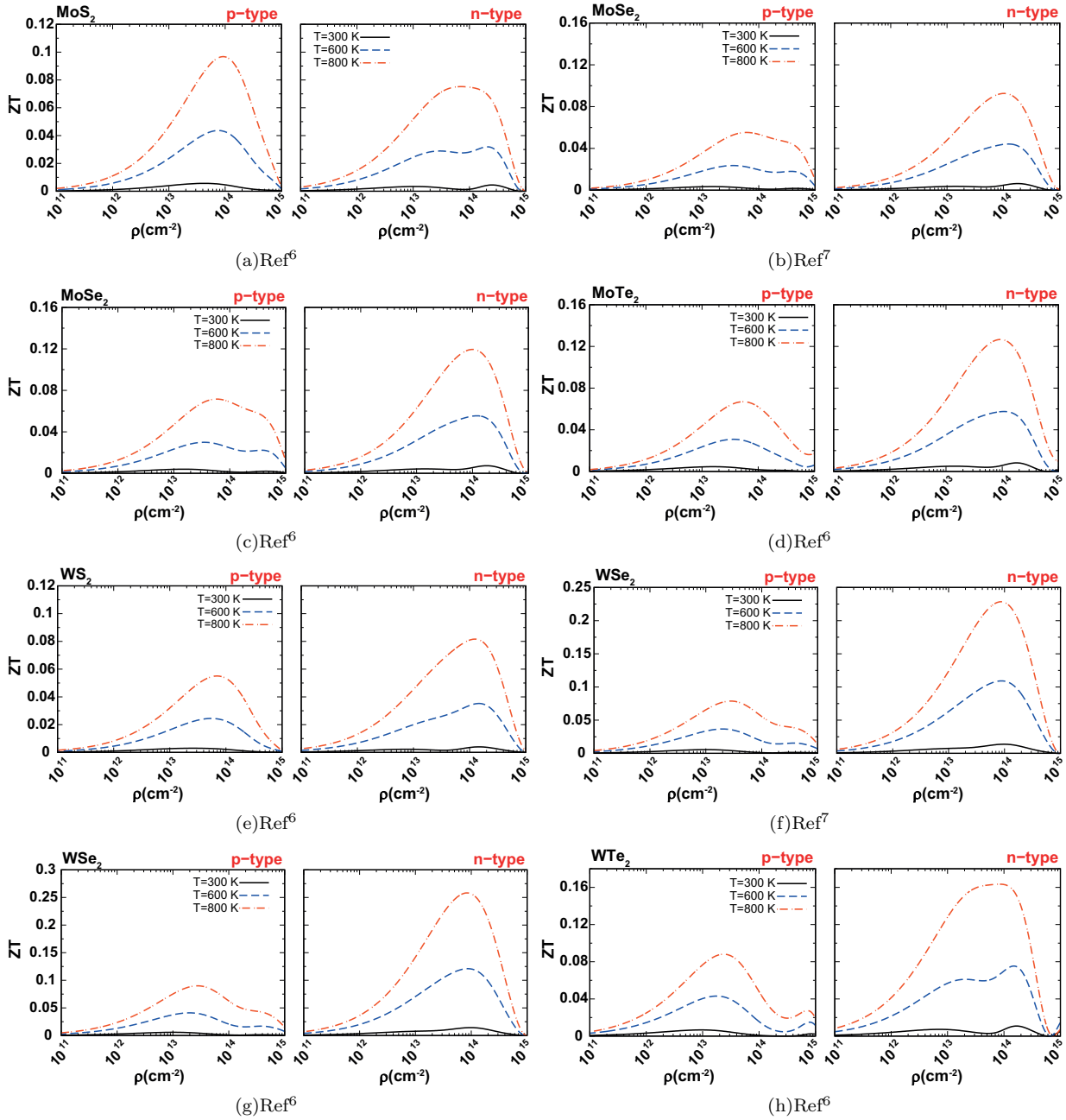


Figure S40. The estimated figure of merit as a function of carrier density using constant relaxation time approximation with τ = 10 fs for p-type and n-type carrier concentration of MoX_2 and WX_2 (X=S, Se, Te). The lattice thermal conductivity values have been provided from literature as cited in captions.

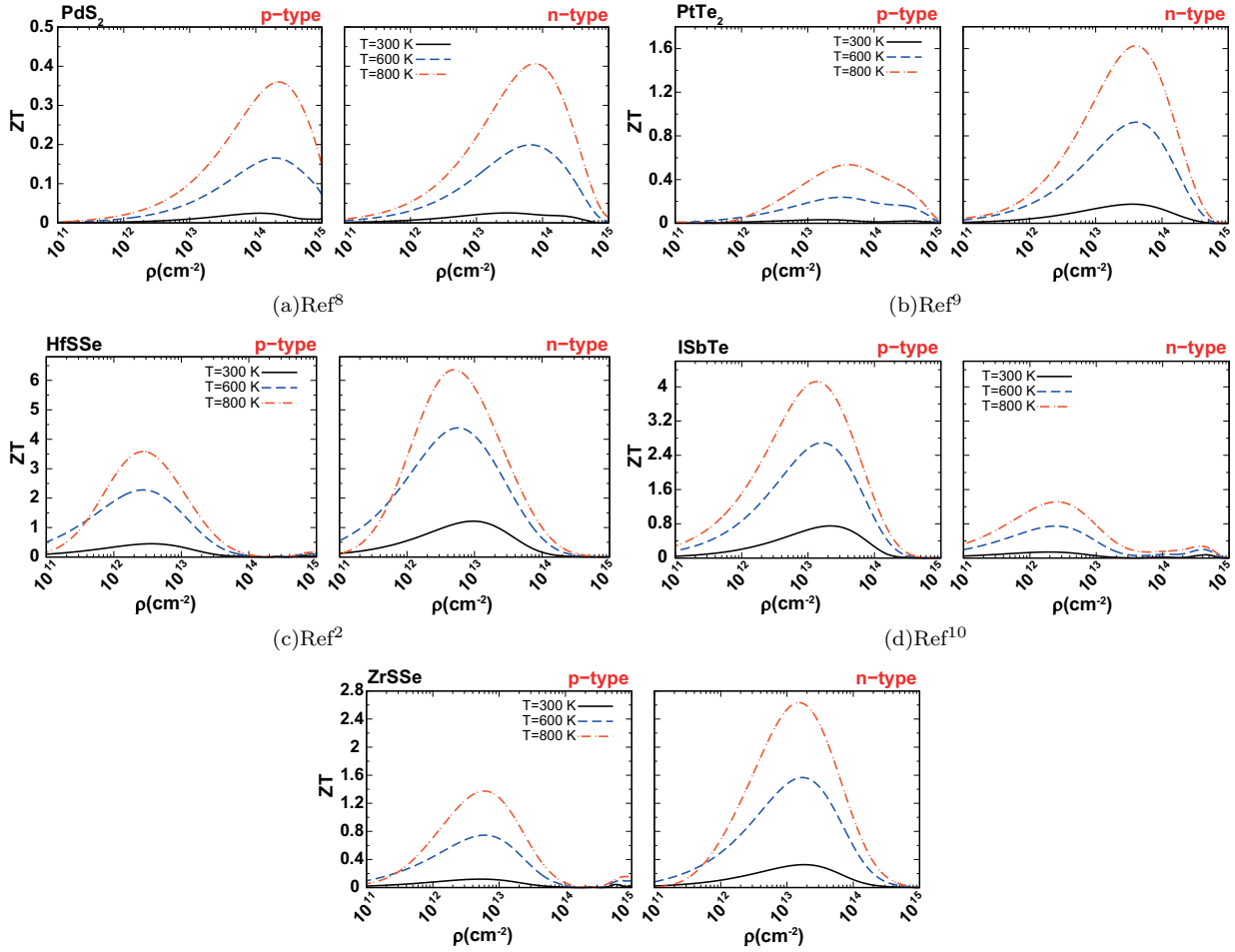


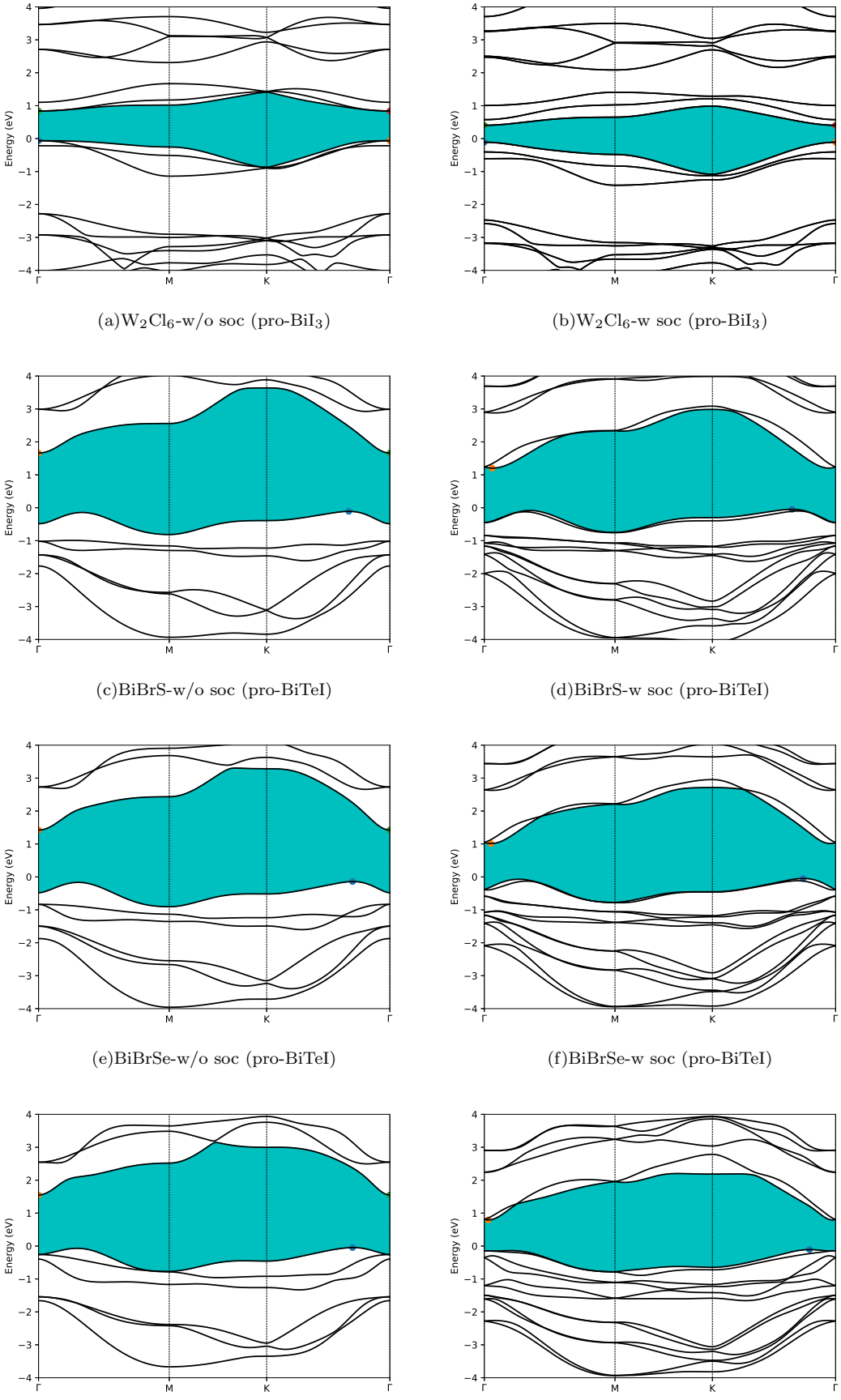
Figure S41. The estimated of figure of merit as a function of carrier density using constant relaxation time approximation with $\tau = 10$ fs for p-type and n-type carrier concentration of PdS_2, $PtTe_2$, HfSSe, ISbTe, ZrSSe. The lattice thermal conductivity values have been provided from literature as cited in captions.

Table S16. Energy band gap (E_{gap}) values of 2D isotropic materials, which includes heavy elements, with and without spin-orbit coupling effect. "D" and "ID" stand for direct and indirect energy bands, respectively. The last two columns correspond to reported energy band gap values in C2DB and previous studies, respectively.

Prototype	Material	Structure	E_g (eV) (PBE)	E_g (eV) (PBE+SOC)	E_g (eV) (C2DB-PBE+SOC)[11]	E_g (eV) (PBE+SOC) (Ref.)
Pro-BiI_3	W_2Cl_6	P-31m	0.90 (D)	0.51 (D)	0.49 (D)	
Pro-BiTeI	BiBrS	P3m1	1.77 (ID)	1.25 (ID)	0.93 (ID)	
	BiBrSe	P3m1	1.56 (ID)	1.06 (ID)	0.77 (ID)	
	BiBrTe	P3m1	1.60 (ID)	0.90 (ID)	0.63 (ID)	
	BiClS	P3m1	1.79 (ID)	1.36 (ID)	1.04 (ID)	
	BiClSe	P3m1	1.65 (ID)	1.17 (ID)	0.88 (ID)	
	BiClTe	P3m1	1.77 (ID)	0.93 (ID)	0.64 (D)	
	BiIS	P3m1	1.76 (ID)	1.16 (ID)	0.82 (ID)	
	BiISe	P3m1	1.64 (ID)	0.95 (D)	0.65 (ID)	
	BiITe	P3m1	1.51 (ID)	0.73 (ID)	0.45 (ID)	0.69 (ID)[10]
	HfSSe	P3m1	0.81 (ID)	0.68 (ID)	0.68 (ID)	
Pro-CdI_2	HfS_2	P-3m1	1.28 (ID)	1.22 (ID)	1.22 (ID)	1.23 (ID)[12] 1.16 (ID)[13]
	$HfSe_2$	P-3m1	0.60 (ID)	0.43 (ID)	0.43 (ID)	0.45 (ID)[12] 0.42 (ID)[13]
	$HgBr_2$	P-3m1	2.02 (D)	1.91 (D)	1.98 (ID)	
	$PbBr_2$	P-3m1	2.74 (ID)	2.34 (ID)	2.06 (ID)	
	PbO_2	P-3m1	1.26 (ID)	1.28 (ID)	1.35 (ID)	
	PtO_2	P-3m1	1.74 (ID)	1.76 (ID)	1.67 (ID)	
	PtS_2	P-3m1	1.81 (ID)	1.77 (ID)	1.69 (ID)	1.73 (ID)[13]
	$PtSe_2$	P-3m1	1.40 (ID)	1.21 (ID)	1.17 (ID)	1.20 (ID)[13]
	$PtTe_2$	P-3m1	0.76 (ID)	0.38 (ID)	0.31 (ID)	0.38 (ID)[9]
Pro-CH	Pb_2Te_2	P-1	1.44 (ID)	0.76 (ID)	0.46 (ID)	
Pro-GaSe	Hg_2I_2	P1	1.33 (ID)	1.24 (ID)	1.28 (ID)	
	Pt_2Cl_2	P1	1.68 (ID)	1.43 (D)	1.31 (D)	
Pro-GeSe	HgTe	P3m1	0.04 (D)	0.15 (ID)	0.15 (D)	
	PbTe	P3m1	1.62 (D)	1.14 (D)	0.93 (D)	
Pro-MoS_2	$HfBr_2$	P-6m2	0.86 (ID)	0.76 (ID)	0.73 (ID)	
	$HfCl_2$	P-6m2	1.01 (ID)	0.93 (ID)	0.90 (ID)	
	HfI_2	P-6m2	0.78 (ID)	0.64 (ID)	0.63 (ID)	
	$HfTe_2$	P-6m2	0.38 (ID)	0.14 (ID)	0.13 (ID)	
	WO_2	P-6m2	1.36 (ID)	1.33 (ID)	1.34 (ID)	
	WS_2	P-6m2	1.81 (D)	1.55 (D)	1.53 (D)	1.54 (D)[12,14] 1.60 (D)[13]
	WSe_2	P-6m2	1.54 (D)	1.26 (D)	1.24 (D)	1.32 (D)[12] 1.28 (D)[13] 1.20 (D)[14]
	WTe_2	P-6m2	1.04 (D)	0.73 (D)	0.73 (D)	0.74 (D)[12] 0.78 (D)[13]
Pro-MoSSe	BiBrS	P3m1	2.11 (ID)	1.63 (ID)	1.25 (ID)	
	BiBrSe	P3m1	2.08 (ID)	1.41 (ID)	1.07 (ID)	
	BiBrTe	P3m1	1.84 (ID)	0.91 (D)	0.58 (D)	
	BiClS	P3m1	2.31 (ID)	1.87 (ID)	1.50 (ID)	
	BiClSe	P3m1	2.28 (ID)	1.63 (ID)	1.29 (ID)	
	BiISe	P3m1	1.72 (ID)	0.85 (ID)	0.48 (ID)	
	BiITe	P3m1	1.66 (ID)	0.70 (ID)	0.39 (ID)	
	HfBrCl	P3m1	0.94 (ID)	0.85 (ID)	0.82 (ID)	
	HfBrI	P3m1	0.85 (ID)	0.73 (ID)	0.71 (ID)	
	HfClI	P3m1	0.96 (ID)	0.84 (ID)	0.81 (ID)	
	HfSeTe	P3m1	0.29 (ID)	0.14 (ID)	0.14 (ID)	
	WSSe	P3m1	1.69 (ID)	1.42 (D)	1.40 (D)	1.44 (D)[14] 1.42 (D)[15] 1.46 (D)[16]
	WSTe	P3m1	1.23 (ID)	1.15 (ID)	1.14 (ID)	1.15 (ID)[16]
	WSeTe	P3m1	1.35 (D)	1.06 (ID)	1.04 (ID)	1.09 (ID)[16]
Pro-PbS	Pb_2Se_2	Pmn2_1	1.27 (ID)	0.94 (ID)	0.82 (ID)	
Pro-Ti_2CO_2	Hf_2CO_2	P-3m1	1.02 (ID)	0.98 (ID)	0.94 (ID)	

Table S17. Energy band gap (E_{gap}) values of 2D anisotropic materials, which includes heavy elements, with and without spin-orbit coupling effect. "D" and "ID" stand for direct and indirect energy bands, respectively. The last column corresponds to reported energy band gap values in C2DB.

Prototype	Material	Structure	E_g (eV) (PBE)	E_g (eV) (PBE+SOC)	E_g (eV) (C2DB-PBE+SOC)[11]
Pro-AuSe	Au_2O_2	P2/m	0.17 (ID)	0.20 (ID)	0.18 (ID)
	Au_2S_2	P2/m	1.54 (ID)	1.31 (ID)	1.22 (ID)
	Au_2Se_2	P2/m	1.21 (ID)	1.00 (ID)	0.96 (ID)
	Au_2Te_2	P2/m	0.96 (ID)	0.67 (ID)	0.62 (ID)
Pro-FeOCl	$Hf_2Br_2N_2$	Pmmn	2.11 (D)	2.11 (D)	2.07 (D)
	$Hf_2Cl_2N_2$	Pmmn	2.16 (D)	2.16 (D)	2.11 (D)
	$Ir_2Cl_2O_2$	Pmmn	0.44 (ID)	0.54 (ID)	0.45 (ID)
Pro-PdS_2	Pt_2S_4	P2_1/c	1.94 (D)	1.87 (ID)	1.80 (ID)
	Pt_2Se_4	P2_1/c	1.50 (ID)	1.45 (ID)	1.44 (ID)
	Pt_2Te_4	P2_1/c	1.38 (ID)	1.33 (ID)	1.31 (ID)
Pro-TiS_3	Hf_2O_6	Pmmn	3.29 (ID)	3.29 (ID)	3.47 (ID)
Pro-WTe_2	Hf_2Br_4	P2_1/m	0.85 (D)	0.84 (D)	0.85 (ID)
	Hf_2Cl_4	P2_1/m	0.85 (D)	0.85 (D)	0.84 (ID)
	Os_2O_4	P2_1/m	0.38 (ID)	0.23 (D)	0.17 (D)
	Os_2S_4	P2_1/m	0.70 (ID)	0.58 (ID)	0.53 (ID)
	Os_2Se_4	P2_1/m	0.77 (ID)	0.63 (ID)	0.57 (ID)
	Os_2Te_4	P2_1/m	0.76 (ID)	0.71 (ID)	0.71 (ID)



(a)W_2Cl_6-w/o soc (pro-BiI_3)

(b)W_2Cl_6-w soc (pro-BiI_3)

(c)BiBrS-w/o soc (pro-BiTeI)

(d)BiBrS-w soc (pro-BiTeI)

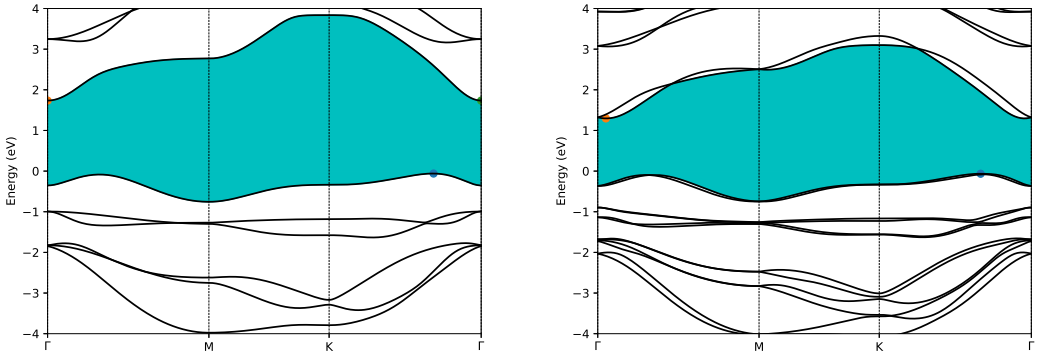
(e)BiBrSe-w/o soc (pro-BiTeI)

(f)BiBrSe-w soc (pro-BiTeI)

(g)BiBrTe-w/o soc (pro-BiTeI)

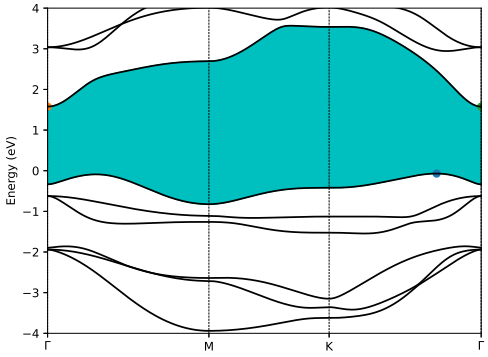
(h)BiBrTe-w soc (pro-BiTeI)

Figure S42. Electronic band structures by using PBE (w/o SOC) and PBE+SOC (w SOC)

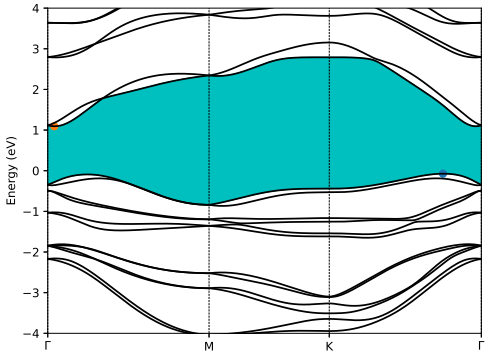


(a)BiClS-w/o soc (pro-BiTeI)

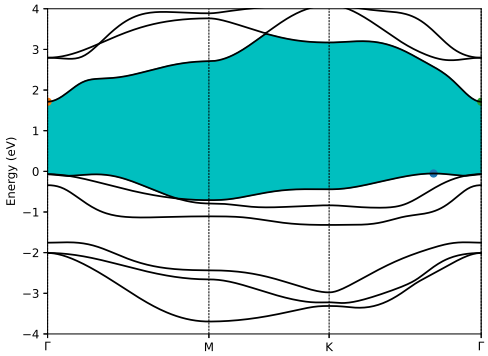
(b)BiClS-w soc (pro-BiTeI)



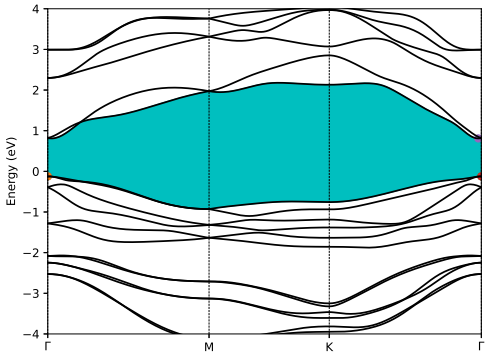
(c)BiClSe-w/o soc (pro-BiTeI)



(d)BiClSe-w soc (pro-BiTeI)

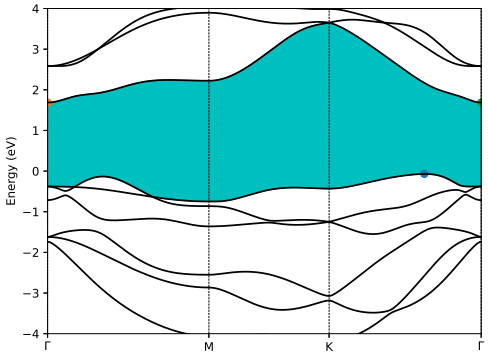


(e)BiClTe-w/o soc (pro-BiTeI)

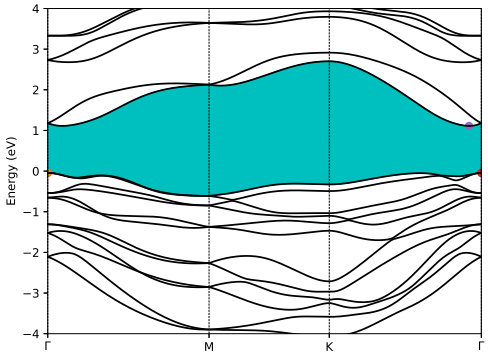


(f)BiClTe-w soc (pro-BiTeI)

