

Supplementary Information

Physically guided discovery of high-performance photocatalytic and photovoltaic heterostructures

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Table S1. Correspondence between abbreviations and their full names in the heat map.

Abbreviation	Full Name	Unit
ehull	Energy above convex hull	eV/atom
hform	Heat of formation	eV/atom
gap_pbe	Band gap (PBE)	eV
cbm_pbe	CBM (PBE)	eV
energ	Energy	eV
Inporx	Interband polarizability at (x)	Å
Inpory	Interband polarizability at (y)	Å
Inporz	Interband polarizability at (z