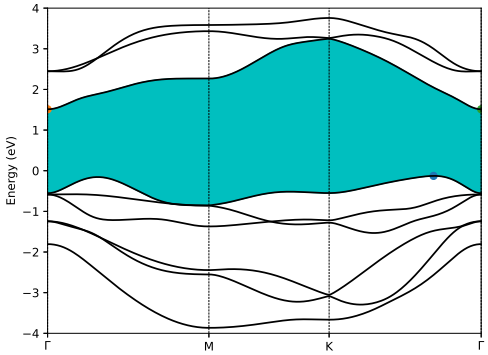
Figure S43. Electronic band structures by using PBE (w/o SOC) and PBE+SOC (w SOC)



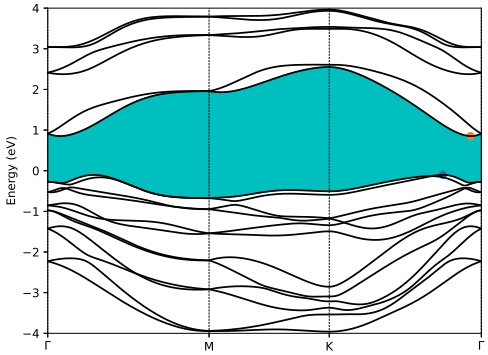
(a)BiIS-w/o soc (pro-BiTeI)



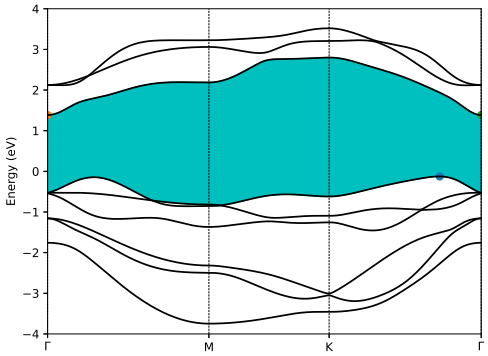
(b)BiIS-w soc (pro-BiTeI)



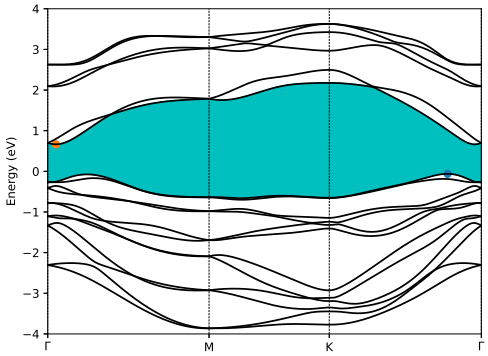
(c)BiISe-w/o soc (pro-BiTeI)



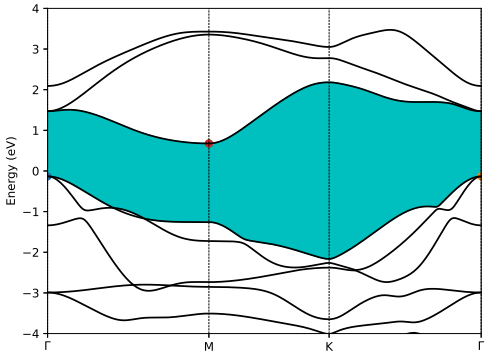
(d)BiISe-w soc (pro-BiTeI)



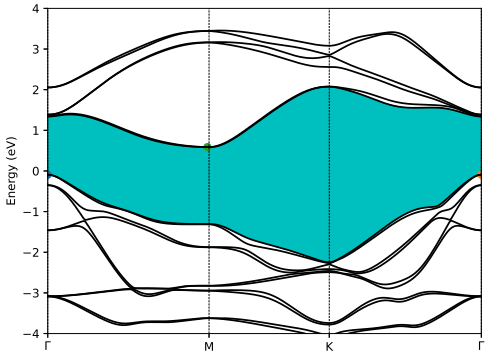
(e)BiITe-w/o soc (pro-BiTeI)



(f)BiITe-w soc (pro-BiTeI)

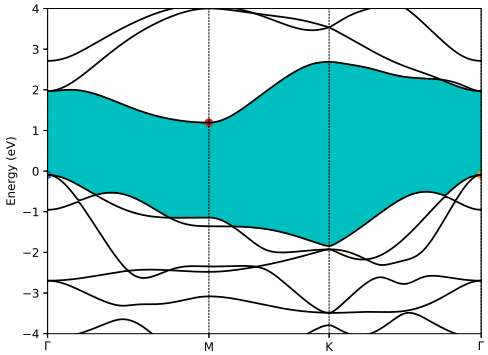


(g)HfSSe-w/o soc (pro-BiTeI)

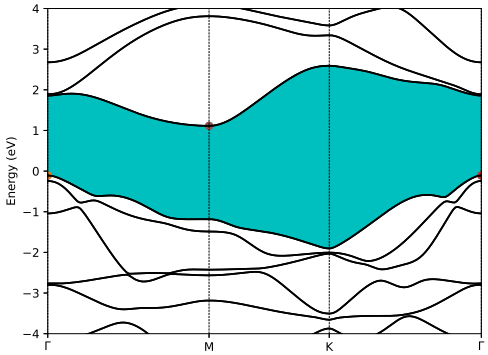


(h)HfSSe-w soc (pro-BiTeI)

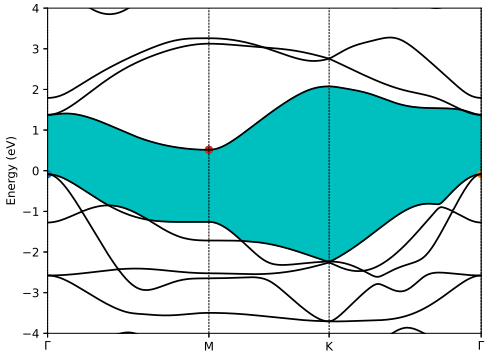
Figure S44. Electronic band structures by using PBE (w/o SOC) and PBE+SOC (w SOC)



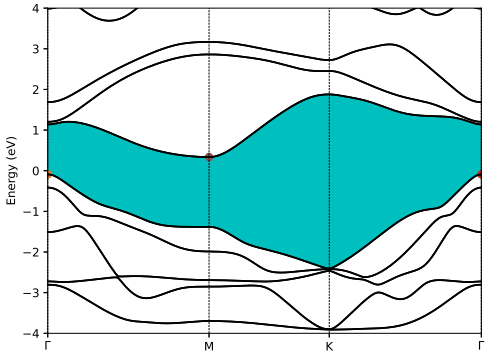
(a)HfS_2-w/o soc (pro-CdI_2)



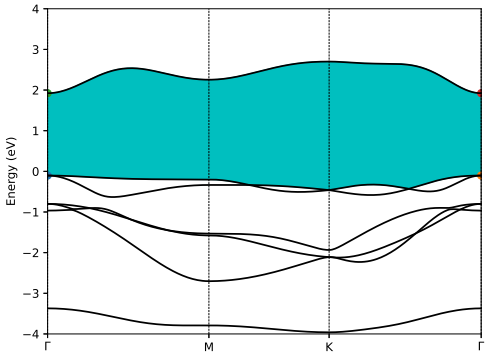
(b)HfS_2-w soc (pro-CdI_2)



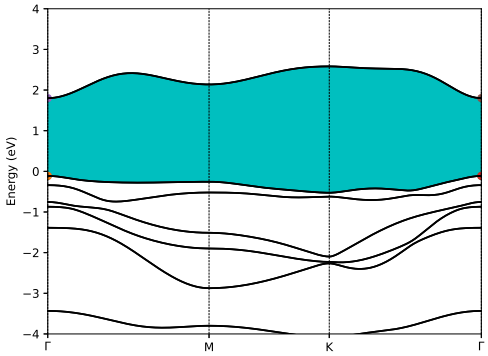
(c)$HfSe_2$-w/o soc (pro-CdI_2)



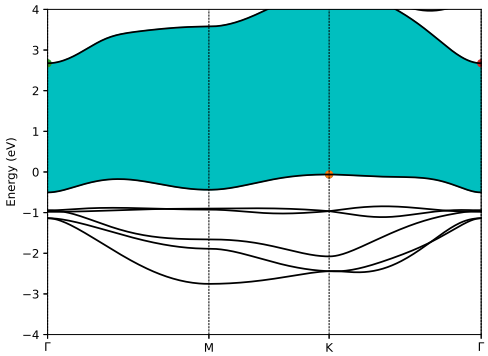
(d)$HfSe_2$-w soc (pro-CdI_2)



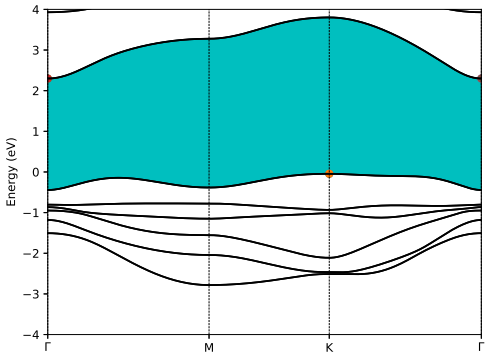
(e)$HgBr_2$-w/o soc (pro-CdI_2)



(f)$HgBr_2$-w soc (pro-CdI_2)

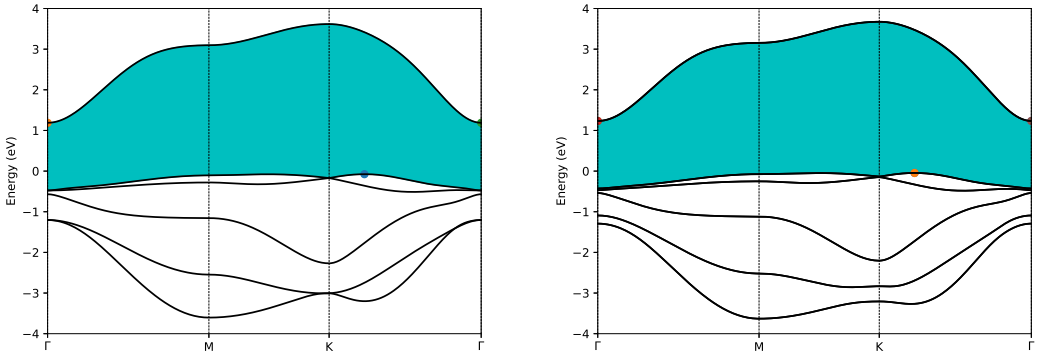


(g)$PbBr_2$-w/o soc (pro-CdI_2)

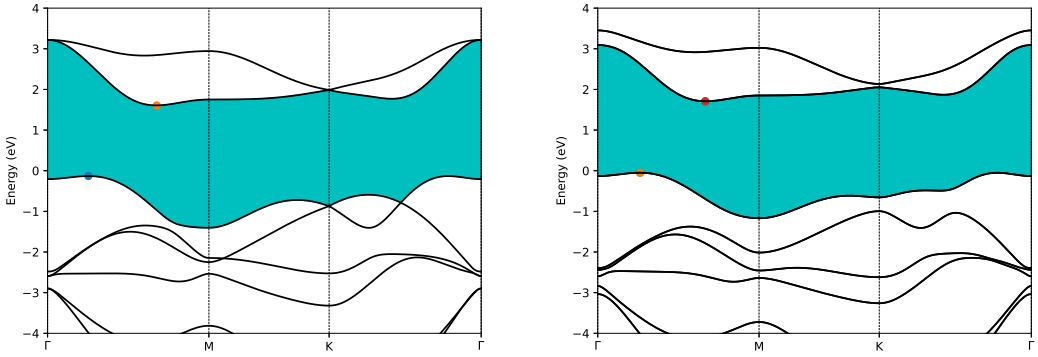


(h)$PbBr_2$-w soc (pro-CdI_2)

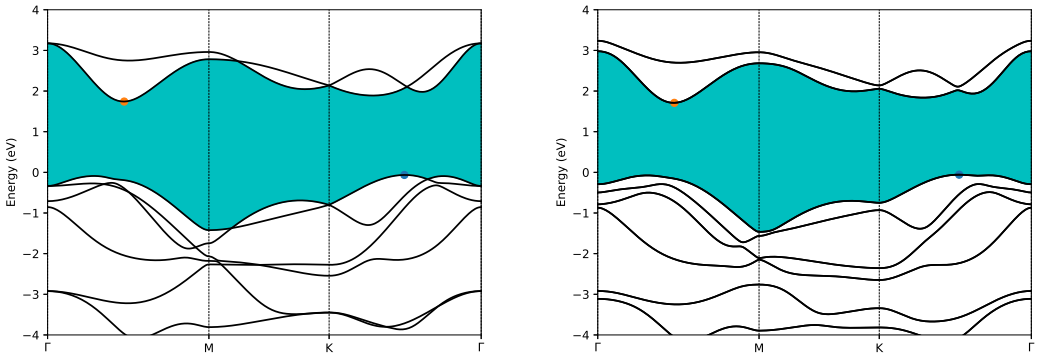
Figure S45. Electronic band structures by using PBE (w/o SOC) and PBE+SOC (w SOC)



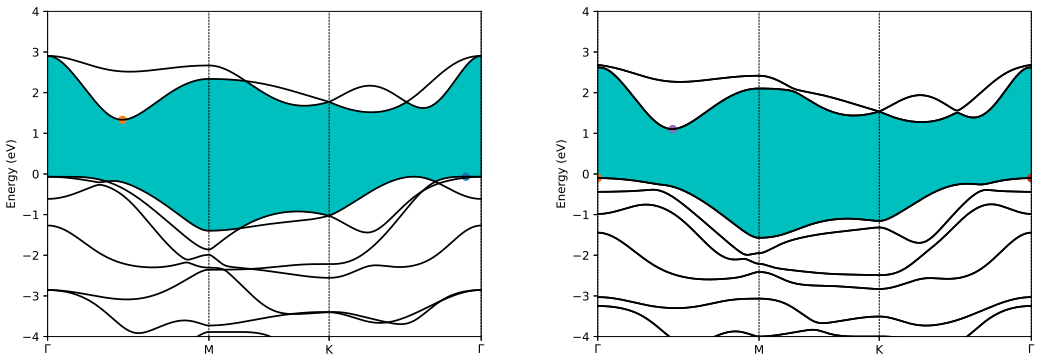
(a)PbO_2-w/o soc (pro-CdI_2) (b)PbO_2-w soc (pro-CdI_2)



(c)PtO_2-w/o soc (pro-CdI_2) (d)PtO_2-w soc (pro-CdI_2)

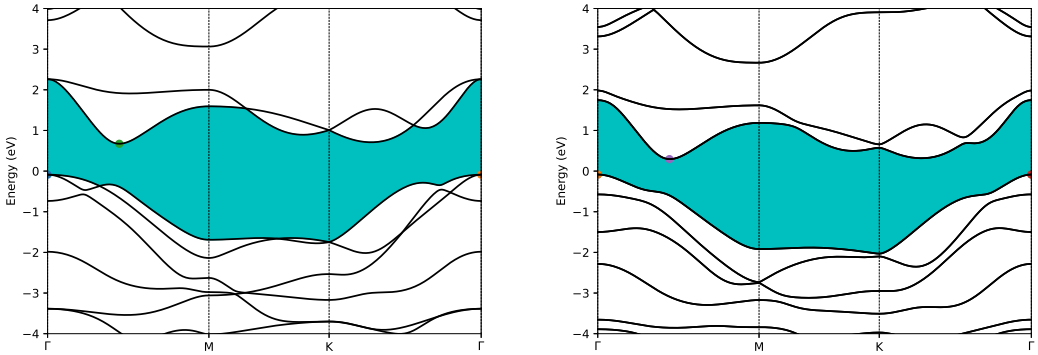


(e)PtS_2-w/o soc (pro-CdI_2) (f)PtS_2-w soc (pro-CdI_2)



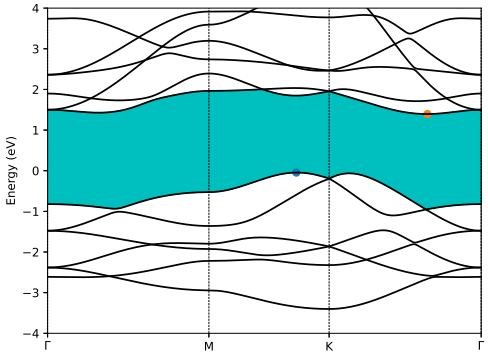
(g)$PtSe_2$-w/o soc (pro-CdI_2) (h)$PtSe_2$-w soc (pro-CdI_2)

Figure S46. Electronic band structures by using PBE (w/o SOC) and PBE+SOC (w SOC)

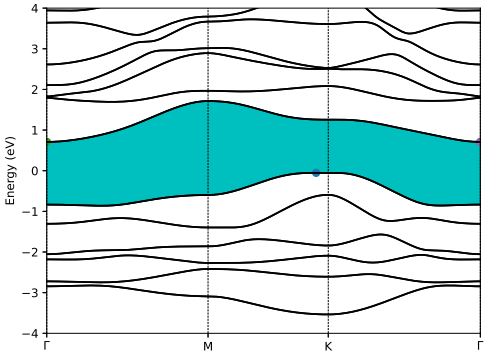


(a)$PtTe_2$-w/o soc (pro-CdI_2)

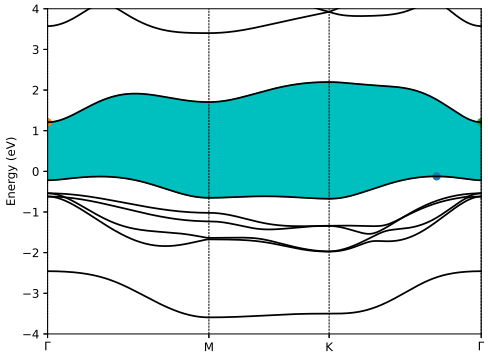
(b)$PtTe_2$-w soc (pro-CdI_2)



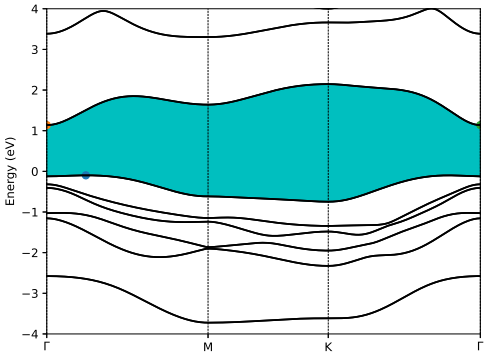
(c)Pb_2Te_2-w/o soc (pro-CH)



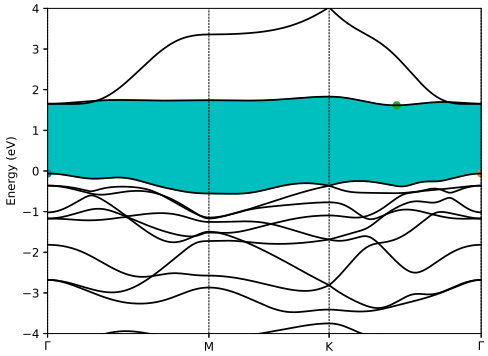
(d)Pb_2Te_2-w soc (pro-CH)



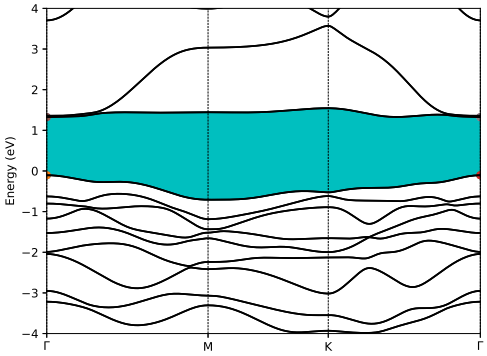
(e)Hg_2I_2-w/o soc (pro-GaSe)



(f)Hg_2I_2-w soc (pro-GaSe)

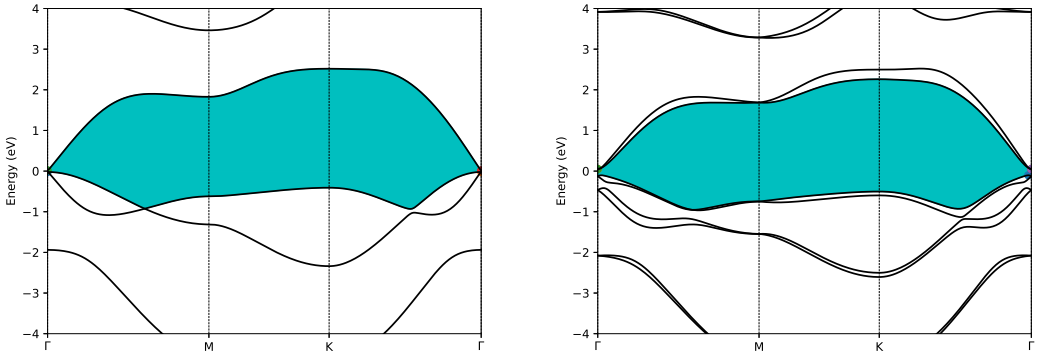


(g)Pt_2Cl_2-w/o soc (pro-GaSe)



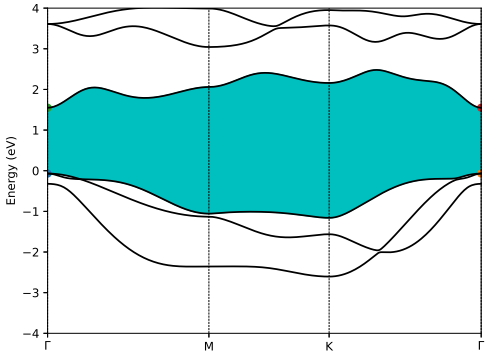
(h)Pt_2Cl_2-w soc (pro-GaSe)

Figure S47. Electronic band structures by using PBE (w/o SOC) and PBE+SOC (w SOC)

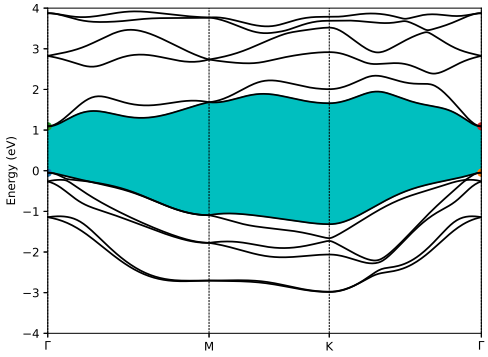


(a)HgTe-w/o soc (pro-GeSe)

(b)HgTe-w soc (pro-GeSe)

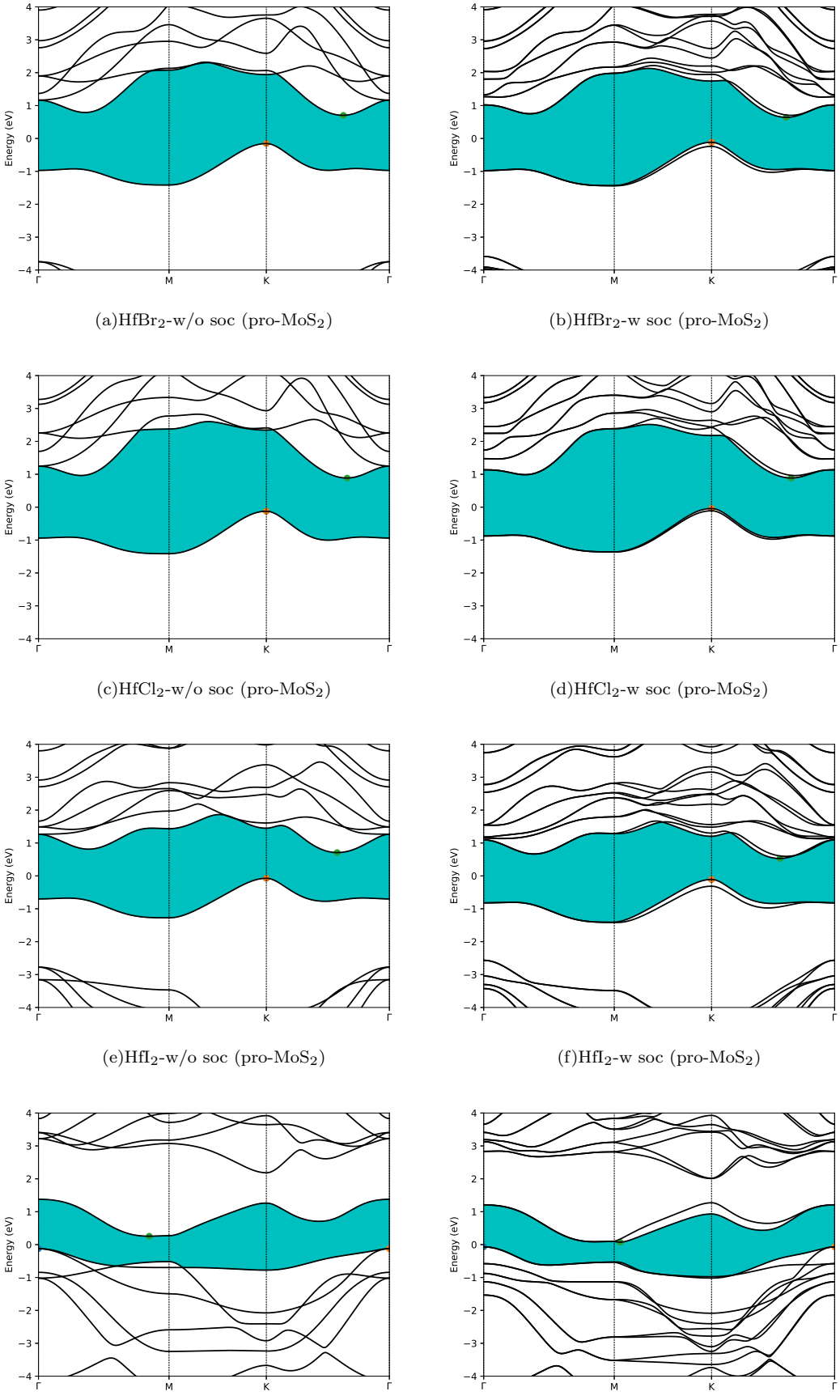


(c)PbTe-w/o soc (pro-GeSe)



(d)PbTe-w soc (pro-GeSe)

Figure S48. Electronic band structures by using PBE (w/o SOC) and PBE+SOC (w SOC)



(a)$HfBr_2$-w/o soc (pro-MoS_2)

(b)$HfBr_2$-w soc (pro-MoS_2)

(c)$HfCl_2$-w/o soc (pro-MoS_2)

(d)$HfCl_2$-w soc (pro-MoS_2)

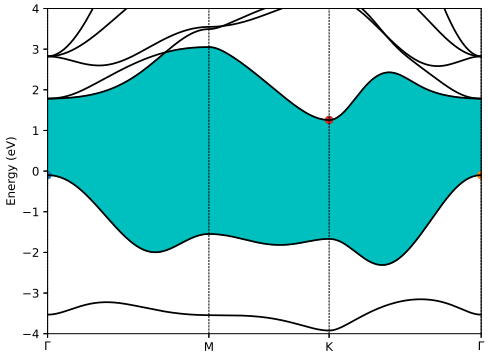
(e)HfI_2-w/o soc (pro-MoS_2)

(f)HfI_2-w soc (pro-MoS_2)

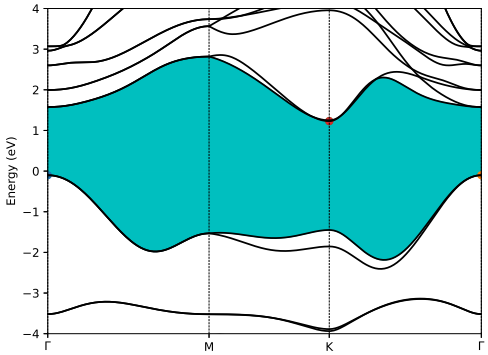
(g)$HfTe_2$-w/o soc (pro-MoS_2)

(h)$HfTe_2$-w soc (pro-MoS_2)

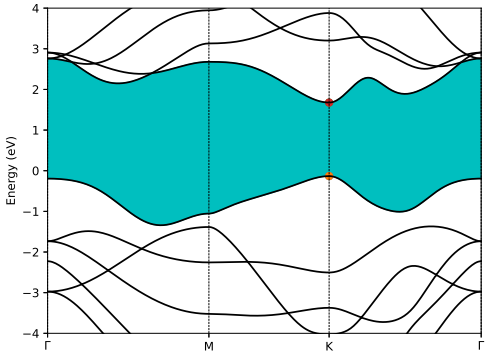
Figure S49. Electronic band structures by using PBE (w/o SOC) and PBE+SOC (w SOC)



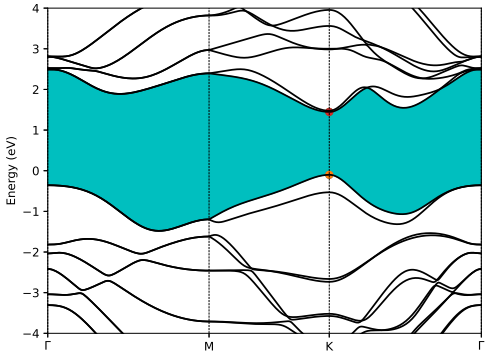
(a)WO_2-w/o soc (pro-MoS_2)



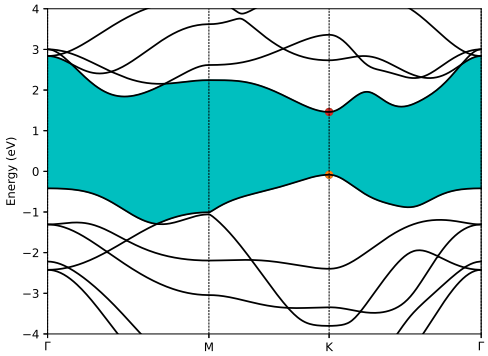
(b)WO_2-w soc (pro-MoS_2)



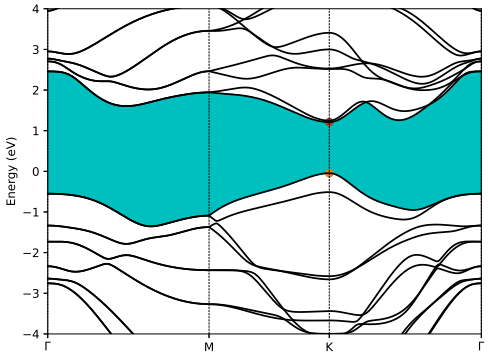
(c)WS_2-w/o soc (pro-MoS_2)



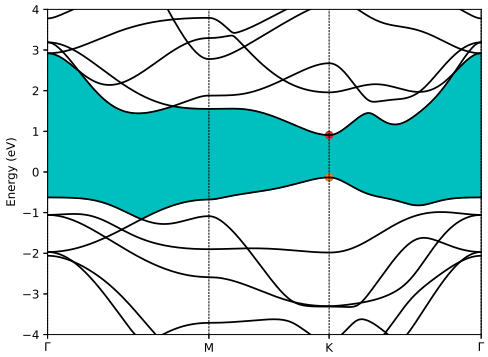
(d)WS_2-w soc (pro-MoS_2)



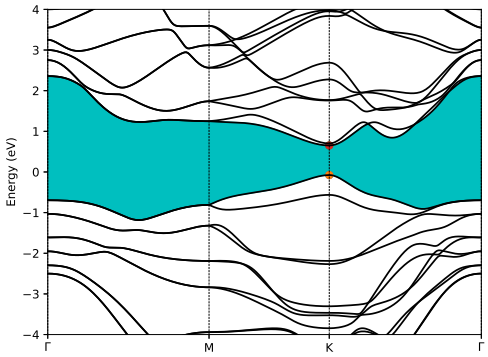
(e)WSe_2-w/o soc (pro-MoS_2)



(f)WSe_2-w soc (pro-MoS_2)

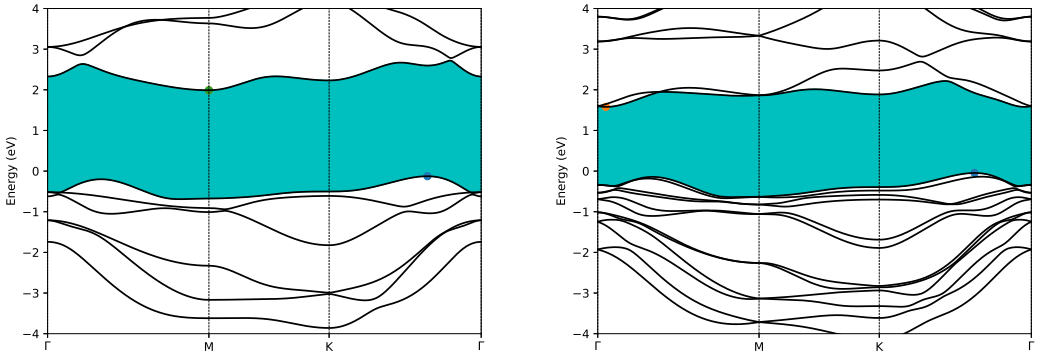


(g)WTe_2-w/o soc (pro-MoS_2)



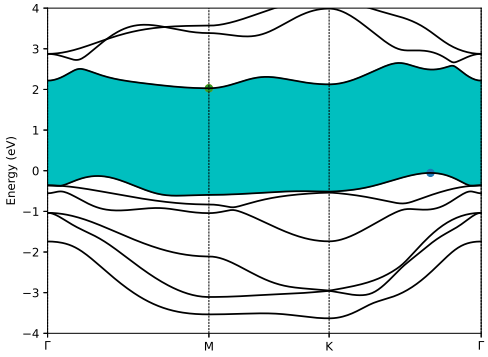
(h)WTe_2-w soc (pro-MoS_2)

Figure S50. Electronic band structures by using PBE (w/o SOC) and PBE+SOC (w SOC)

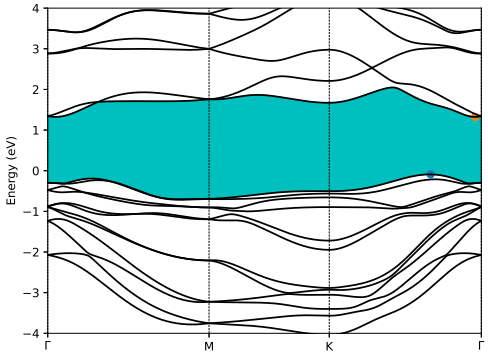


(a)BiBrS-w/o soc (pro-MoSSe)

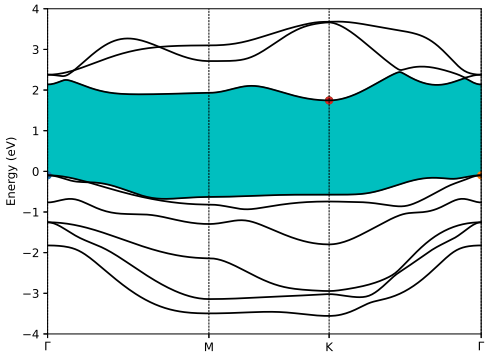
(b)BiBrS-w soc (pro-MoSSe)



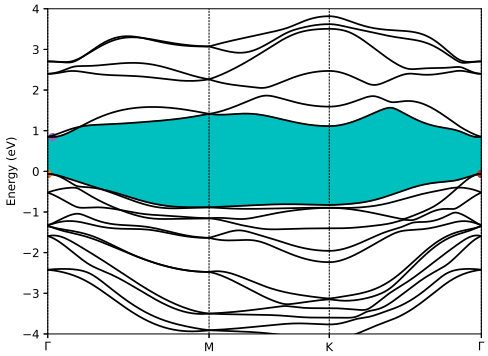
(c)BiBrSe-w/o soc (pro-MoSSe)



(d)BiBrSe-w soc (pro-MoSSe)

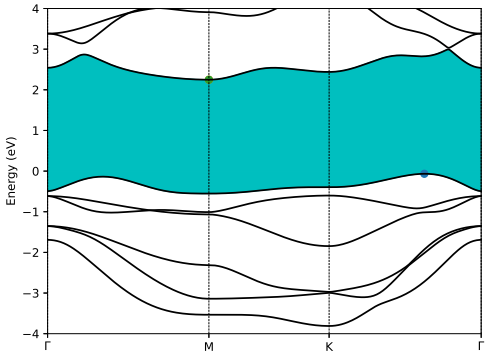


(e)BiBrTe-w/o soc (pro-MoSSe)

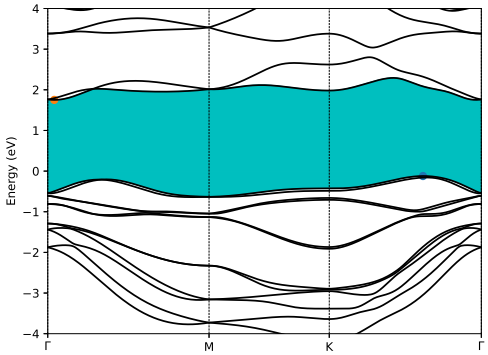


(f)BiBrTe-w soc (pro-MoSSe)

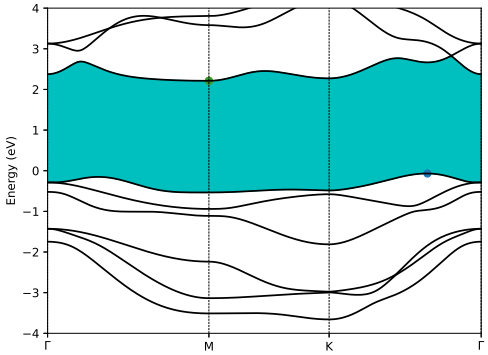
Figure S51. Electronic band structures by using PBE (w/o SOC) and PBE+SOC (w SOC)



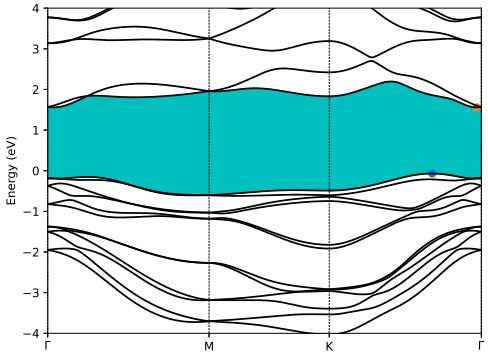
(a)BiClS-w/o soc (pro-MoSSe)



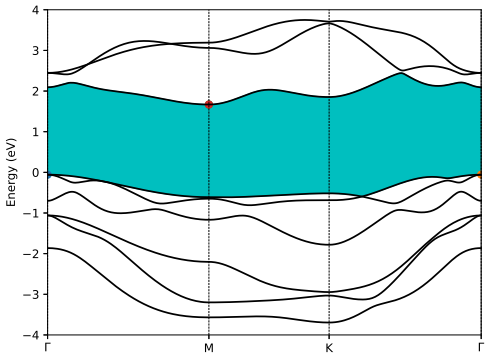
(b)BiClS-w soc (pro-MoSSe)



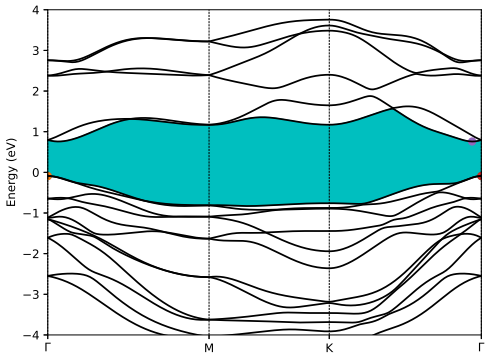
(c)BiClSe-w/o soc (pro-MoSSe)



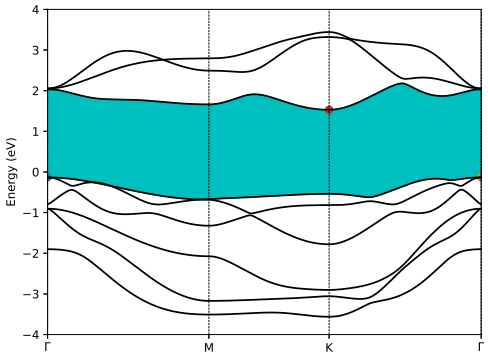
(d)BiClSe-w soc (pro-MoSSe)



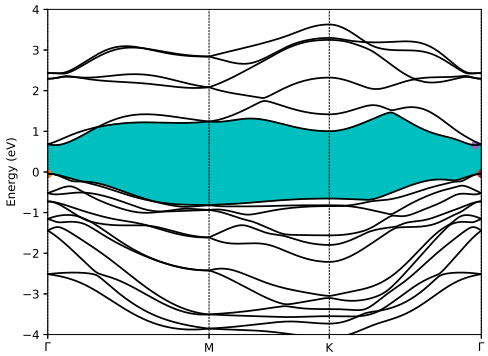
(e)BiISe-w/o soc (pro-MoSSe)



(f)BiISe-w soc (pro-MoSSe)

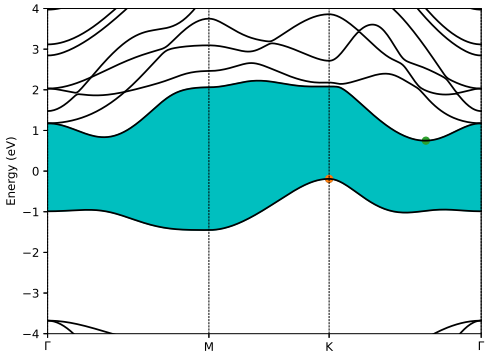


(g)BiITe-w/o soc (pro-MoSSe)

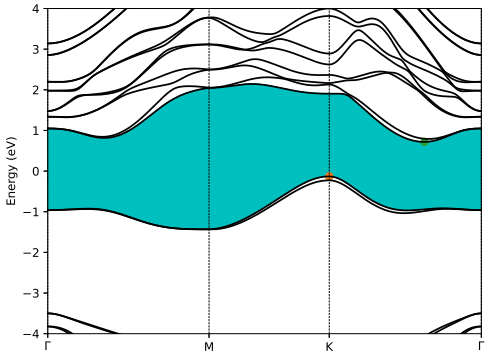


(h)BiITe-w soc (pro-MoSSe)

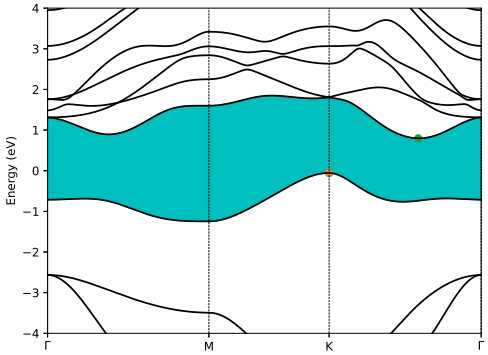
Figure S52. Electronic band structures by using PBE (w/o SOC) and PBE+SOC (w SOC)



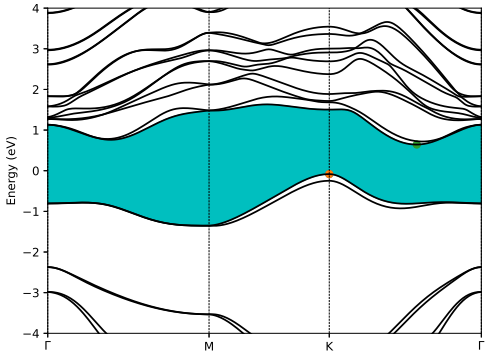
(a)HfBrCl-w/o soc (pro-MoSSe)



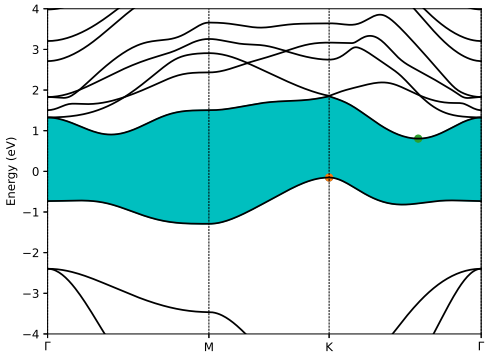
(b)HfBrCl-w soc (pro-MoSSe)



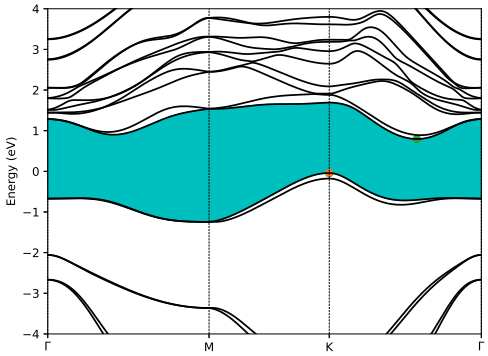
(c)HfBrI-w/o soc (pro-MoSSe)



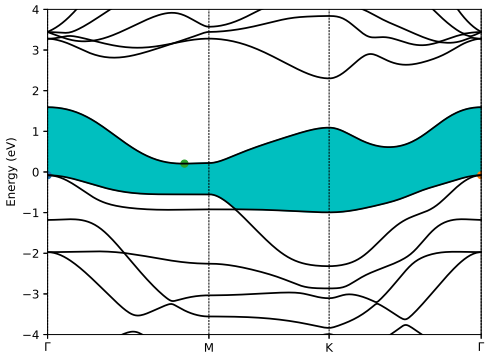
(d)HfBrI-w soc (pro-MoSSe)



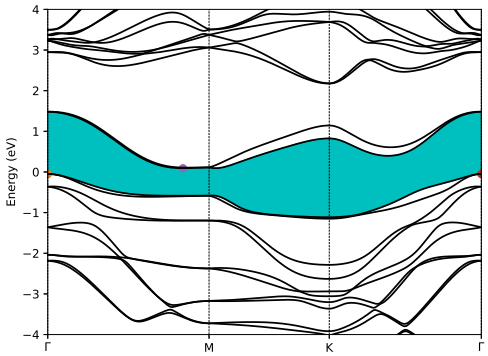
(e)HfClI-w/o soc (pro-MoSSe)



(f)HfClI-w soc (pro-MoSSe)

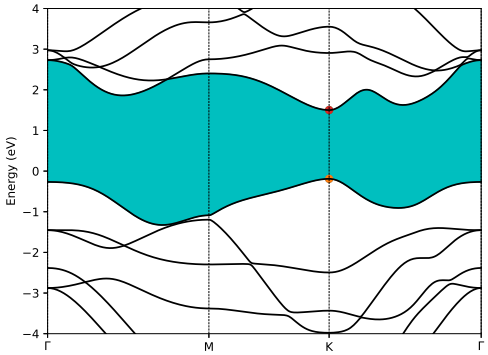


(g)HfSeTe-w/o soc (pro-MoSSe)

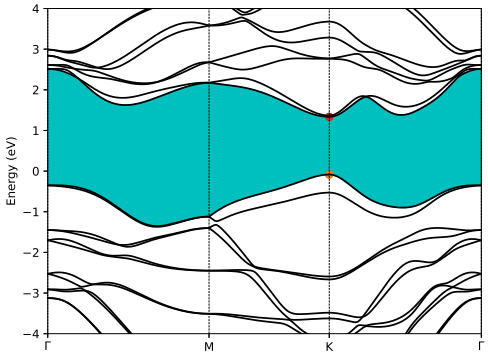


(h)HfSeTe-w soc (pro-MoSSe)

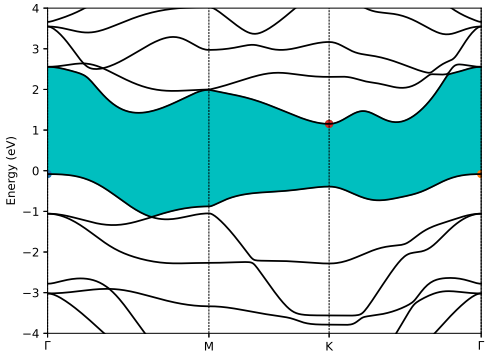
Figure S53. Electronic band structures by using PBE (w/o SOC) and PBE+SOC (w SOC)



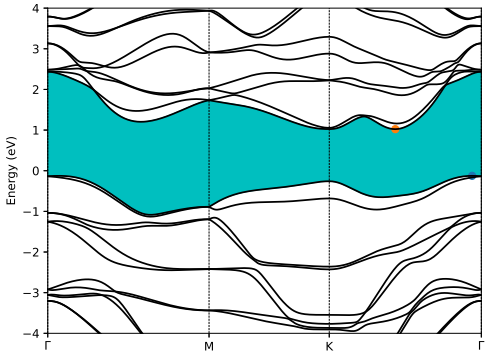
(a)WSSe-w/o soc (pro-MoSSe)



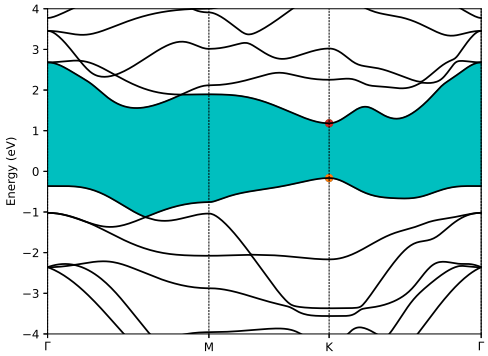
(b)WSSe-w soc (pro-MoSSe)



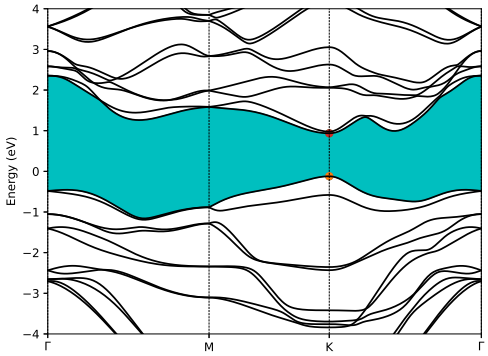
(c)WSTe-w/o soc (pro-MoSSe)



(d)WSTe-w soc (pro-MoSSe)

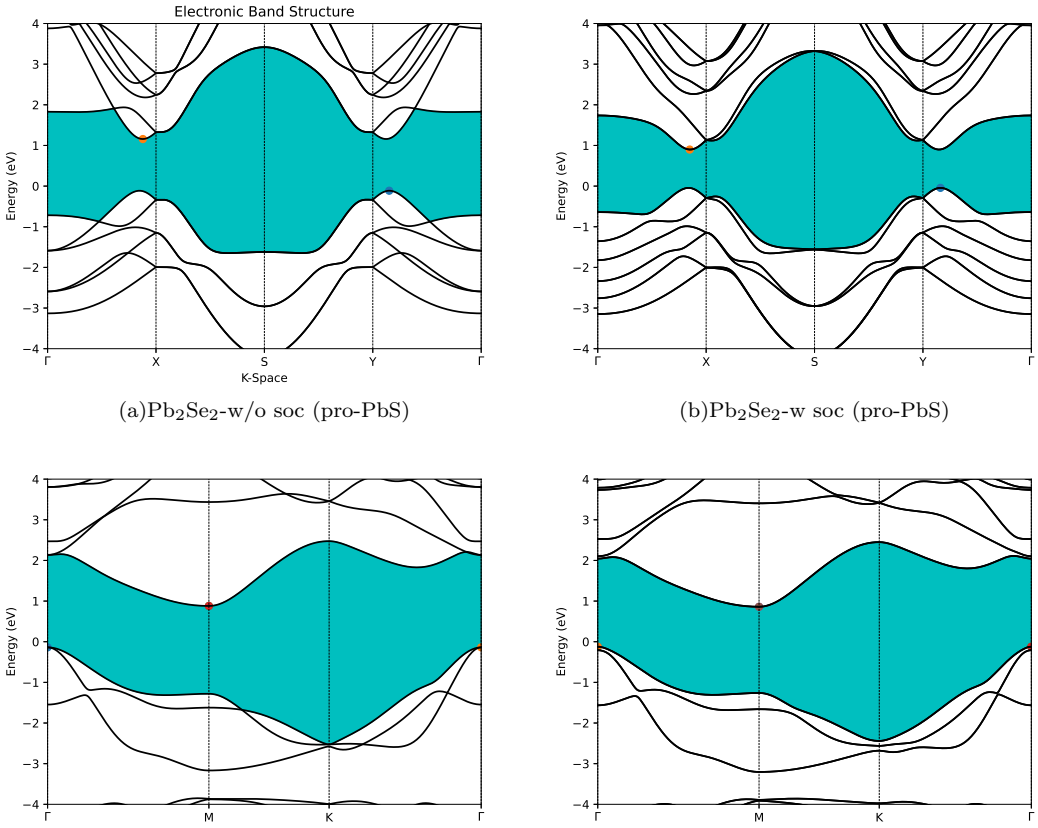


(e)WSeTe-w/o soc (pro-MoSSe)



(f)WSeTe-w soc (pro-MoSSe)

Figure S54. Electronic band structures by using PBE (w/o SOC) and PBE+SOC (w SOC)



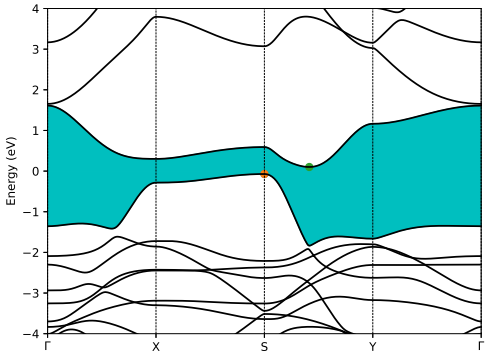
(a)Pb_2Se_2-w/o soc (pro-PbS)

(b)Pb_2Se_2-w soc (pro-PbS)

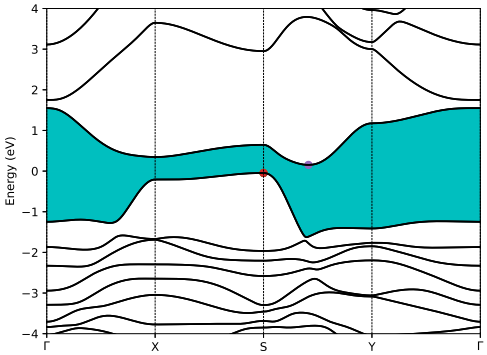
(c)Hf_2CO_2-w/o soc (pro-Ti_2CO_2)

(d)Hf_2CO_2-w soc (pro-Ti_2CO_2)

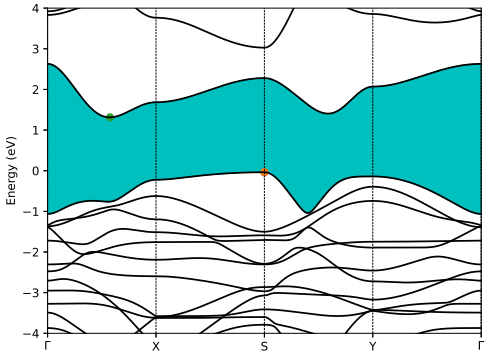
Figure S55. Electronic band structures by using PBE (w/o SOC) and PBE+SOC (w SOC)



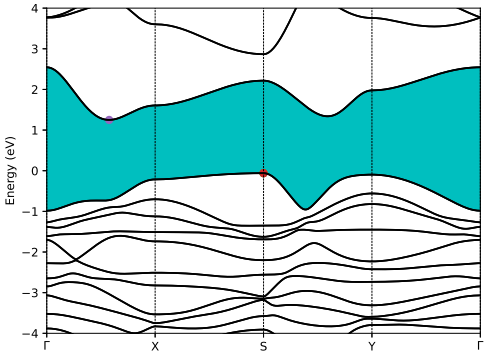
(a)Au_2O_2-w/o soc (pro-AuSe)



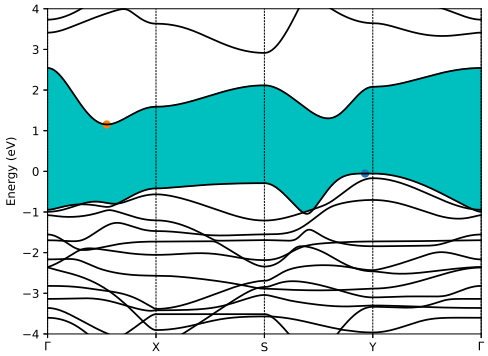
(b)Au_2O_2-w soc (pro-AuSe)



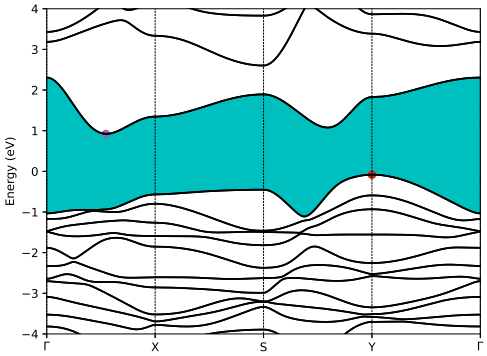
(c)Au_2S_2-w/o soc (pro-AuSe)



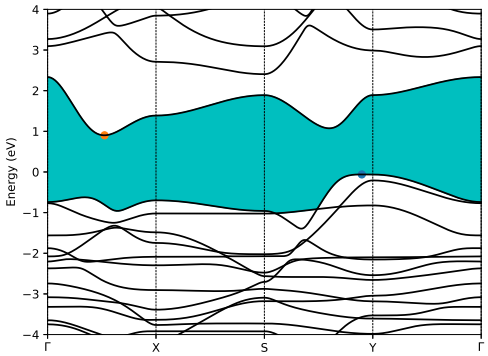
(d)Au_2S_2-w soc (pro-AuSe)



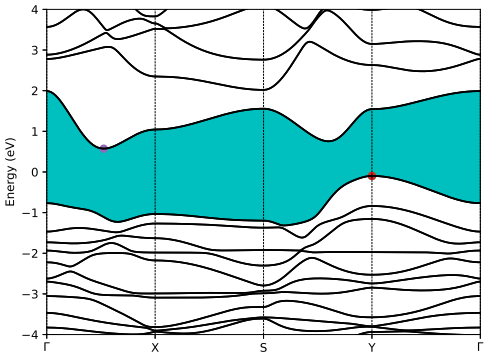
(e)Au_2Se_2-w/o soc (pro-AuSe)



(f)Au_2Se_2-w soc (pro-AuSe)

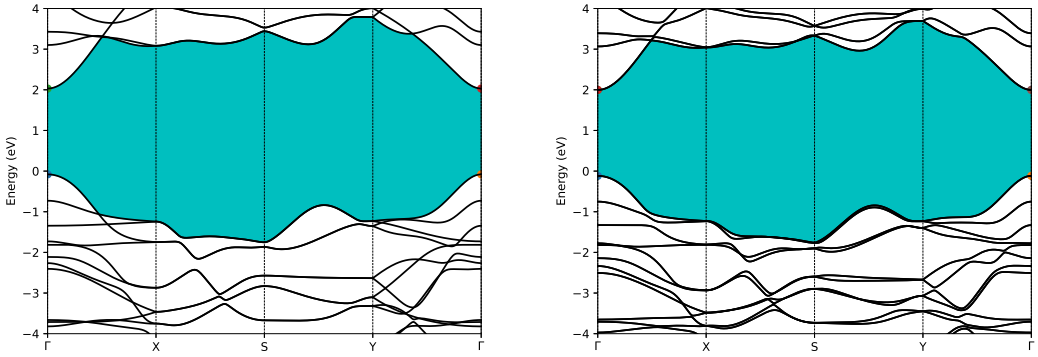


(g)Au_2Te_2-w/o soc (pro-AuSe)



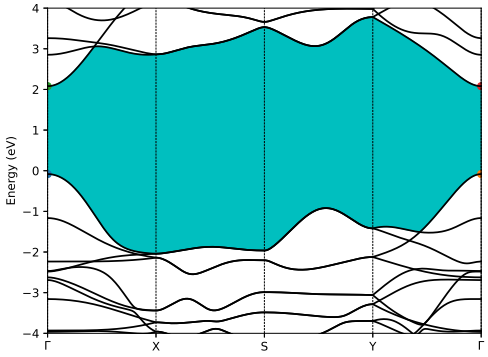
(h)Au_2Te_2-w soc (pro-AuSe)

Figure S56. Electronic band structures by using PBE (w/o SOC) and PBE+SOC (w SOC)

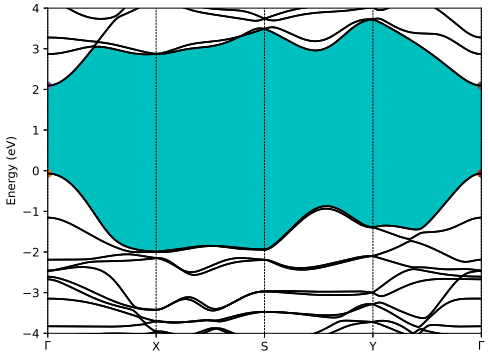


(a)$Hf_2Br_2N_2$-w/o soc (pro-FeOCl)

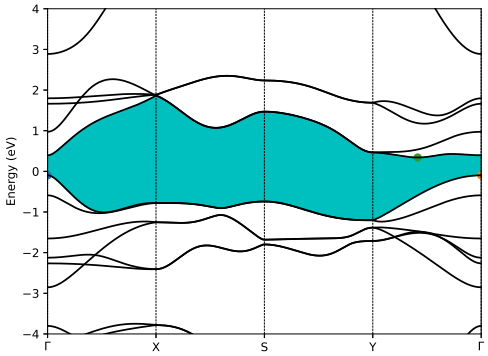
(b)$Hf_2Br_2N_2$-w soc (pro-FeOCl)



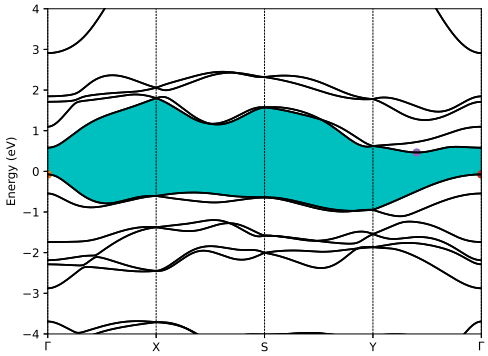
(c)$Hf_2Cl_2N_2$-w/o soc (pro-FeOCl)



(d)$Hf_2Cl_2N_2$-w soc (pro-FeOCl)

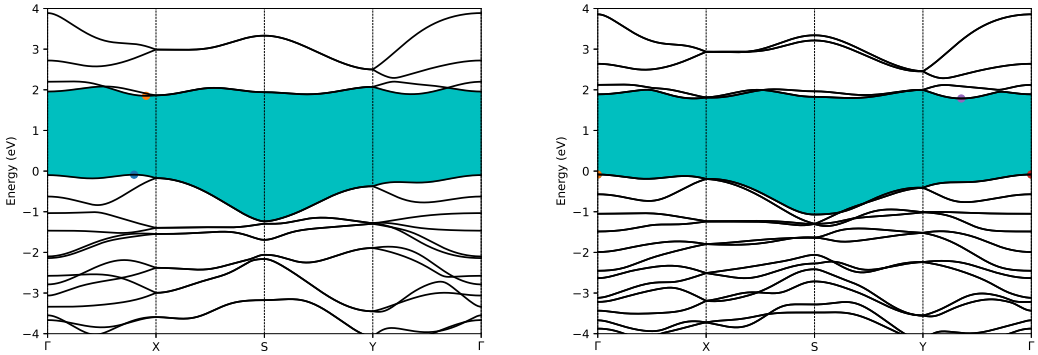


(e)$Ir_2Cl_2O_2$-w/o soc (pro-FeOCl)



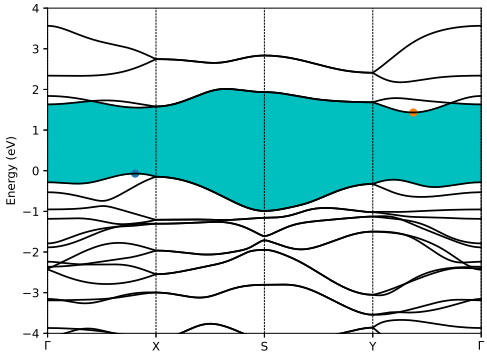
(f)$Ir_2Cl_2O_2$-w soc (pro-FeOCl)

Figure S57. Electronic band structures by using PBE (w/o SOC) and PBE+SOC (w SOC)

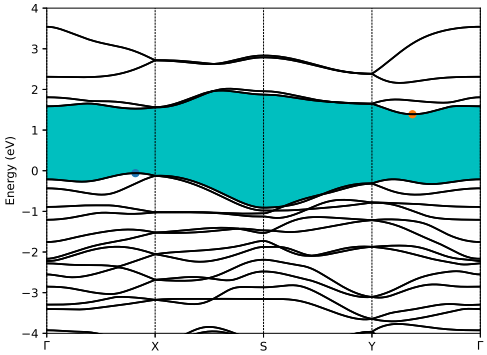


(a)Pt_2S_4-w/o soc (pro-PdS_2)

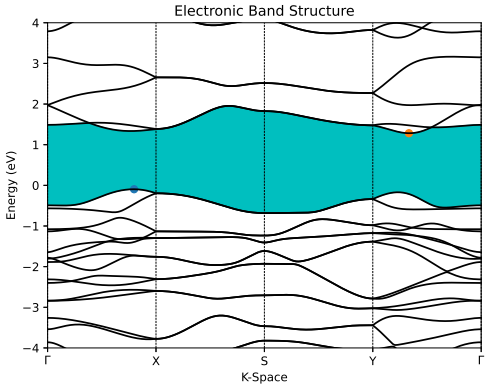
(b)Pt_2S_4-w soc (pro-PdS_2)



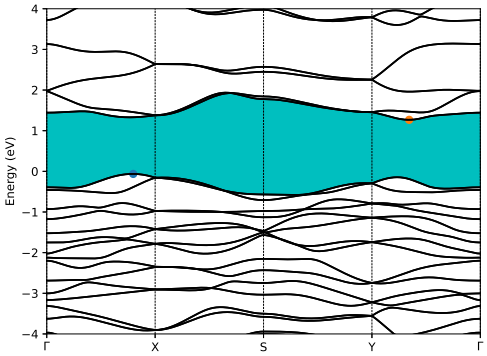
(c)Pt_2Se_4-w/o soc (pro-PdS_2)



(d)Pt_2Se_4-w soc (pro-PdS_2)

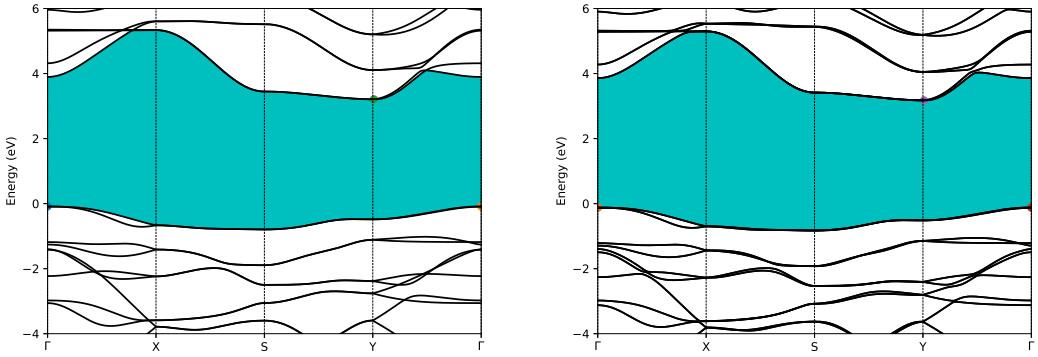


(e)Pt_2Te_4-w/o soc (pro-PdS_2)

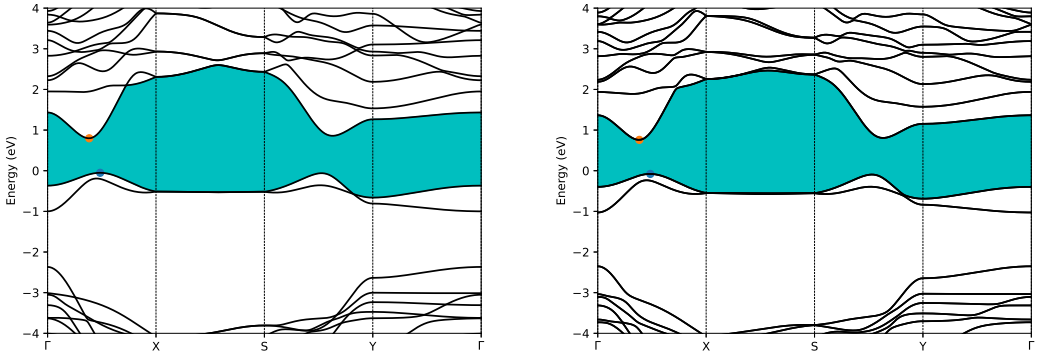


(f)Pt_2Te_4-w soc (pro-PdS_2)

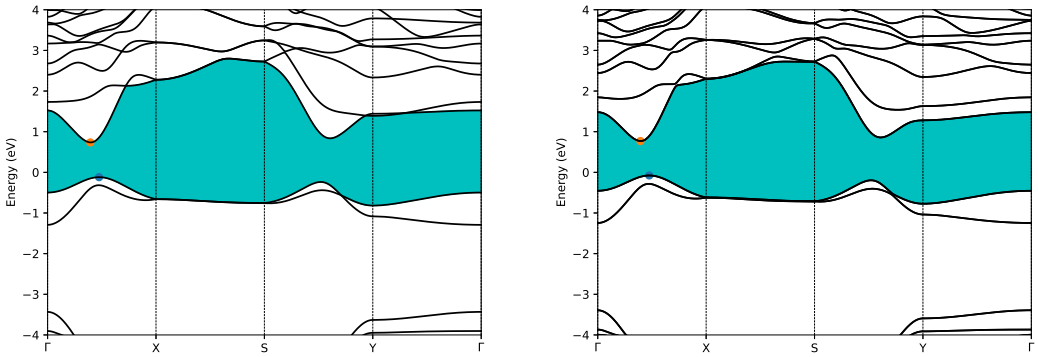
Figure S58. Electronic band structures by using PBE (w/o SOC) and PBE+SOC (w SOC)



(a)Hf_2O_6-w/o soc (pro-TiS_3) (b)Hf_2O_6-w soc (pro-TiS_3)

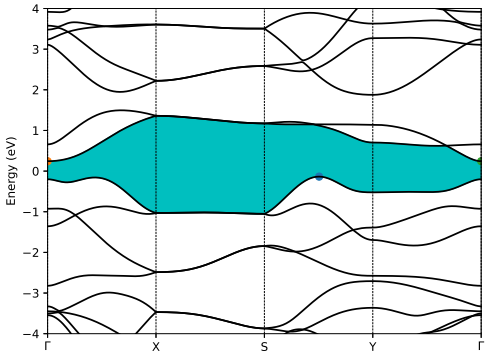


(c)Hf_2Br_4-w/o soc (pro-WTe_2) (d)Hf_2Br_4-w soc (pro-WTe_2)

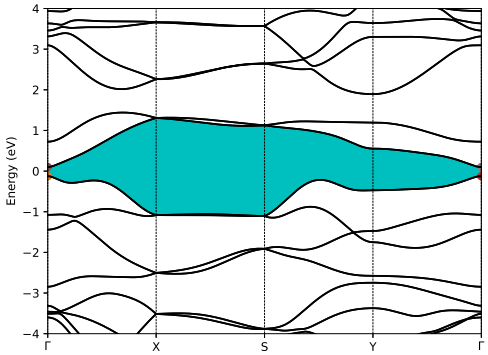


(e)Hf_2Cl_4-w/o soc (proWTe_2-) (f)Hf_2Cl_4-w soc (pro-WTe_2)

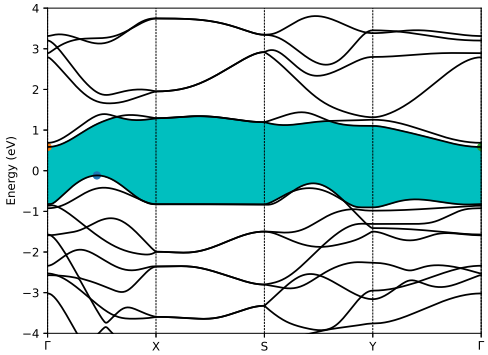
Figure S59. Electronic band structures by using PBE (w/o SOC) and PBE+SOC (w SOC)



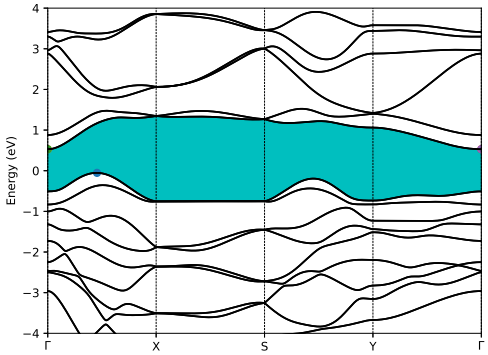
(a)Os_2O_4-w/o soc (pro-WTe_2)



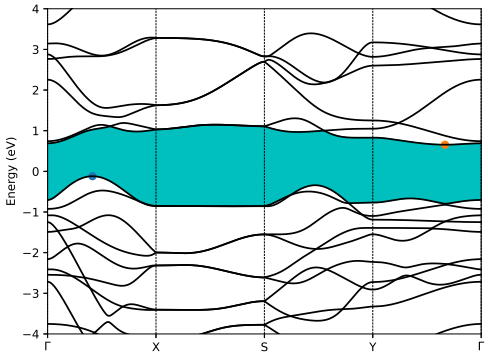
(b)Os_2O_4-w soc (pro-WTe_2)



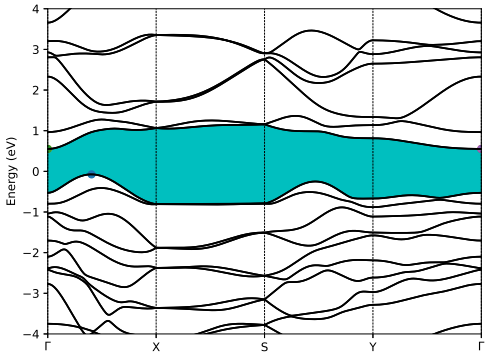
(c)Os_2S_4-w/o soc (pro-WTe_2)



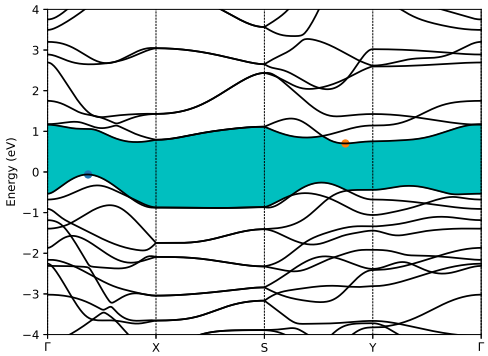
(d)Os_2S_4-w soc (pro-WTe_2)



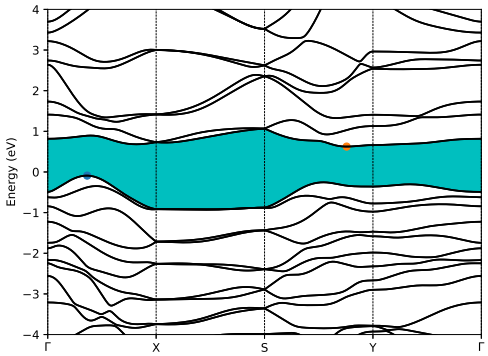
(e)Os_2Se_4-w/o soc (pro-WTe_2)



(f)Os_2Se_4-w soc (pro-WTe_2)

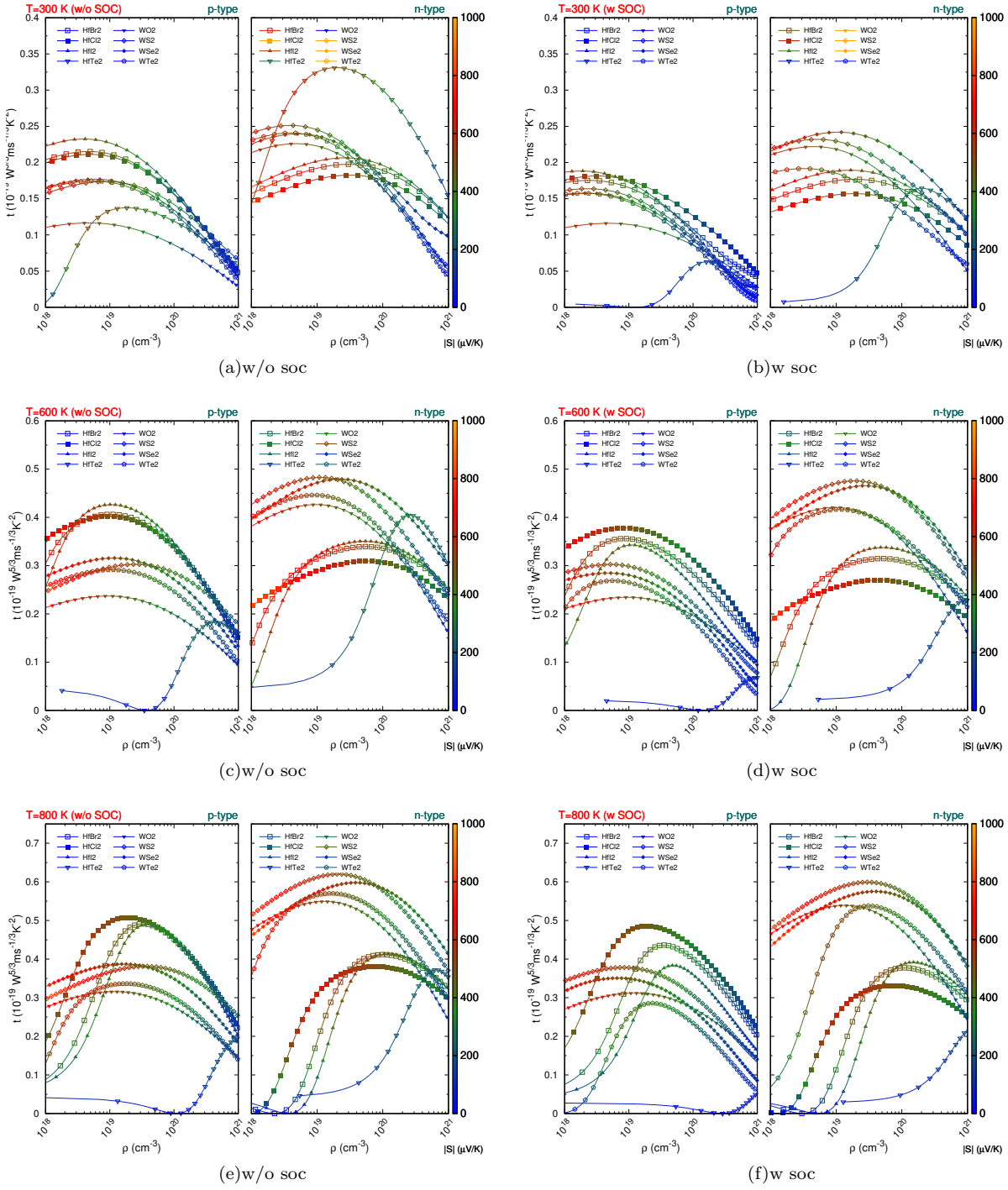


(g)Os_2Te_4-w/o soc (pro-WTe_2)



(h)Os_2Te_4-w soc (pro-WTe_2)

Figure S60. Electronic band structures by using PBE (w/o SOC) and PBE+SOC (w SOC)



(a)w/o soc (b)w soc (c)w/o soc (d)w soc (e)w/o soc (f)w soc

Figure S61. Calculated EFF of 2D isotropic materials with prototype MoS_2 as a function of charge carrier concentration for p-type and n-type carriers at T=300 K (a-b) T=600 K (c-d) T=800 K (e-f) using PBE (w/o SOC) and PBE+SOC (w SOC) . The corresponding Seebeck coefficient at the same carrier concentration is indicated by color.

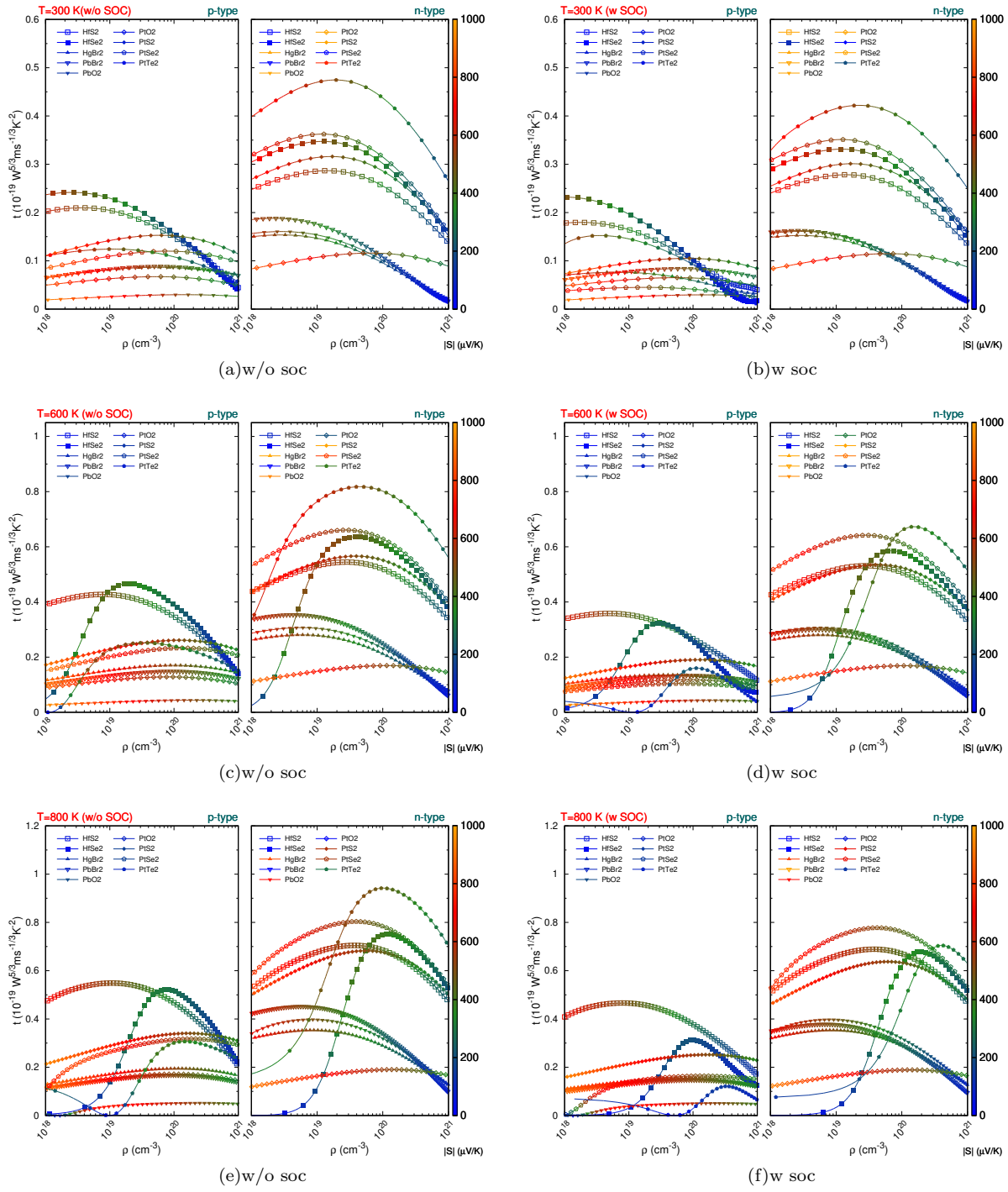


Figure S62. Calculated EFF of 2D isotropic materials with prototype-CdI_2 as a function of charge carrier concentration for p-type and n-type carriers at T=300 K (a-b) T=600 K (c-d) T=800 K (e-f) using PBE (w/o SOC) and PBE+SOC (w SOC). The corresponding Seebeck coefficient at the same carrier concentration is indicated by color.

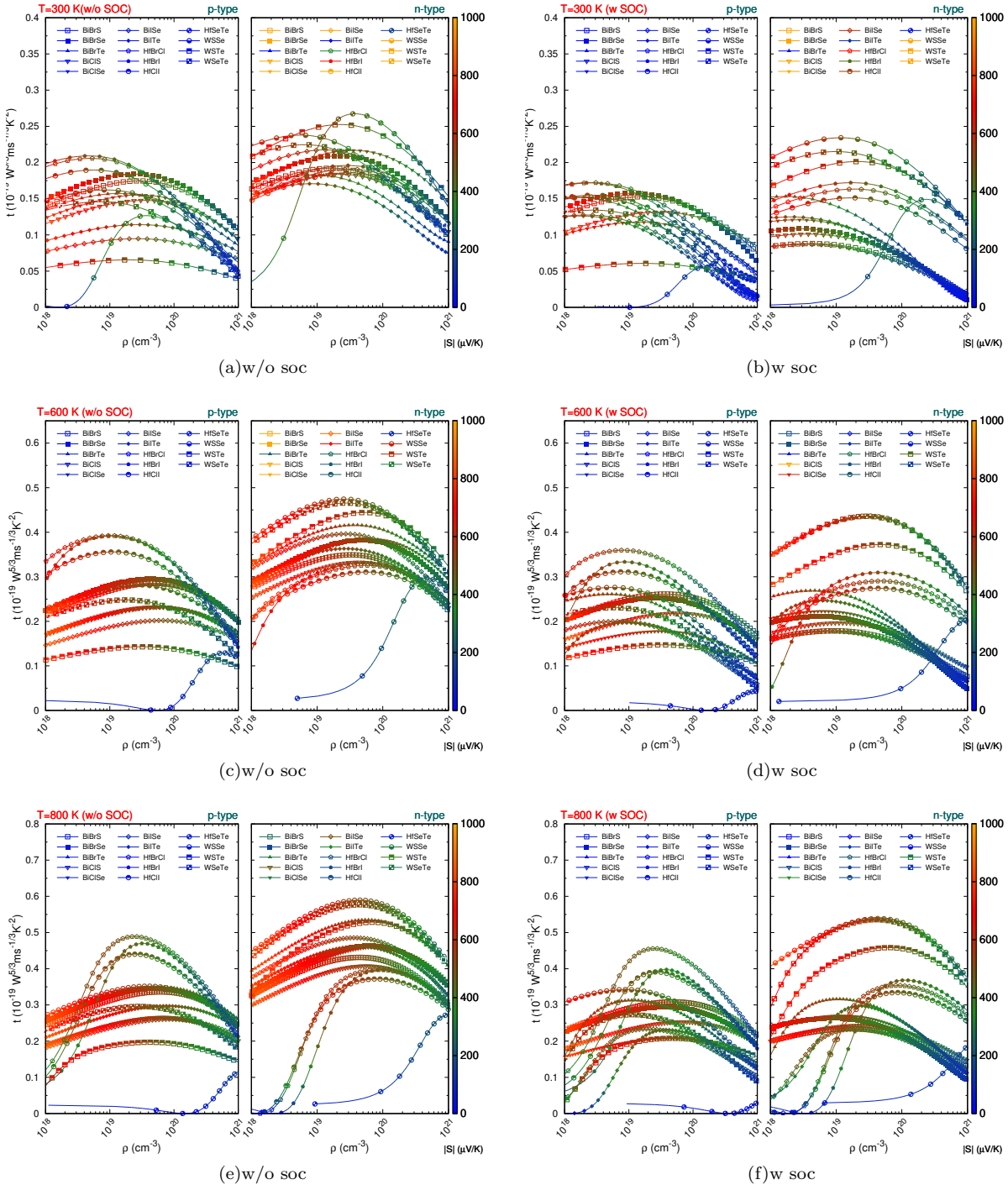


Figure S63. Calculated EFF of 2D isotropic materials with prototype-MoSSe as a function of charge carrier concentration for *p*- type and *n*-type carriers at T=300 K (a-b) T=600 K (c-d) T=800 K (e-f) using PBE (w/o SOC) and PBE+SOC (w SOC). The corresponding Seebeck coefficient at the same carrier concentration is indicated by color.

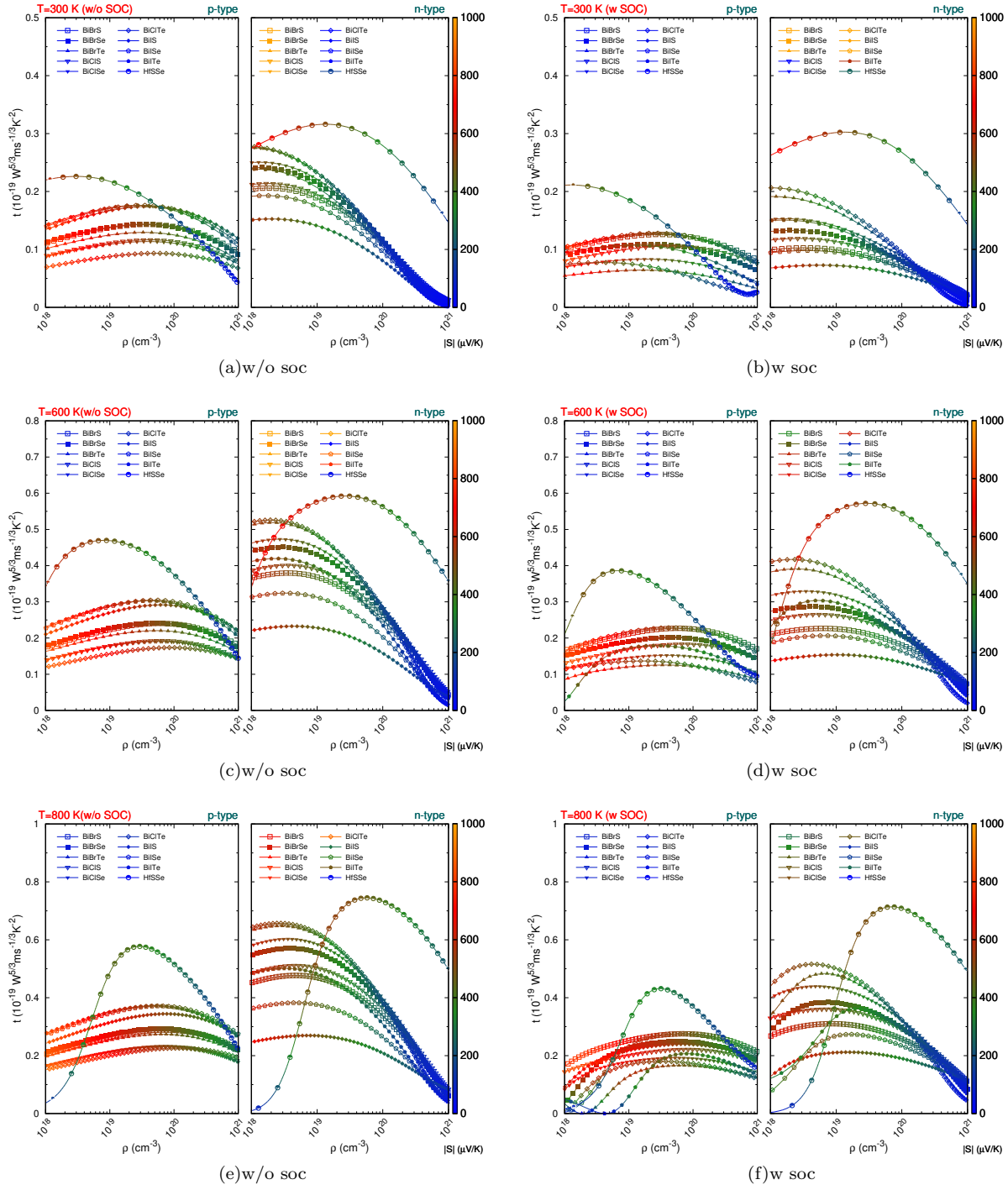
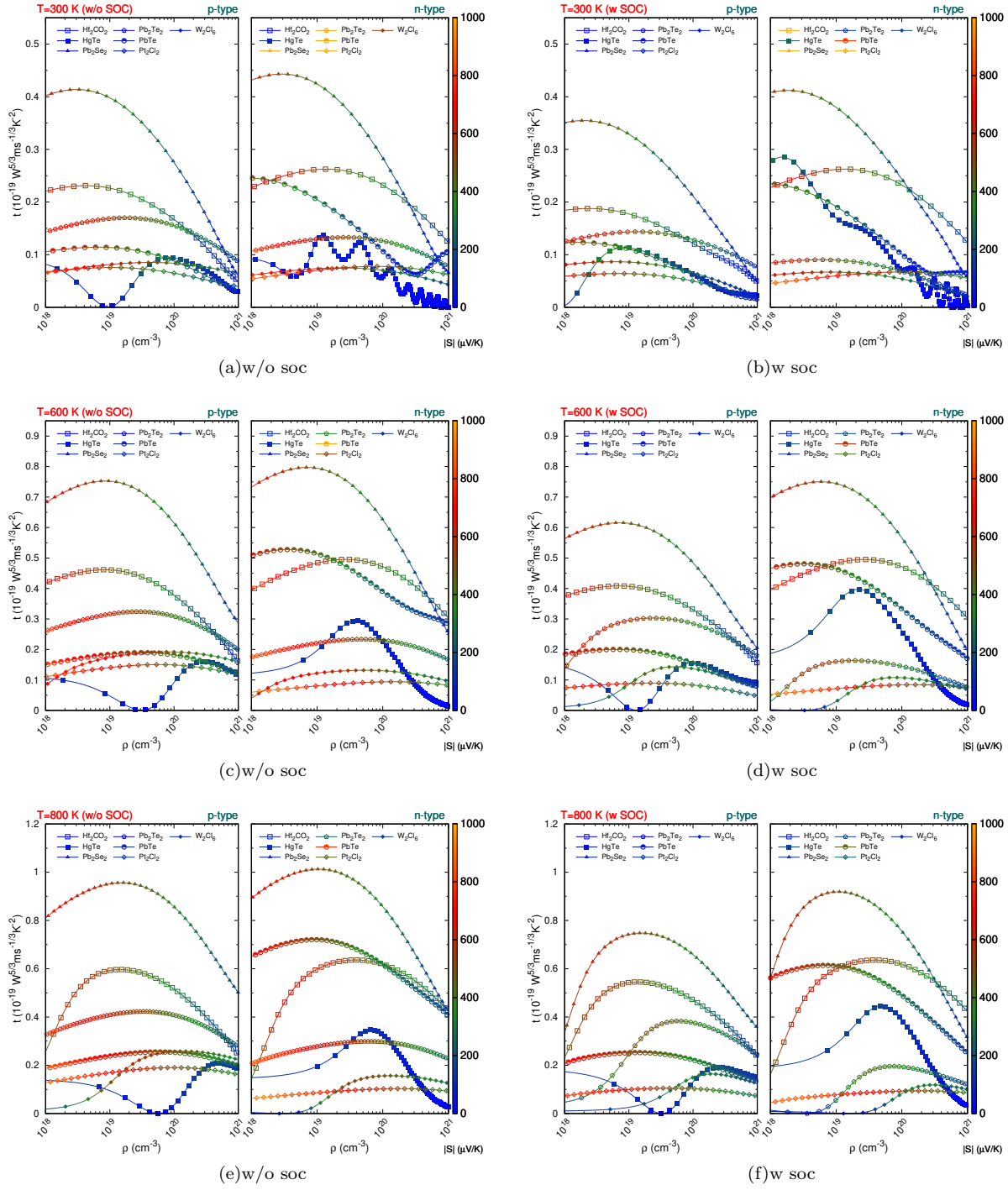


Figure S64. Calculated EFF of 2D isotropic materials with prototype-BiTeI as a function of charge carrier concentration for *p*- type and *n*-type carriers at T=300 K (a-b) T=600 K (c-d) T=800 K (e-f) using PBE (w/o SOC) and PBE+SOC (w SOC). The corresponding Seebeck coefficient at the same carrier concentration is indicated by color.



(a)w/o soc (b)w soc

(c)w/o soc (d)w soc

(e)w/o soc (f)w soc

Figure S65. Calculated EFF of 2D isotropic materials as a function of charge carrier concentration for *p*- type and *n*-type carriers at T=300 K (a-b) T=600 K (c-d) T=800 K (e-f) using PBE (w/o SOC) and PBE+SOC (w SOC). The corresponding Seebeck coefficient at the same carrier concentration is indicated by color.

Table S18. At T=300 K, calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) for p-type carrier concentration of 2D isotropic materials using PBE (w/o SOC) and PBE+SOC (w SOC).

p-type		T=300 K (w/o SOC)				T=300 K (w SOC)			
Prototype	Material	EFF_{max}	ρ	S	$S^2\sigma/\tau$	EFF_{max}	ρ	S	$S^2\sigma/\tau$
pro-BiI_3	W_2Cl_6	0.09	4.20	501.41	0.26	0.09	0.56	510.23	0.07
pro-BiTel	BiBrS	0.14	3.88	507.80	0.41	0.13	3.09	505.72	0.31
pro-BiTel	BiBrSe	0.14	3.40	508.02	0.37	0.11	2.24	506.60	0.21
pro-BiTel	BiBrTe	0.13	3.48	507.90	0.34	0.06	1.68	508.39	0.11
pro-BiTel	BiClS	0.12	4.10	510.48	0.34	0.11	4.55	506.97	0.33
pro-BiTel	BiClSe	0.11	3.81	510.51	0.32	0.08	1.90	509.73	0.15
pro-BiTel	BiClTe	0.09	5.21	508.92	0.32	0.08	0.37	513.50	0.05
pro-BiTel	BiIS	0.17	3.90	509.04	0.50	0.13	2.59	509.90	0.28
pro-BiTel	BiISe	0.18	3.16	507.79	0.44	0.13	2.53	507.27	0.28
pro-BiTel	BiITe	0.18	2.73	507.96	0.40	0.11	1.18	508.56	0.14
pro-BiTel	HfSSe	0.23	0.30	504.66	0.12	0.21	0.13	502.99	0.06
pro-CdI_2	HfS_2	0.21	0.37	504.92	0.13	0.18	0.17	508.79	0.07
pro-CdI_2	$HfSe_2$	0.24	0.26	501.51	0.12	0.23	0.10	495.34	0.06
pro-CdI_2	$HgBr_2$	0.09	5.56	491.60	0.32	0.08	0.64	511.88	0.07
pro-CdI_2	$PbBr_2$	0.09	5.74	504.71	0.33	0.08	6.23	505.83	0.33
pro-CdI_2	PbO_2	0.03	14.28	514.39	0.20	0.03	14.66	512.12	0.20
pro-CdI_2	PtO_2	0.07	5.34	510.70	0.24	0.07	5.65	506.83	0.24
pro-CdI_2	PtS_2	0.15	5.99	512.55	0.59	0.11	7.78	512.85	0.48
pro-CdI_2	$PtSe_2$	0.12	7.68	507.88	0.54	0.04	1.80	506.78	0.08
pro-CdI_2	$PtTe_2$	0.12	1.11	502.36	0.16	0.15	0.34	470.51	0.09
pro-CH	Pb_2Te_2	0.17	1.81	507.62	0.30	0.14	1.38	501.25	0.21
pro-GaSe	Hg_2I_2	0.06	5.31	510.66	0.21	0.04	5.67	506.22	0.16
pro-GaSe	Pt_2Cl_2	0.08	1.08	505.97	0.09	0.06	0.71	509.71	0.06
pro-GeSe	HgTe	0.09	8.13	225.11	0.39	0.11	0.86	311.35	0.12
pro-GeSe	PbTe	0.11	0.66	510.38	0.10	0.12	0.15	512.66	0.04
pro-MoS_2	$HfBr_2$	0.22	0.46	508.86	0.15	0.18	0.24	504.71	0.08
pro-MoS_2	$HfCl_2$	0.21	0.50	505.91	0.15	0.18	0.31	506.18	0.10
pro-MoS_2	HfI_2	0.23	0.39	509.36	0.14	0.19	0.18	507.42	0.07
pro-MoS_2	$HfTe_2$	0.14	1.84	444.18	0.24	0.06	16.13	166.14	0.37
pro-MoS_2	WO_2	0.12	0.48	504.24	0.08	0.12	0.48	505.05	0.08
pro-MoS_2	WS_2	0.17	0.87	507.13	0.18	0.16	0.23	505.63	0.07
pro-MoS_2	WSe_2	0.18	0.56	509.41	0.14	0.16	0.24	504.28	0.07
pro-MoS_2	WTe_2	0.17	0.55	507.21	0.13	0.16	0.19	508.11	0.06
pro-MoSSe	BiBrS	0.17	2.92	508.23	0.41	0.15	1.54	508.06	0.24
pro-MoSSe	BiBrSe	0.18	2.44	511.54	0.38	0.16	1.19	509.96	0.21
pro-MoSSe	BiBrTe	0.16	1.41	510.06	0.23	0.15	0.15	509.06	0.05
pro-MoSSe	BiClS	0.15	3.43	509.47	0.39	0.13	3.08	506.14	0.32
pro-MoSSe	BiClSe	0.16	2.87	511.64	0.36	0.12	1.45	510.90	0.18
pro-MoSSe	BiISe	0.09	2.63	499.83	0.21	0.13	0.22	508.64	0.06
pro-MoSSe	BiITe	0.11	2.79	504.45	0.27	0.13	0.18	508.52	0.05
pro-MoSSe	HfBrCl	0.21	0.50	507.54	0.15	0.17	0.28	502.64	0.09
pro-MoSSe	HfBrI	0.21	0.47	507.90	0.15	0.17	0.23	503.92	0.08
pro-MoSSe	HfClI	0.19	0.56	506.35	0.15	0.15	0.28	506.69	0.08
pro-MoSSe	HfSeTe	0.13	3.78	366.49	0.35	0.06	15.75	161.95	0.33
pro-MoSSe	WSSe	0.16	0.87	507.81	0.17	0.15	0.24	510.38	0.07
pro-MoSSe	WSTe	0.07	1.96	502.43	0.12	0.06	1.59	498.68	0.10
pro-MoSSe	WSeTe	0.15	0.72	507.58	0.14	0.13	0.27	510.48	0.07
pro-PbS	Pb_2Se_2	0.41	0.30	507.52	0.22	0.35	0.20	508.59	0.15
pro-Ti_2CO_2	Hf_2CO_2	0.23	0.42	505.54	0.15	0.19	0.24	503.03	0.09

Table S19. At T=300 K, calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) for n-type carrier concentration of 2D isotropic materials using PBE (w/o SOC) and PBE+SOC (w SOC).

n-type		T=300 K (w/o SOC)				T=300 K (w SOC)			
Prototype	Material	EFF_{max}	ρ	S	$S^2\sigma/\tau$	EFF_{max}	ρ	S	$S^2\sigma/\tau$
pro-BiI_3	$W2Cl_6$	0.07	2.35	509.18	0.15	0.07	0.82	508.47	0.07
pro-BiTel	BiBrS	0.21	0.18	507.19	0.07	0.10	0.33	504.64	0.06
pro-BiTel	BiBrSe	0.24	0.14	508.13	0.07	0.13	0.21	502.26	0.05
pro-BiTel	BiBrTe	0.28	0.09	508.45	0.06	0.19	0.11	503.70	0.05
pro-BiTel	BiClS	0.21	0.17	508.80	0.07	0.12	0.27	502.12	0.06
pro-BiTel	BiClSe	0.25	0.13	506.82	0.07	0.15	0.17	505.67	0.05
pro-BiTel	BiClTe	0.28	0.09	505.77	0.06	0.21	0.10	501.76	0.05
pro-BiTel	BiIS	0.15	0.20	510.15	0.06	0.07	0.59	504.71	0.06
pro-BiTel	BiISe	0.19	0.16	508.43	0.06	0.10	0.37	502.93	0.06
pro-BiTel	BiITe	0.24	0.12	507.84	0.06	0.15	0.16	505.05	0.05
pro-BiTel	HfSSe	0.32	1.34	509.14	0.42	0.30	1.39	506.11	0.42
pro-CdI_2	HfS_2	0.29	1.46	506.02	0.41	0.28	1.42	508.58	0.39
pro-CdI_2	$HfSe_2$	0.35	1.19	509.40	0.43	0.33	1.25	504.97	0.43
pro-CdI_2	$HgBr_2$	0.15	0.29	506.60	0.07	0.15	0.28	509.13	0.07
pro-CdI_2	$PbBr_2$	0.19	0.22	507.66	0.08	0.16	0.25	509.35	0.07
pro-CdI_2	PbO_2	0.16	0.29	507.82	0.08	0.16	0.28	509.02	0.08
pro-CdI_2	PtO_2	0.12	6.32	513.81	0.44	0.11	6.32	510.24	0.43
pro-CdI_2	PtS_2	0.32	1.60	510.11	0.48	0.30	1.76	507.27	0.49
pro-CdI_2	$PtSe_2$	0.36	1.18	508.65	0.45	0.35	1.19	509.40	0.44
pro-CdI_2	$PtTe_2$	0.47	1.95	505.12	0.83	0.42	2.25	507.45	0.83
pro-CH	Pb_2Te_2	0.13	2.74	510.72	0.29	0.09	0.60	507.40	0.07
pro-GaSe	Hg_2I_2	0.20	0.18	508.10	0.07	0.20	0.17	508.13	0.07
pro-GaSe	Pt_2Cl_2	0.08	8.20	513.70	0.35	0.07	9.89	513.76	0.34
pro-GeSe	HgTe	0.14	1.21	88.71	0.11	0.29	0.15	263.88	0.10
pro-GeSe	PbTe	0.25	0.08	506.04	0.05	0.24	0.07	506.44	0.05
pro-MoS_2	$HfBr_2$	0.20	2.99	508.81	0.45	0.18	1.96	507.40	0.31
pro-MoS_2	$HfCl_2$	0.18	3.14	510.37	0.43	0.16	1.84	511.57	0.26
pro-MoS_2	HfI_2	0.21	2.76	507.00	0.45	0.19	1.67	506.18	0.29
pro-MoS_2	$HfTe_2$	0.33	1.95	494.27	0.58	0.16	20.12	280.01	1.32
pro-MoS_2	WO_2	0.23	0.48	508.74	0.15	0.22	0.45	510.40	0.14
pro-MoS_2	WS_2	0.25	0.40	506.75	0.15	0.23	0.52	503.09	0.17
pro-MoS_2	WSe_2	0.24	0.50	509.54	0.17	0.24	1.04	505.52	0.28
pro-MoS_2	WTe_2	0.24	0.39	509.35	0.14	0.19	0.33	504.33	0.10
pro-MoSSe	BiBrS	0.19	1.68	506.73	0.30	0.09	0.42	503.21	0.06
pro-MoSSe	BiBrSe	0.21	2.19	507.72	0.39	0.11	0.29	505.00	0.05
pro-MoSSe	BiBrTe	0.18	0.93	505.62	0.19	0.15	0.17	504.01	0.06
pro-MoSSe	BiClS	0.18	2.19	507.69	0.35	0.10	0.36	505.86	0.06
pro-MoSSe	BiClSe	0.22	3.59	506.45	0.57	0.12	0.25	506.08	0.05
pro-MoSSe	BiISe	0.22	1.27	509.35	0.28	0.09	0.36	507.23	0.05
pro-MoSSe	BiITe	0.17	0.81	508.59	0.16	0.12	0.21	505.35	0.05
pro-MoSSe	HfBrCl	0.19	3.05	509.74	0.44	0.16	1.95	505.51	0.28
pro-MoSSe	HfBrI	0.20	2.95	507.07	0.45	0.17	1.67	510.27	0.27
pro-MoSSe	HfClI	0.19	2.98	510.69	0.42	0.15	1.69	509.96	0.24
pro-MoSSe	HfSeTe	0.27	3.73	444.08	0.73	0.15	23.54	284.23	1.31
pro-MoSSe	WSSe	0.24	0.55	507.36	0.18	0.23	1.18	503.82	0.29
pro-MoSSe	WSTe	0.25	2.32	504.40	0.49	0.20	2.15	505.74	0.37
pro-MoSSe	WSeTe	0.22	0.66	503.61	0.19	0.22	0.96	501.65	0.23
pro-PbS	Pb_2Se_2	0.44	0.29	508.47	0.22	0.41	0.19	506.28	0.16
pro-Ti_2CO_2	Hf_2CO_2	0.26	1.34	510.13	0.35	0.26	1.34	510.33	0.35

Table S20. At T=600 K, calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) for p-type carrier concentration of 2D isotropic materials using PBE (w/o SOC) and PBE+SOC (w SOC).

p-type		T=600 K (w/o SOC)				T=600 K (w SOC)			
Prototype	Material	EFF_{max}	ρ	S	$S^2\sigma/\tau$	EFF_{max}	ρ	S	$S^2\sigma/\tau$
pro-BiI_3	W_2Cl_6	0.19	8.05	500.71	0.55	0.14	4.99	385.57	0.30
pro-BiTel	BiBrS	0.24	6.12	510.37	0.58	0.23	5.78	509.42	0.53
pro-BiTel	BiBrSe	0.24	5.09	511.13	0.51	0.20	4.52	508.07	0.40
pro-BiTel	BiBrTe	0.22	5.35	510.42	0.48	0.13	3.59	507.27	0.21
pro-BiTel	BiClS	0.19	6.27	511.85	0.48	0.18	6.81	509.82	0.48
pro-BiTel	BiClSe	0.19	5.79	510.46	0.44	0.15	3.96	509.20	0.28
pro-BiTel	BiClTe	0.17	8.95	508.46	0.54	0.14	1.70	509.89	0.14
pro-BiTel	BiIS	0.29	6.38	510.48	0.73	0.20	5.32	512.13	0.45
pro-BiTel	BiISe	0.30	4.91	510.85	0.63	0.23	4.49	508.72	0.45
pro-BiTel	BiITe	0.30	4.15	509.93	0.56	0.18	2.61	495.67	0.25
pro-BiTel	HfSSe	0.47	0.81	485.71	0.30	0.39	0.67	431.58	0.22
pro-CdI_2	HfS_2	0.43	0.77	506.98	0.26	0.36	0.49	507.01	0.16
pro-CdI_2	$HfSe_2$	0.47	1.94	390.26	0.53	0.32	2.92	273.39	0.47
pro-CdI_2	$HgBr_2$	0.17	9.92	508.22	0.57	0.14	4.08	511.85	0.25
pro-CdI_2	$PbBr_2$	0.15	9.28	511.08	0.47	0.13	9.40	512.72	0.43
pro-CdI_2	PbO_2	0.09	0.00	938.10	0.00	0.08	0.00	948.92	0.00
pro-CdI_2	PtO_2	0.13	8.26	507.42	0.38	0.12	8.07	507.89	0.34
pro-CdI_2	PtS_2	0.26	11.98	511.15	0.99	0.19	12.86	510.05	0.75
pro-CdI_2	$PtSe_2$	0.23	13.85	508.10	0.97	0.11	0.00	896.49	0.00
pro-CdI_2	$PtTe_2$	0.25	3.40	467.49	0.41	0.16	11.20	215.71	0.53
pro-CH	Pb_2Te_2	0.32	2.76	507.98	0.47	0.30	2.44	495.98	0.40
pro-GaSe	Hg_2I_2	0.11	7.87	508.63	0.31	0.09	8.51	504.84	0.27
pro-GaSe	Pt_2Cl_2	0.15	5.70	507.93	0.35	0.09	2.17	515.59	0.11
pro-GeSe	HgTe	0.16	29.18	176.23	0.87	0.16	0.02	168.58	0.14
pro-GeSe	PbTe	0.19	2.99	512.60	0.29	0.20	0.66	512.45	0.11
pro-MoS_2	$HfBr_2$	0.41	1.05	498.08	0.30	0.36	0.86	477.27	0.23
pro-MoS_2	$HfCl_2$	0.40	1.00	506.21	0.29	0.38	0.86	504.31	0.25
pro-MoS_2	HfI_2	0.43	1.04	483.74	0.32	0.34	1.09	418.53	0.26
pro-MoS_2	$HfTe_2$	0.18	42.57	238.95	1.45	0.07	95.43	100.03	0.64
pro-MoS_2	WO_2	0.24	0.93	506.07	0.16	0.23	0.94	505.93	0.16
pro-MoS_2	WS_2	0.30	2.51	509.94	0.40	0.30	0.51	508.10	0.14
pro-MoS_2	WSe_2	0.32	1.18	508.83	0.25	0.28	0.47	510.32	0.12
pro-MoS_2	WTe_2	0.29	1.10	510.29	0.22	0.27	0.57	481.43	0.13
pro-MoSSe	BiBrS	0.29	5.00	512.04	0.60	0.26	3.68	511.02	0.45
pro-MoSSe	BiBrSe	0.30	4.28	512.34	0.56	0.25	2.70	512.60	0.35
pro-MoSSe	BiBrTe	0.28	4.25	511.25	0.54	0.26	0.49	512.01	0.12
pro-MoSSe	BiClS	0.23	5.78	512.03	0.54	0.22	5.76	510.92	0.50
pro-MoSSe	BiClSe	0.23	4.87	514.31	0.48	0.18	3.05	514.71	0.27
pro-MoSSe	BiISe	0.20	6.44	504.75	0.51	0.20	0.65	509.15	0.11
pro-MoSSe	BiITe	0.23	5.83	507.56	0.55	0.20	0.93	492.56	0.14
pro-MoSSe	HfBrCl	0.39	1.02	506.22	0.29	0.36	0.82	497.55	0.23
pro-MoSSe	HfBrI	0.39	1.06	498.10	0.29	0.33	0.86	465.18	0.22
pro-MoSSe	HfClI	0.36	1.12	507.76	0.28	0.31	0.80	495.84	0.19
pro-MoSSe	HfSeTe	0.13	58.10	183.85	1.19	0.06	993.05	77.79	1.78
pro-MoSSe	WSSe	0.28	2.57	512.19	0.38	0.28	0.56	508.01	0.14
pro-MoSSe	WSTe	0.14	3.22	502.12	0.23	0.15	3.24	497.91	0.23
pro-MoSSe	WSeTe	0.25	1.76	511.69	0.26	0.23	0.59	509.79	0.12
pro-PbS	Pb_2Se_2	0.75	0.84	511.13	0.49	0.62	0.72	511.15	0.38
pro-Ti_2CO_2	Hf_2CO_2	0.46	0.83	506.20	0.29	0.41	0.69	505.58	0.23

Table S21. At T=600 K, calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) for n-type carrier concentration of 2D isotropic materials using PBE (w/o SOC) and PBE+SOC (w SOC).

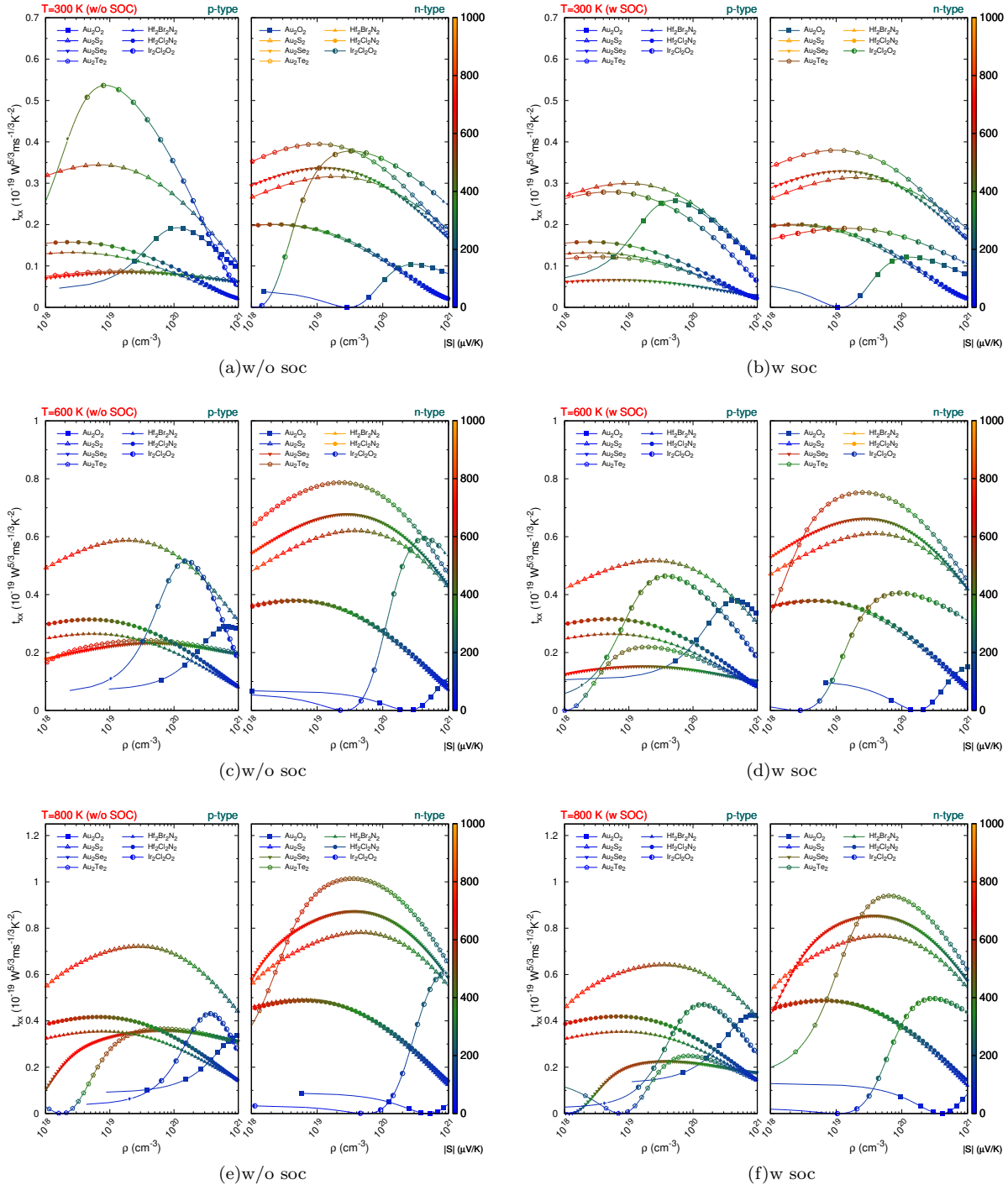
n-type		T=600 K (w/o SOC)				T=600 K (w SOC)			
Prototype	Material	EFF_{max}	ρ	S	$S^2\sigma/\tau$	EFF_{max}	ρ	S	$S^2\sigma/\tau$
pro-BiI_3	W_2Cl_6	0.13	5.24	508.01	0.28	0.11	8.02	391.26	0.30
pro-BiTel	BiBrS	0.38	0.36	508.56	0.14	0.23	0.63	503.36	0.12
pro-BiTel	BiBrSe	0.45	0.28	509.40	0.14	0.29	0.41	503.39	0.11
pro-BiTel	BiBrTe	0.52	0.21	508.06	0.13	0.39	0.24	502.79	0.11
pro-BiTel	BiClS	0.40	0.35	508.99	0.14	0.27	0.54	502.58	0.13
pro-BiTel	BiClSe	0.47	0.27	508.14	0.14	0.33	0.35	504.82	0.12
pro-BiTel	BiClTe	0.53	0.20	507.82	0.13	0.42	0.22	506.93	0.11
pro-BiTel	BiIS	0.23	0.44	513.62	0.10	0.15	1.06	503.68	0.11
pro-BiTel	BiISe	0.32	0.33	512.09	0.11	0.21	0.65	501.73	0.11
pro-BiTel	BiITe	0.42	0.25	509.52	0.12	0.30	0.54	455.04	0.14
pro-BiTel	HfSSe	0.59	2.70	506.06	0.81	0.57	2.89	500.80	0.82
pro-CdI_2	HfS_2	0.54	2.79	508.55	0.76	0.53	2.83	508.19	0.75
pro-CdI_2	$HfSe_2$	0.64	3.89	461.59	1.11	0.59	6.85	409.29	1.48
pro-CdI_2	$HgBr_2$	0.28	0.58	509.01	0.14	0.28	0.58	510.18	0.14
pro-CdI_2	$PbBr_2$	0.35	0.43	508.75	0.14	0.30	0.51	509.61	0.14
pro-CdI_2	PbO_2	0.31	0.56	509.65	0.15	0.31	0.58	507.37	0.15
pro-CdI_2	PtO_2	0.17	11.48	514.70	0.61	0.17	11.15	513.71	0.59
pro-CdI_2	PtS_2	0.57	3.84	510.51	0.98	0.54	4.32	510.01	1.01
pro-CdI_2	$PtSe_2$	0.66	2.74	509.26	0.92	0.64	2.90	509.39	0.93
pro-CdI_2	$PtTe_2$	0.82	4.50	506.54	1.58	0.67	15.31	400.82	2.99
pro-CH	Pb_2Te_2	0.23	4.80	509.61	0.47	0.16	1.82	476.11	0.17
pro-GaSe	Hg_2I_2	0.36	0.37	508.61	0.13	0.36	0.35	509.54	0.13
pro-GaSe	Pt_2Cl_2	0.09	14.61	515.95	0.40	0.08	16.06	516.09	0.38
pro-GeSe	HgTe	0.29	3.92	116.06	0.41	0.40	2.16	182.81	0.45
pro-GeSe	PbTe	0.53	0.37	504.43	0.20	0.48	0.32	507.63	0.16
pro-MoS_2	$HfBr_2$	0.34	5.60	508.93	0.75	0.31	4.95	506.24	0.64
pro-MoS_2	$HfCl_2$	0.31	5.72	511.01	0.70	0.27	4.57	512.42	0.52
pro-MoS_2	HfI_2	0.35	5.28	507.41	0.75	0.34	5.08	492.99	0.70
pro-MoS_2	$HfTe_2$	0.40	25.92	298.45	2.51	0.23	96.26	191.95	3.03
pro-MoS_2	WO_2	0.43	0.95	510.13	0.29	0.42	0.97	509.25	0.29
pro-MoS_2	WS_2	0.48	1.12	508.30	0.37	0.48	1.92	507.49	0.52
pro-MoS_2	WSe_2	0.48	2.22	508.57	0.57	0.47	2.79	508.01	0.65
pro-MoS_2	WTe_2	0.45	0.91	509.10	0.30	0.42	1.14	496.93	0.32
pro-MoSSe	BiBrS	0.35	3.31	509.05	0.55	0.18	0.92	505.95	0.12
pro-MoSSe	BiBrSe	0.38	4.78	509.81	0.77	0.21	0.57	508.11	0.10
pro-MoSSe	BiBrTe	0.42	3.72	501.93	0.71	0.27	0.45	510.26	0.11
pro-MoSSe	BiClS	0.33	4.28	509.47	0.62	0.20	1.13	508.38	0.15
pro-MoSSe	BiClSe	0.38	6.42	510.59	0.94	0.22	0.64	509.26	0.12
pro-MoSSe	BiISe	0.40	2.73	509.36	0.55	0.18	0.76	503.00	0.11
pro-MoSSe	BiITe	0.36	2.70	505.29	0.50	0.25	0.63	479.55	0.13
pro-MoSSe	HfBrCl	0.33	5.62	510.76	0.72	0.29	4.63	510.86	0.57
pro-MoSSe	HfBrI	0.33	5.44	510.14	0.72	0.31	4.77	502.88	0.62
pro-MoSSe	HfClI	0.31	5.71	509.95	0.70	0.27	4.36	509.96	0.52
pro-MoSSe	HfSeTe	0.30	46.49	256.98	2.68	0.20	105.07	195.54	2.87
pro-MoSSe	WSSe	0.47	2.54	508.71	0.62	0.44	3.10	508.29	0.65
pro-MoSSe	WSTe	0.44	5.32	509.76	0.95	0.37	4.69	508.62	0.73
pro-MoSSe	WSeTe	0.47	2.80	505.92	0.65	0.44	2.87	507.11	0.62
pro-PbS	Pb_2Se_2	0.80	0.70	510.06	0.45	0.75	0.59	509.67	0.39
pro-Ti_2CO_2	Hf_2CO_2	0.50	2.70	509.09	0.68	0.50	2.72	508.42	0.68

Table S22. At T=800 K, calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) for p-type carrier concentration of 2D isotropic materials using PBE (w/o SOC) and PBE+SOC (w SOC).

p-type		T=800 K (w/o SOC)				T=800 K (w SOC)			
Prototype	Material	EFF_{max}	ρ	S	$S^2\sigma/\tau$	EFF_{max}	ρ	S	$S^2\sigma/\tau$
pro-BiI_3	W_2Cl_6	0.26	13.51	478.34	0.87	0.16	19.28	309.56	0.69
pro-BiTel	BiBrS	0.29	7.14	512.90	0.64	0.28	7.09	510.33	0.61
pro-BiTel	BiBrSe	0.29	6.06	511.41	0.58	0.25	5.83	506.73	0.48
pro-BiTel	BiBrTe	0.27	6.59	510.89	0.57	0.17	0.00	442.74	0.03
pro-BiTel	BiClS	0.23	7.53	511.45	0.53	0.22	7.95	511.31	0.53
pro-BiTel	BiClSe	0.23	6.81	511.49	0.50	0.19	5.49	507.75	0.36
pro-BiTel	BiClTe	0.23	11.09	507.79	0.67	0.18	3.41	495.24	0.24
pro-BiTel	BiIS	0.34	7.51	512.55	0.79	0.24	6.86	512.26	0.52
pro-BiTel	BiISe	0.37	5.86	511.27	0.72	0.27	6.19	497.75	0.55
pro-BiTel	BiITe	0.37	4.93	511.59	0.64	0.21	7.91	420.64	0.49
pro-BiTel	HfSSe	0.58	2.87	396.81	0.69	0.43	3.09	328.75	0.54
pro-CdI_2	HfS_2	0.55	1.08	506.62	0.35	0.47	0.79	505.09	0.24
pro-CdI_2	$HfSe_2$	0.52	7.52	295.29	1.16	0.31	10.11	200.27	0.78
pro-CdI_2	$HgBr_2$	0.19	11.67	512.13	0.61	0.15	6.63	514.78	0.32
pro-CdI_2	$PbBr_2$	0.17	9.91	513.27	0.46	0.15	9.90	514.33	0.41
pro-CdI_2	PbO_2	0.17	0.00	703.37	0.02	0.17	0.00	714.02	0.02
pro-CdI_2	PtO_2	0.17	9.95	506.14	0.47	0.15	9.40	507.85	0.40
pro-CdI_2	PtS_2	0.34	16.98	509.00	1.34	0.25	16.76	507.34	0.98
pro-CdI_2	$PtSe_2$	0.32	19.08	504.80	1.35	0.19	0.00	658.63	0.02
pro-CdI_2	$PtTe_2$	0.31	14.64	373.75	1.08	0.12	33.45	146.76	0.62
pro-CH	Pb_2Te_2	0.42	3.33	507.98	0.57	0.38	5.91	430.69	0.75
pro-GaSe	Hg_2I_2	0.14	9.02	509.42	0.35	0.15	0.00	631.94	0.01
pro-GaSe	Pt_2Cl_2	0.19	10.14	511.00	0.53	0.11	4.39	515.52	0.17
pro-GeSe	HgTe	0.21	50.21	165.10	1.29	0.19	25.11	185.16	0.81
pro-GeSe	PbTe	0.26	5.87	508.95	0.50	0.25	1.34	510.86	0.19
pro-MoS_2	$HfBr_2$	0.49	3.20	420.83	0.63	0.44	3.54	385.64	0.60
pro-MoS_2	$HfCl_2$	0.51	1.87	474.80	0.46	0.49	1.95	461.79	0.45
pro-MoS_2	HfI_2	0.49	3.98	387.03	0.73	0.38	4.88	320.19	0.65
pro-MoS_2	$HfTe_2$	0.20	116.44	192.10	2.36	0.07	172.69	91.97	0.84
pro-MoS_2	WO_2	0.32	1.21	506.90	0.21	0.31	1.23	506.74	0.21
pro-MoS_2	WS_2	0.38	3.63	510.60	0.53	0.38	0.81	511.19	0.20
pro-MoS_2	WSe_2	0.39	1.66	510.34	0.32	0.35	0.67	508.23	0.16
pro-MoS_2	WTe_2	0.34	1.76	497.87	0.29	0.29	2.27	383.42	0.29
pro-MoSSe	BiBrS	0.34	6.10	512.31	0.67	0.31	4.89	512.91	0.53
pro-MoSSe	BiBrSe	0.35	5.13	514.13	0.61	0.29	3.74	513.97	0.42
pro-MoSSe	BiBrTe	0.35	5.82	510.76	0.68	0.31	1.15	486.02	0.21
pro-MoSSe	BiClS	0.27	6.77	513.65	0.56	0.25	6.78	513.89	0.54
pro-MoSSe	BiClSe	0.26	5.99	514.44	0.52	0.21	4.35	514.55	0.33
pro-MoSSe	BiISe	0.26	8.24	507.98	0.64	0.23	1.91	462.94	0.22
pro-MoSSe	BiITe	0.30	7.59	507.70	0.70	0.23	3.94	422.05	0.35
pro-MoSSe	HfBrCl	0.49	2.42	452.91	0.53	0.46	2.49	431.72	0.50
pro-MoSSe	HfBrI	0.47	3.31	419.93	0.62	0.40	3.76	368.82	0.57
pro-MoSSe	HfClI	0.44	2.51	460.21	0.48	0.39	2.64	424.33	0.44
pro-MoSSe	HfSeTe	0.12	133.22	144.52	1.49	0.09	993.04	89.98	2.43
pro-MoSSe	WSSe	0.35	3.90	510.82	0.52	0.34	0.88	510.40	0.19
pro-MoSSe	WSTe	0.20	4.13	501.78	0.30	0.21	4.60	494.62	0.34
pro-MoSSe	WSeTe	0.30	2.93	511.40	0.36	0.27	1.13	488.97	0.18
pro-PbS	Pb_2Se_2	0.96	1.53	509.56	0.76	0.75	1.57	495.98	0.63
pro-Ti_2CO_2	Hf_2CO_2	0.60	1.46	480.10	0.46	0.55	1.40	474.68	0.40

Table S23. At T=800 K, calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) for n-type carrier concentration of 2D isotropic materials using PBE (w/o SOC) and PBE+SOC (w SOC).

n-type		T=800 K (w/o SOC)				T=800 K (w SOC)			
Prototype	Material	EFF_{max}	ρ	S	$S^2\sigma/\tau$	EFF_{max}	ρ	S	$S^2\sigma/\tau$
pro-BiI_3	W_2Cl_6	0.16	12.84	455.83	0.50	0.12	30.51	315.06	0.66
pro-BiTel	BiBrS	0.48	0.47	510.25	0.17	0.31	0.86	499.71	0.17
pro-BiTel	BiBrSe	0.57	0.37	510.05	0.17	0.38	0.73	477.09	0.18
pro-BiTel	BiBrTe	0.65	0.27	510.60	0.16	0.48	0.67	439.27	0.22
pro-BiTel	BiClS	0.51	0.47	508.86	0.18	0.36	0.70	503.07	0.17
pro-BiTel	BiClSe	0.60	0.36	508.70	0.18	0.44	0.50	498.19	0.16
pro-BiTel	BiClTe	0.66	0.26	510.62	0.16	0.52	0.44	473.57	0.18
pro-BiTel	BiIS	0.27	0.73	513.87	0.13	0.21	1.52	494.37	0.17
pro-BiTel	BiISe	0.38	0.46	513.03	0.13	0.27	1.65	439.79	0.23
pro-BiTel	BiITe	0.50	0.33	512.63	0.14	0.36	2.09	357.23	0.35
pro-BiTel	HfSSe	0.74	5.65	461.88	1.38	0.71	6.97	443.77	1.52
pro-CdI_2	HfS_2	0.70	3.70	508.31	0.99	0.69	3.74	508.39	0.97
pro-CdI_2	$HfSe_2$	0.75	12.08	380.66	2.29	0.68	19.22	338.48	2.79
pro-CdI_2	$HgBr_2$	0.35	0.85	510.11	0.19	0.35	0.85	510.25	0.19
pro-CdI_2	$PbBr_2$	0.45	0.57	508.80	0.18	0.38	0.67	510.07	0.17
pro-CdI_2	PbO_2	0.40	0.81	502.73	0.20	0.40	0.80	503.96	0.20
pro-CdI_2	PtO_2	0.19	14.06	516.57	0.65	0.19	13.62	515.57	0.63
pro-CdI_2	PtS_2	0.68	5.53	512.38	1.25	0.64	6.13	512.74	1.25
pro-CdI_2	$PtSe_2$	0.80	3.94	511.82	1.18	0.78	4.20	511.76	1.19
pro-CdI_2	$PtTe_2$	0.94	10.22	455.44	2.62	0.70	39.96	333.21	4.91
pro-CH	Pb_2Te_2	0.30	6.04	509.16	0.59	0.20	7.19	383.22	0.42
pro-GaSe	Hg_2I_2	0.44	0.51	509.31	0.17	0.45	0.50	506.38	0.17
pro-GaSe	Pt_2Cl_2	0.10	18.12	517.37	0.42	0.09	20.10	515.49	0.41
pro-GeSe	HgTe	0.35	6.71	115.57	0.60	0.45	4.87	162.02	0.70
pro-GeSe	PbTe	0.72	0.90	505.36	0.40	0.61	0.69	507.80	0.29
pro-MoS_2	$HfBr_2$	0.41	10.12	473.33	1.12	0.38	10.99	457.10	1.09
pro-MoS_2	$HfCl_2$	0.38	7.82	501.81	0.88	0.33	7.48	494.75	0.74
pro-MoS_2	HfI_2	0.41	12.02	450.87	1.26	0.39	14.72	420.70	1.37
pro-MoS_2	$HfTe_2$	0.37	64.31	231.57	3.44	0.23	150.63	166.46	3.42
pro-MoS_2	WO_2	0.55	1.30	509.07	0.38	0.54	1.34	509.74	0.38
pro-MoS_2	WS_2	0.62	2.12	507.88	0.60	0.60	3.05	508.89	0.74
pro-MoS_2	WSe_2	0.60	3.94	509.11	0.87	0.58	3.87	510.95	0.83
pro-MoS_2	WTe_2	0.57	1.64	501.87	0.46	0.54	3.17	452.18	0.68
pro-MoSSe	BiBrS	0.43	4.42	509.86	0.68	0.23	1.62	507.33	0.19
pro-MoSSe	BiBrSe	0.46	6.30	510.71	0.93	0.26	0.86	510.25	0.14
pro-MoSSe	BiBrTe	0.53	5.60	506.64	0.99	0.32	1.07	484.49	0.20
pro-MoSSe	BiClS	0.41	5.60	510.45	0.75	0.24	2.27	510.45	0.25
pro-MoSSe	BiClSe	0.46	7.78	512.03	1.06	0.27	1.20	511.04	0.18
pro-MoSSe	BiISe	0.49	3.75	510.68	0.69	0.23	1.94	451.54	0.21
pro-MoSSe	BiITe	0.46	4.22	508.15	0.71	0.30	2.33	396.82	0.31
pro-MoSSe	HfBrCl	0.40	8.49	492.08	0.96	0.35	8.51	481.16	0.86
pro-MoSSe	HfBrI	0.40	9.97	473.44	1.07	0.37	11.27	449.85	1.08
pro-MoSSe	HfClI	0.37	8.22	495.79	0.88	0.33	8.26	479.54	0.80
pro-MoSSe	HfSeTe	0.27	99.57	204.02	3.29	0.20	163.59	170.11	3.23
pro-MoSSe	WSSe	0.59	4.39	510.31	0.92	0.54	4.40	510.32	0.84
pro-MoSSe	WSTe	0.53	6.85	513.47	1.11	0.46	6.39	509.58	0.92
pro-MoSSe	WSeTe	0.58	4.42	509.78	0.91	0.54	4.12	508.74	0.80
pro-PbS	Pb_2Se_2	1.01	1.05	510.21	0.62	0.92	1.08	492.39	0.59
pro-Ti_2CO_2	Hf_2CO_2	0.64	3.92	500.64	0.92	0.64	3.84	502.61	0.91

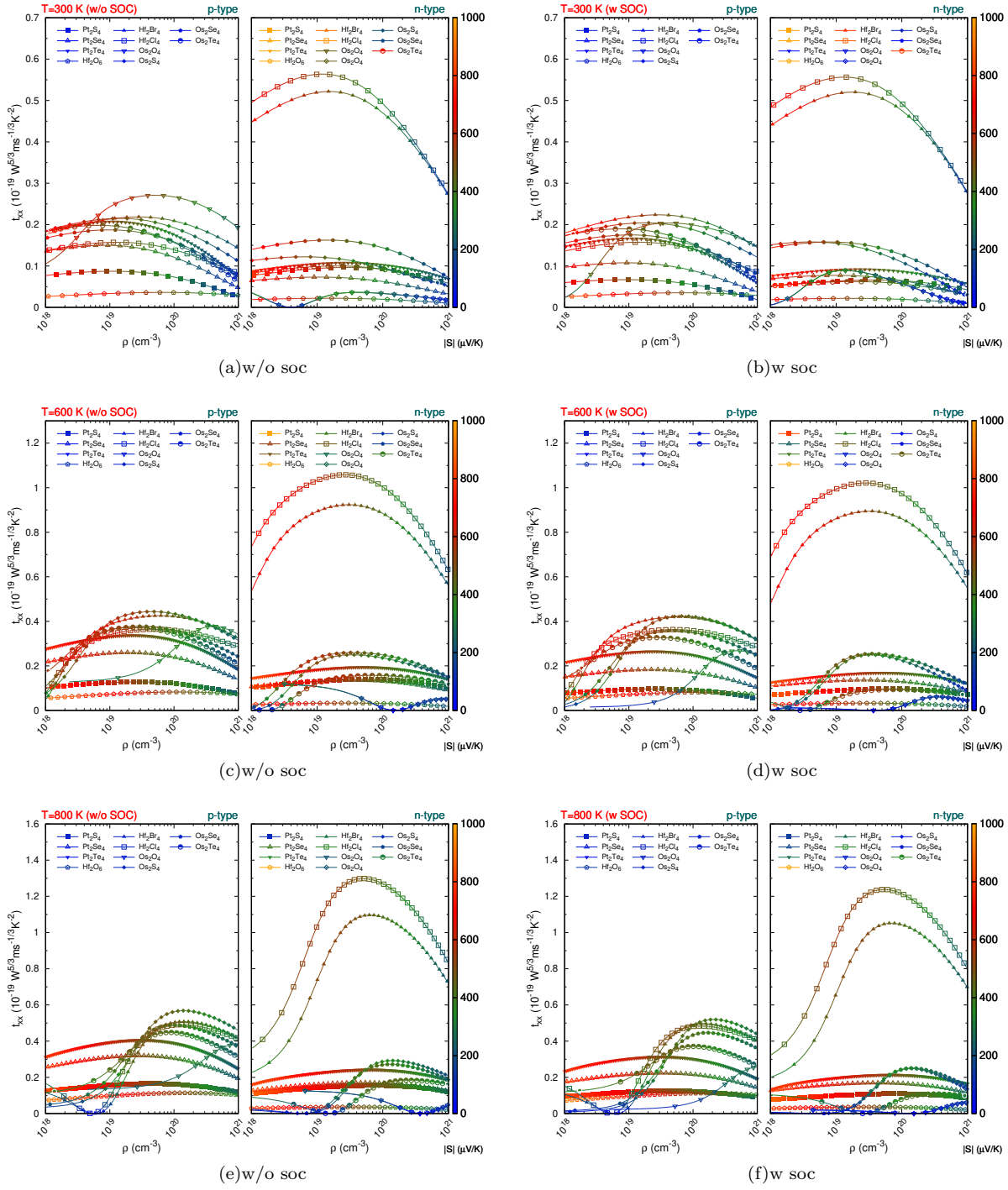


(a)w/o soc (b)w soc

(c)w/o soc (d)w soc

(e)w/o soc (f)w soc

Figure S66. Calculated EFF of 2D anisotropic materials with prototypes AuSe and FeOCl as a function of charge carrier concentration through x-direction for p- type and n-type carriers at T=300 K (a-b) T=600 K (c-d) T=800 K (e-f) using PBE (w/o SOC) and PBE+SOC (w SOC). The corresponding Seebeck coefficient at the same carrier concentration is indicated by color.

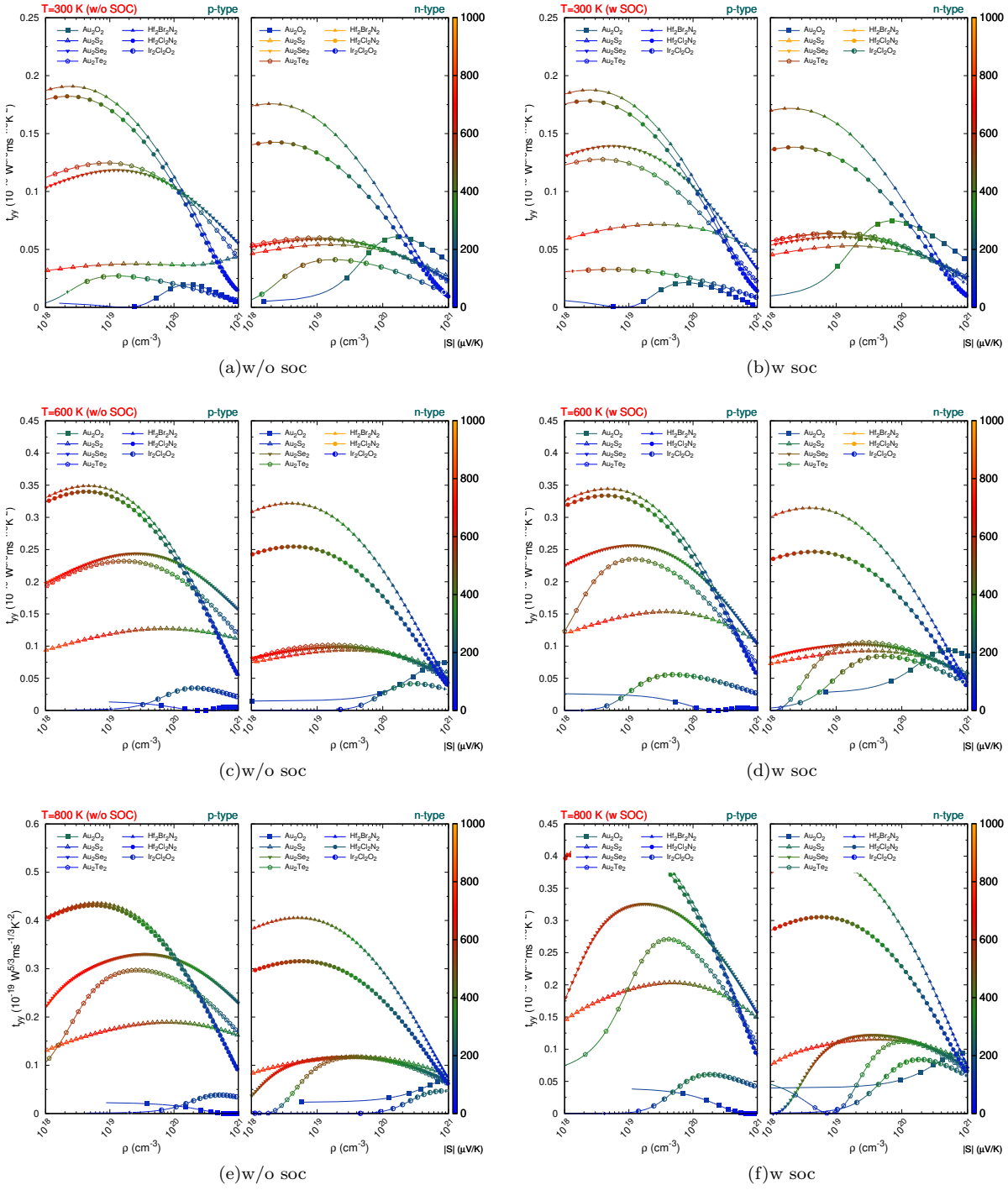


(a)w/o soc (b)w soc

(c)w/o soc (d)w soc

(e)w/o soc (f)w soc

Figure S67. Calculated EFF of 2D anisotropic materials with prototypes PdS_2, TiS_3 and WTe_2 as a function of charge carrier concentration through x-direction for *p*- type and *n*-type carriers at T=300 K (a-b) T=600 K (c-d) T=800 K (e-f) using PBE (w/o SOC) and PBE+SOC (w SOC). The corresponding Seebeck coefficient at the same carrier concentration is indicated by color.

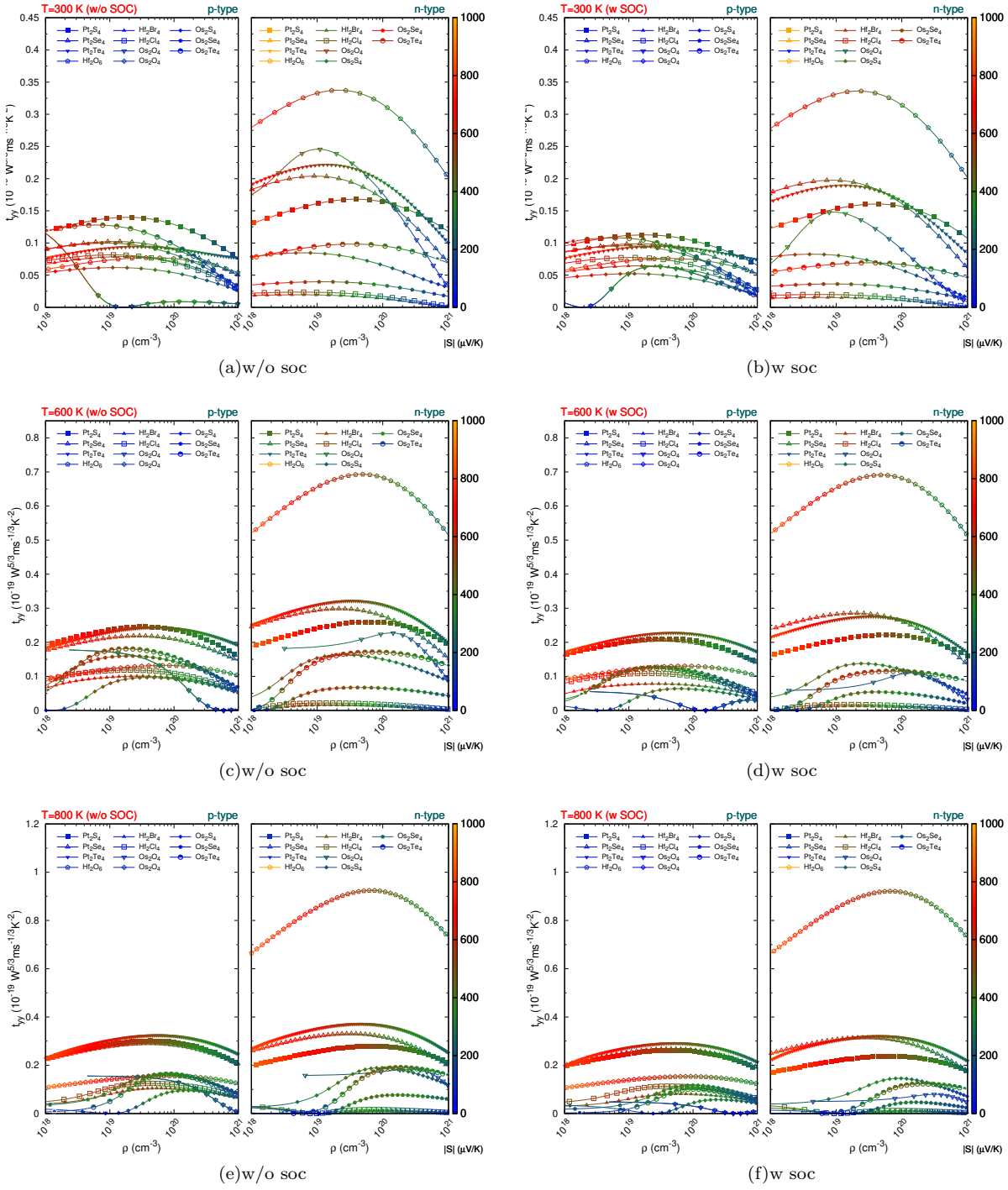


(a)w/o soc (b)w soc

(c)w/o soc (d)w soc

(e)w/o soc (f)w soc

Figure S68. Calculated EFF of 2D anisotropic materials with prototypes AuSe and FeOCl as a function of charge carrier concentration through y-direction for p- type and n-type carriers at T=300 K (a-b) T=600 K (c-d) T=800 K (e-f) using PBE (w/o SOC) and PBE+SOC (w SOC). The corresponding Seebeck coefficient at the same carrier concentration is indicated by color.



(a)w/o soc (b)w soc

(c)w/o soc (d)w soc

(e)w/o soc (f)w soc

Figure S69. Calculated EFF of 2D anisotropic materials with prototypes PdS_2, TiS_3 and WTe_2 as a function of charge carrier concentration through y-direction for *p*- type and *n*-type carriers at T=300 K (a-b) T=600 K (c-d) T=800 K (e-f) using PBE (w/o SOC) and PBE+SOC (w SOC). The corresponding Seebeck coefficient at the same carrier concentration is indicated by color.

Table S24. At T=300 K, calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) through x-direction for p-type carrier concentration of 2D anisotropic materials using PBE (w/o SOC) and PBE+SOC (w SOC).

p-type		T=300 K (w/o SOC)				T=300 K (w SOC)			
Prototype	Material	t_x^p(max)	ρ	S_{xx}	$S_{xx}^2\sigma_{xx}/\tau$	t_x^p(max)	ρ	S_{xx}	$S_{xx}^2\sigma_{xx}/\tau$
pro-AuSe	Au_2O_2	0.19	11.16	221.55	1.00	0.26	4.72	302.73	0.82
pro-AuSe	Au_2S_2	0.34	0.70	506.47	0.31	0.30	0.94	512.07	0.33
pro-AuSe	Au_2Se_2	0.08	2.19	493.62	0.16	0.07	0.62	505.82	0.06
pro-AuSe	Au_2Te_2	0.09	1.79	493.12	0.15	0.12	0.35	507.52	0.07
pro-FeOCl	$Hf_2Br_2N_2$	0.13	0.27	504.44	0.06	0.13	0.27	503.70	0.06
pro-FeOCl	$Hf_2Cl_2N_2$	0.16	0.24	506.12	0.07	0.16	0.23	508.48	0.07
pro-FeOCl	$Ir_2Cl_2O_2$	0.54	0.85	393.28	0.56	0.28	0.53	505.70	0.21
pro-PdS_2	Pt_2S_4	0.09	1.12	512.34	0.11	0.07	0.92	514.94	0.07
pro-PdS_2	Pt_2Se_4	0.15	0.84	510.11	0.15	0.11	0.93	510.69	0.12
pro-PdS_2	Pt_2Te_4	0.21	1.08	512.30	0.25	0.17	1.12	512.34	0.21
pro-TiS_3	Hf_2O_6	0.04	6.40	500.23	0.14	0.04	6.66	498.09	0.14
pro-WTe_2	Hf_2Br_4	0.22	2.82	502.25	0.50	0.22	2.91	501.58	0.52
pro-WTe_2	Hf_2Cl_4	0.16	1.35	504.16	0.22	0.16	1.43	503.76	0.23
pro-WTe_2	Os_2O_4	0.27	5.18	497.14	0.94	0.20	4.10	474.09	0.60
pro-WTe_2	Os_2S_4	0.21	1.44	505.78	0.31	0.20	1.80	503.42	0.35
pro-WTe_2	Os_2Se_4	0.19	0.96	508.61	0.21	0.18	1.06	505.61	0.21
pro-WTe_2	Os_2Te_4	0.20	0.68	506.97	0.18	0.19	0.79	504.72	0.19

Table S25. At T=300 K, calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) through x-direction for n-type carrier concentration of 2D anisotropic materials using PBE (w/o SOC) and PBE+SOC (w SOC).

n-type		T=300 K (w/o SOC)				T=300 K (w SOC)			
Prototype	Material	t_x^n(max)	ρ	S_{xx}	$S_{xx}^2\sigma_{xx}/\tau$	t_x^n(max)	ρ	S_{xx}	$S_{xx}^2\sigma_{xx}/\tau$
pro-AuSe	Au_2O_2	0.10	29.42	236.75	0.99	0.12	13.35	304.73	0.72
pro-AuSe	Au_2S_2	0.32	1.91	504.44	0.54	0.31	2.01	505.40	0.55
pro-AuSe	Au_2Se_2	0.34	1.25	506.42	0.43	0.33	1.28	503.96	0.43
pro-AuSe	Au_2Te_2	0.39	1.04	506.23	0.45	0.38	0.98	508.44	0.41
pro-FeOCl	$Hf_2Br_2N_2$	0.20	0.20	508.70	0.08	0.20	0.21	508.20	0.08
pro-FeOCl	$Hf_2Cl_2N_2$	0.20	0.24	508.57	0.08	0.20	0.24	509.71	0.08
pro-FeOCl	$Ir_2Cl_2O_2$	0.38	3.26	445.67	0.91	0.19	1.52	503.22	0.28
pro-PdS_2	Pt_2S_4	0.10	3.02	509.77	0.22	0.07	3.75	512.48	0.18
pro-PdS_2	Pt_2Se_4	0.07	1.06	509.68	0.08	0.08	0.97	509.42	0.08
pro-PdS_2	Pt_2Te_4	0.11	2.68	500.83	0.23	0.09	2.32	502.07	0.18
pro-TiS_3	Hf_2O_6	0.02	1.47	513.52	0.03	0.02	1.57	508.72	0.03
pro-WTe_2	Hf_2Br_4	0.52	1.49	509.27	0.75	0.52	1.74	509.85	0.83
pro-WTe_2	Hf_2Cl_4	0.56	1.24	504.47	0.72	0.56	1.34	506.44	0.75
pro-WTe_2	Os_2O_4	0.06	0.01	457.73	0.04	0.09	1.38	335.45	0.12
pro-WTe_2	Os_2S_4	0.12	0.65	506.26	0.10	0.16	0.42	508.06	0.10
pro-WTe_2	Os_2Se_4	0.16	1.45	509.07	0.23	0.16	0.82	506.62	0.15
pro-WTe_2	Os_2Te_4	0.10	2.03	511.80	0.18	0.06	1.88	513.92	0.10

Table S26. At T=600 K, calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) through x-direction for p-type carrier concentration of 2D isotropic materials using PBE (w/o SOC) and PBE+SOC (w SOC).

p-type		T=600 K (w/o SOC)				T=600 K (w SOC)			
Prototype	Material	t_x^p(max)	ρ	S_{xx}	$S_{xx}^2\sigma_{xx}/\tau$	t_x^p(max)	ρ	S_{xx}	$S_{xx}^2\sigma_{xx}/\tau$
pro-AuSe	Au_2O_2	0.29	68.51	142.26	2.55	0.38	45.88	182.65	2.95
pro-AuSe	Au_2S_2	0.59	1.88	512.31	0.64	0.52	2.51	510.06	0.69
pro-AuSe	Au_2Se_2	0.23	4.71	489.83	0.47	0.15	1.68	501.74	0.15
pro-AuSe	Au_2Te_2	0.24	3.61	489.66	0.41	0.22	1.91	422.18	0.24
pro-FeOCl	$Hf_2Br_2N_2$	0.26	0.55	506.47	0.13	0.26	0.56	505.97	0.13
pro-FeOCl	$Hf_2Cl_2N_2$	0.31	0.49	507.42	0.14	0.32	0.49	506.96	0.14
pro-FeOCl	$Ir_2Cl_2O_2$	0.52	15.67	196.47	2.16	0.46	3.89	381.92	0.82
pro-PdS_2	Pt_2S_4	0.13	2.73	513.39	0.18	0.10	2.52	515.68	0.13
pro-PdS_2	Pt_2Se_4	0.26	1.94	511.73	0.29	0.18	2.24	511.59	0.23
pro-PdS_2	Pt_2Te_4	0.34	2.30	511.94	0.42	0.26	2.42	512.11	0.34
pro-TiS_3	Hf_2O_6	0.08	11.94	501.94	0.31	0.08	12.12	501.78	0.31
pro-WTe_2	Hf_2Br_4	0.43	6.07	503.62	1.02	0.42	5.85	503.12	0.98
pro-WTe_2	Hf_2Cl_4	0.36	4.93	496.29	0.76	0.36	5.00	497.13	0.76
pro-WTe_2	Os_2O_4	0.38	40.10	342.64	3.26	0.27	48.20	325.89	2.55
pro-WTe_2	Os_2S_4	0.44	4.45	486.83	0.86	0.42	6.83	468.91	1.09
pro-WTe_2	Os_2Se_4	0.38	2.91	490.69	0.55	0.36	4.67	465.72	0.72
pro-WTe_2	Os_2Te_4	0.37	2.29	488.26	0.46	0.33	2.80	491.20	0.47

Table S27. At T=600 K, calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) through x-direction for n-type carrier concentration of 2D isotropic materials using PBE (w/o SOC) and PBE+SOC (w SOC).

n-type		T=600 K (w/o SOC)				T=600 K (w SOC)			
Prototype	Material	t_x^n(max)	ρ	S_{xx}	$S_{xx}^2\sigma_{xx}/\tau$	t_x^n(max)	ρ	S_{xx}	$S_{xx}^2\sigma_{xx}/\tau$
pro-AuSe	Au_2O_2	0.14	176.55	155.05	2.38	0.15	124.25	178.64	2.20
pro-AuSe	Au_2S_2	0.62	3.75	508.65	1.06	0.61	3.87	508.86	1.06
pro-AuSe	Au_2Se_2	0.68	2.86	506.02	0.96	0.66	2.85	506.09	0.94
pro-AuSe	Au_2Te_2	0.79	2.27	507.65	0.96	0.75	2.51	496.12	0.98
pro-FeOCl	$Hf_2Br_2N_2$	0.38	0.42	507.30	0.15	0.38	0.43	507.94	0.15
pro-FeOCl	$Hf_2Cl_2N_2$	0.38	0.49	508.27	0.16	0.38	0.50	507.69	0.17
pro-FeOCl	$Ir_2Cl_2O_2$	0.59	43.90	277.07	4.90	0.41	9.21	426.04	1.24
pro-PdS_2	Pt_2S_4	0.14	5.86	513.33	0.32	0.10	6.48	513.28	0.24
pro-PdS_2	Pt_2Se_4	0.14	3.31	509.01	0.21	0.14	2.73	510.59	0.19
pro-PdS_2	Pt_2Te_4	0.19	5.03	509.54	0.40	0.17	5.02	509.91	0.35
pro-TiS_3	Hf_2O_6	0.03	2.74	514.50	0.05	0.03	2.76	514.70	0.05
pro-WTe_2	Hf_2Br_4	0.92	3.05	507.53	1.37	0.89	3.24	508.16	1.38
pro-WTe_2	Hf_2Cl_4	1.06	2.65	507.32	1.43	1.02	2.83	507.40	1.44
pro-WTe_2	Os_2O_4	0.12	0.32	273.92	0.53	0.06	34.59	150.98	0.38
pro-WTe_2	Os_2S_4	0.25	3.43	444.28	0.40	0.25	3.41	380.10	0.40
pro-WTe_2	Os_2Se_4	0.26	3.54	489.53	0.42	0.25	3.51	430.71	0.41
pro-WTe_2	Os_2Te_4	0.16	6.90	495.36	0.40	0.09	7.86	475.72	0.26

Table S28. At T=800 K, calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) through x-direction for p-type carrier concentration of 2D isotropic materials using PBE (w/o SOC) and PBE+SOC (w SOC).

p-type		T=800 K (w/o SOC)				T=800 K (w SOC)			
Prototype	Material	t_x^p(max)	ρ	S_{xx}	$S_{xx}^2\sigma_{xx}/\tau$	t_x^p(max)	ρ	S_{xx}	$S_{xx}^2\sigma_{xx}/\tau$
pro-AuSe	Au_2O_2	0.34	110.52	127.37	3.33	0.42	81.30	155.88	3.86
pro-AuSe	Au_2S_2	0.72	2.90	511.07	0.87	0.64	3.42	511.33	0.86
pro-AuSe	Au_2Se_2	0.36	6.78	486.56	0.76	0.23	3.82	467.61	0.32
pro-AuSe	Au_2Te_2	0.37	6.52	459.88	0.75	0.25	8.58	318.17	0.59
pro-FeOCl	$Hf_2Br_2N_2$	0.35	0.77	506.75	0.18	0.35	0.78	506.26	0.18
pro-FeOCl	$Hf_2Cl_2N_2$	0.42	0.67	506.77	0.19	0.42	0.68	507.16	0.19
pro-FeOCl	$Ir_2Cl_2O_2$	0.43	36.11	147.20	2.45	0.47	13.82	289.46	1.58
pro-PdS_2	Pt_2S_4	0.17	4.59	510.44	0.27	0.12	4.51	511.35	0.20
pro-PdS_2	Pt_2Se_4	0.32	2.89	510.95	0.38	0.22	3.33	512.26	0.30
pro-PdS_2	Pt_2Te_4	0.41	3.15	511.73	0.52	0.31	3.27	512.43	0.41
pro-TiS_3	Hf_2O_6	0.11	15.52	501.63	0.42	0.11	15.55	502.41	0.41
pro-WTe_2	Hf_2Br_4	0.51	14.52	445.89	1.79	0.50	14.57	440.90	1.75
pro-WTe_2	Hf_2Cl_4	0.49	12.78	448.84	1.58	0.48	13.18	446.45	1.59
pro-WTe_2	Os_2O_4	0.38	87.57	279.67	4.55	0.26	107.85	265.47	3.42
pro-WTe_2	Os_2S_4	0.57	13.91	420.51	1.94	0.52	21.07	396.34	2.33
pro-WTe_2	Os_2Se_4	0.49	10.03	421.03	1.34	0.45	16.50	391.58	1.70
pro-WTe_2	Os_2Te_4	0.45	8.67	416.32	1.13	0.37	10.36	418.90	1.06

Table S29. At T=800 K, calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) through x-direction for n-type carrier concentration of 2D isotropic materials using PBE (w/o SOC) and PBE+SOC (w SOC).

n-type		T=800 K (w/o SOC)				T=800 K (w SOC)			
Prototype	Material	t_x^n(max)	ρ	S_{xx}	$S_{xx}^2\sigma_{xx}/\tau$	t_x^n(max)	ρ	S_{xx}	$S_{xx}^2\sigma_{xx}/\tau$
pro-AuSe	Au_2O_2	0.13	293.18	130.52	2.63	0.15	231.63	145.99	2.58
pro-AuSe	Au_2S_2	0.78	4.57	508.96	1.26	0.77	4.68	509.04	1.25
pro-AuSe	Au_2Se_2	0.87	3.71	506.79	1.22	0.85	3.80	504.55	1.21
pro-AuSe	Au_2Te_2	1.01	3.49	494.29	1.37	0.94	6.45	435.40	1.91
pro-FeOCl	$Hf_2Br_2N_2$	0.49	0.56	509.06	0.19	0.49	0.57	509.03	0.20
pro-FeOCl	$Hf_2Cl_2N_2$	0.49	0.66	508.53	0.22	0.49	0.67	509.49	0.22
pro-FeOCl	$Ir_2Cl_2O_2$	0.61	93.10	225.76	6.65	0.50	30.05	347.92	2.72
pro-PdS_2	Pt_2S_4	0.16	7.21	516.13	0.34	0.11	7.78	514.04	0.25
pro-PdS_2	Pt_2Se_4	0.17	5.00	511.05	0.29	0.17	4.23	511.94	0.26
pro-PdS_2	Pt_2Te_4	0.24	6.44	510.00	0.49	0.21	6.66	509.50	0.44
pro-TiS_3	Hf_2O_6	0.04	3.39	514.74	0.05	0.04	3.38	515.36	0.05
pro-WTe_2	Hf_2Br_4	1.10	6.49	455.14	2.25	1.05	6.90	453.21	2.24
pro-WTe_2	Hf_2Cl_4	1.30	5.00	470.26	2.23	1.24	5.35	468.40	2.22
pro-WTe_2	Os_2O_4	0.13	0.66	218.43	0.89	0.06	119.62	123.59	0.63
pro-WTe_2	Os_2S_4	0.29	13.91	348.53	0.97	0.25	13.87	280.92	0.81
pro-WTe_2	Os_2Se_4	0.27	13.13	394.47	0.88	0.25	14.15	325.14	0.85
pro-WTe_2	Os_2Te_4	0.18	24.84	414.84	0.91	0.11	0.04	356.51	0.13

Table S30. At T=300 K, calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) through y-direction for p-type carrier concentration of 2D isotropic materials using PBE (w/o SOC) and PBE+SOC (w SOC).

p-type		T=300 K (w/o SOC)				T=300 K (w SOC)			
Prototype	Material	t_y^p(max)	ρ	S_{yy}	$S_{yy}^2\sigma_{yy}/\tau$	t_y^p(max)	ρ	S_{yy}	$S_{yy}^2\sigma_{yy}/\tau$
pro-AuSe	Au_2O_2	0.03	998.38	226.36	0.71	0.03	997.06	203.81	0.56
pro-AuSe	Au_2S_2	0.04	119.98	177.88	0.75	0.07	2.64	487.13	0.16
pro-AuSe	Au_2Se_2	0.12	1.29	506.27	0.16	0.14	0.55	507.27	0.11
pro-AuSe	Au_2Te_2	0.12	0.91	510.58	0.13	0.13	0.37	506.51	0.08
pro-FeOCl	$Hf_2Br_2N_2$	0.19	0.24	507.73	0.08	0.19	0.24	508.31	0.08
pro-FeOCl	$Hf_2Cl_2N_2$	0.18	0.23	506.51	0.08	0.18	0.22	509.49	0.07
pro-FeOCl	$Ir_2Cl_2O_2$	0.03	1.29	372.30	0.04	0.03	0.53	507.72	0.02
pro-PdS_2	Pt_2S_4	0.14	1.85	508.73	0.24	0.11	1.79	500.95	0.19
pro-PdS_2	Pt_2Se_4	0.10	1.22	502.26	0.13	0.10	1.40	503.15	0.14
pro-PdS_2	Pt_2Te_4	0.09	2.83	490.36	0.21	0.09	2.90	491.63	0.22
pro-TiS_3	Hf_2O_6	0.08	4.15	509.84	0.23	0.08	4.34	505.52	0.23
pro-WTe_2	Hf_2Br_4	0.08	1.65	509.96	0.13	0.06	1.50	513.17	0.10
pro-WTe_2	Hf_2Cl_4	0.08	1.07	509.04	0.10	0.08	1.04	512.18	0.09
pro-WTe_2	Os_2O_4	0.14	0.02	544.95	0.09	0.06	2.69	385.82	0.14
pro-WTe_2	Os_2S_4	0.06	1.26	505.79	0.08	0.05	1.15	509.06	0.07
pro-WTe_2	Os_2Se_4	0.10	0.85	510.90	0.10	0.10	0.84	510.52	0.10
pro-WTe_2	Os_2Te_4	0.13	0.60	509.69	0.11	0.11	0.58	512.96	0.09

Table S31. At T=300 K, calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) through y-direction for n-type carrier concentration of 2D isotropic materials using PBE (w/o SOC) and PBE+SOC (w SOC).

p-type		T=300 K (w/o SOC)				T=300 K (w SOC)			
Prototype	Material	t_y^n(max)	ρ	S_{yy}	$S_{yy}^2\sigma_{yy}/\tau$	t_y^n(max)	ρ	S_{yy}	$S_{yy}^2\sigma_{yy}/\tau$
pro-AuSe	Au_2O_2	0.06	17.14	279.34	0.43	0.07	7.20	356.19	0.31
pro-AuSe	Au_2S_2	0.05	1.61	506.68	0.08	0.05	1.67	509.06	0.08
pro-AuSe	Au_2Se_2	0.06	1.13	507.00	0.07	0.06	1.13	506.74	0.07
pro-AuSe	Au_2Te_2	0.06	0.94	509.56	0.06	0.06	0.93	508.72	0.07
pro-FeOCl	$Hf_2Br_2N_2$	0.18	0.20	506.26	0.07	0.17	0.20	510.26	0.06
pro-FeOCl	$Hf_2Cl_2N_2$	0.14	0.22	509.00	0.06	0.14	0.22	510.91	0.06
pro-FeOCl	$Ir_2Cl_2O_2$	0.04	1.76	446.97	0.07	0.06	1.01	510.40	0.07
pro-PdS_2	Pt_2S_4	0.17	3.77	509.36	0.45	0.16	4.24	509.29	0.46
pro-PdS_2	Pt_2Se_4	0.20	0.95	509.22	0.22	0.20	0.86	511.85	0.20
pro-PdS_2	Pt_2Te_4	0.22	1.37	514.72	0.30	0.19	1.32	512.26	0.25
pro-TiS_3	Hf_2O_6	0.34	2.13	506.14	0.62	0.34	2.13	507.03	0.61
pro-WTe_2	Hf_2Br_4	0.02	0.54	518.12	0.01	0.02	0.59	519.46	0.01
pro-WTe_2	Hf_2Cl_4	0.02	0.59	514.56	0.02	0.02	0.59	514.37	0.02
pro-WTe_2	Os_2O_4	0.25	1.03	429.47	0.29	0.15	0.91	374.06	0.16
pro-WTe_2	Os_2S_4	0.08	0.61	508.03	0.07	0.08	0.42	510.11	0.05
pro-WTe_2	Os_2Se_4	0.04	1.21	512.65	0.05	0.04	0.87	508.86	0.04
pro-WTe_2	Os_2Te_4	0.10	3.57	503.52	0.25	0.07	3.11	507.55	0.16

Table S32. At T=600 K, calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) through y-direction for p-type carrier concentration of 2D isotropic materials using PBE (w/o SOC) and PBE+SOC (w SOC).

p-type		T=600 K (w/o SOC)				T=600 K (w SOC)			
Prototype	Material	t_y^p(max)	ρ	S_{yy}	$S_{yy}^2\sigma_{yy}/\tau$	t_y^p(max)	ρ	S_{yy}	$S_{yy}^2\sigma_{yy}/\tau$
pro-AuSe	Au_2O_2	0.08	997.35	272.28	1.51	0.06	998.17	245.08	1.05
pro-AuSe	Au_2S_2	0.13	6.90	478.06	0.33	0.15	3.73	504.95	0.26
pro-AuSe	Au_2Se_2	0.24	2.55	506.54	0.33	0.26	1.12	507.82	0.20
pro-AuSe	Au_2Te_2	0.23	1.66	508.68	0.23	0.24	1.16	466.84	0.19
pro-FeOCl	$Hf_2Br_2N_2$	0.35	0.47	508.12	0.15	0.34	0.47	510.16	0.15
pro-FeOCl	$Hf_2Cl_2N_2$	0.34	0.44	507.89	0.14	0.33	0.44	509.16	0.14
pro-FeOCl	$Ir_2Cl_2O_2$	0.03	20.99	197.79	0.16	0.06	5.08	363.62	0.12
pro-PdS_2	Pt_2S_4	0.25	3.52	509.36	0.41	0.21	3.63	510.41	0.36
pro-PdS_2	Pt_2Se_4	0.22	2.83	504.83	0.31	0.21	3.19	505.91	0.32
pro-PdS_2	Pt_2Te_4	0.24	5.08	497.01	0.51	0.23	4.89	499.11	0.47
pro-TiS_3	Hf_2O_6	0.13	7.05	510.39	0.35	0.13	6.99	511.24	0.34
pro-WTe_2	Hf_2Br_4	0.10	2.94	515.25	0.15	0.08	2.75	515.52	0.11
pro-WTe_2	Hf_2Cl_4	0.12	2.03	513.31	0.14	0.11	1.99	514.22	0.12
pro-WTe_2	Os_2O_4	0.18	0.23	295.68	0.79	0.06	0.25	190.55	0.21
pro-WTe_2	Os_2S_4	0.10	3.91	460.72	0.17	0.06	6.01	416.19	0.15
pro-WTe_2	Os_2Se_4	0.16	1.96	492.87	0.18	0.13	2.70	458.33	0.18
pro-WTe_2	Os_2Te_4	0.18	1.78	471.25	0.19	0.12	2.17	460.09	0.15

Table S33. At T=600 K, calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) through y-direction for n-type carrier concentration of 2D isotropic materials using PBE (w/o SOC) and PBE+SOC (w SOC).

n-type		T=600 K (w/o SOC)				T=600 K (w SOC)			
Prototype	Material	t_y^n(max)	ρ	S_{yy}	$S_{yy}^2\sigma_{yy}/\tau$	t_y^n(max)	ρ	S_{yy}	$S_{yy}^2\sigma_{yy}/\tau$
pro-AuSe	Au_2O_2	0.07	83.32	196.11	0.93	0.09	50.95	236.75	0.89
pro-AuSe	Au_2S_2	0.09	3.16	509.65	0.14	0.09	3.32	510.20	0.15
pro-AuSe	Au_2Se_2	0.10	2.07	511.70	0.11	0.10	2.09	511.63	0.12
pro-AuSe	Au_2Te_2	0.10	1.74	510.06	0.10	0.11	2.83	462.63	0.15
pro-FeOCl	$Hf_2Br_2N_2$	0.32	0.39	509.05	0.12	0.31	0.39	510.44	0.12
pro-FeOCl	$Hf_2Cl_2N_2$	0.25	0.44	509.91	0.10	0.25	0.44	510.81	0.10
pro-FeOCl	$Ir_2Cl_2O_2$	0.04	30.82	266.67	0.28	0.08	5.20	417.54	0.18
pro-PdS_2	Pt_2S_4	0.26	6.20	513.86	0.62	0.22	5.92	513.50	0.51
pro-PdS_2	Pt_2Se_4	0.30	2.20	514.20	0.36	0.29	1.91	515.24	0.31
pro-PdS_2	Pt_2Te_4	0.32	3.42	514.29	0.52	0.28	3.39	514.36	0.44
pro-TiS_3	Hf_2O_6	0.69	4.80	506.52	1.39	0.69	4.93	504.63	1.41
pro-WTe_2	Hf_2Br_4	0.02	0.00	551.59	0.00	0.02	0.00	545.45	0.00
pro-WTe_2	Hf_2Cl_4	0.03	0.00	534.50	0.00	0.03	0.00	570.16	0.00
pro-WTe_2	Os_2O_4	0.23	13.74	245.27	1.14	0.11	14.57	198.34	0.51
pro-WTe_2	Os_2S_4	0.16	2.57	461.98	0.22	0.14	2.56	409.57	0.18
pro-WTe_2	Os_2Se_4	0.07	4.25	481.33	0.12	0.05	4.21	404.91	0.10
pro-WTe_2	Os_2Te_4	0.17	7.12	502.48	0.45	0.12	6.94	494.41	0.29

Table S34. At T=800 K, calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) through y-direction for p-type carrier concentration of 2D isotropic materials using PBE (w/o SOC) and PBE+SOC (w SOC).

p-type		T=800 K (w/o SOC)				T=800 K (w SOC)			
Prototype	Material	t_y^p(max)	ρ	S_{yy}	$S_{yy}^2\sigma_{yy}/\tau$	t_y^p(max)	ρ	S_{yy}	$S_{yy}^2\sigma_{yy}/\tau$
pro-AuSe	Au_2O_2	0.11	998.05	273.20	1.83	0.07	9.78E+02	252.27	1.10
pro-AuSe	Au_2S_2	0.19	8.03	489.41	0.45	0.20	4.81E+00	505.39	0.34
pro-AuSe	Au_2Se_2	0.33	3.58	503.73	0.46	0.33	1.78E+00	494.25	0.28
pro-AuSe	Au_2Te_2	0.30	2.73	486.36	0.34	0.27	4.11E+00	376.09	0.42
pro-FeOCl	$Hf_2Br_2N_2$	0.44	0.60	510.66	0.18	0.43	6.13E-01	510.55	0.18
pro-FeOCl	$Hf_2Cl_2N_2$	0.43	0.57	509.98	0.17	0.42	5.77E-01	509.41	0.17
pro-FeOCl	$Ir_2Cl_2O_2$	0.04	51.28	158.02	0.24	0.06	1.85E+01	278.78	0.24
pro-PdS_2	Pt_2S_4	0.30	4.40	511.61	0.48	0.26	4.72E+00	511.06	0.44
pro-PdS_2	Pt_2Se_4	0.29	4.08	505.08	0.44	0.27	4.43E+00	508.03	0.43
pro-PdS_2	Pt_2Te_4	0.32	5.51	502.91	0.60	0.29	5.20E+00	505.72	0.52
pro-TiS_3	Hf_2O_6	0.16	8.27	513.03	0.38	0.15	8.37E+00	512.26	0.38
pro-WTe_2	Hf_2Br_4	0.10	5.85	478.81	0.20	0.08	6.00E+00	473.09	0.16
pro-WTe_2	Hf_2Cl_4	0.13	4.19	477.64	0.19	0.11	4.20E+00	476.72	0.18
pro-WTe_2	Os_2O_4	0.16	0.45	230.73	1.10	0.05	4.91E-01	154.22	0.31
pro-WTe_2	Os_2S_4	0.10	15.68	357.67	0.35	0.06	2.49E+01	316.79	0.29
pro-WTe_2	Os_2Se_4	0.16	6.63	404.69	0.35	0.12	9.94E+00	363.97	0.33
pro-WTe_2	Os_2Te_4	0.16	8.27	362.21	0.40	0.10	1.06E+01	348.90	0.29

Table S35. At T=800 K, calculated maximum EFF (10^{-19} $W^{5/3}ms^{-1/3}K^{-2}$) and corresponding carrier concentration ($10^{19}cm^{-3}$), Seebeck coefficient ($\mu V/K$) and power factor (10^{11} W/mK^{2}s) through y-direction for n-type carrier concentration of 2D isotropic materials using PBE (w/o SOC) and PBE+SOC (w SOC).

n-type		T=800 K (w/o SOC)				T=800 K (w SOC)			
Prototype	Material	t_y^n(max)	ρ	S_{yy}	$S_{yy}^2\sigma_{yy}/\tau$	t_y^n(max)	ρ	S_{yy}	$S_{yy}^2\sigma_{yy}/\tau$
pro-AuSe	Au_2O_2	0.07	126.11	174.97	1.04	0.09	8.39E+01	208.54	1.06
pro-AuSe	Au_2S_2	0.12	4.11	510.31	0.18	0.12	4.27E+00	511.33	0.18
pro-AuSe	Au_2Se_2	0.12	2.92	505.05	0.14	0.12	3.63E+00	485.08	0.17
pro-AuSe	Au_2Te_2	0.12	3.89	457.21	0.17	0.11	1.05E+01	362.74	0.31
pro-FeOCl	$Hf_2Br_2N_2$	0.41	0.52	509.23	0.15	0.40	5.22E-01	510.00	0.15
pro-FeOCl	$Hf_2Cl_2N_2$	0.32	0.58	510.45	0.13	0.31	5.86E-01	511.38	0.12
pro-FeOCl	$Ir_2Cl_2O_2$	0.05	86.96	228.18	0.50	0.08	1.88E+01	333.72	0.35
pro-PdS_2	Pt_2S_4	0.28	6.92	515.66	0.59	0.24	6.63E+00	515.73	0.49
pro-PdS_2	Pt_2Se_4	0.33	3.19	515.81	0.42	0.31	2.78E+00	516.66	0.36
pro-PdS_2	Pt_2Te_4	0.37	4.57	514.13	0.60	0.32	4.56E+00	515.10	0.52
pro-TiS_3	Hf_2O_6	0.92	6.67	506.56	1.91	0.92	6.74E+00	505.88	1.92
pro-WTe_2	Hf_2Br_4	0.03	0.00	467.23	0.02	0.03	3.84E-03	453.19	0.02
pro-WTe_2	Hf_2Cl_4	0.04	0.01	449.97	0.02	0.04	2.01E-03	477.78	0.02
pro-WTe_2	Os_2O_4	0.18	26.10	198.27	1.34	0.08	3.10E+01	155.64	0.54
pro-WTe_2	Os_2S_4	0.19	9.09	377.13	0.48	0.15	9.07E+00	321.18	0.38
pro-WTe_2	Os_2Se_4	0.08	16.46	393.11	0.29	0.05	1.58E+01	295.26	0.17
pro-WTe_2	Os_2Te_4	0.19	18.32	433.89	0.77	0.12	2.05E+01	412.89	0.54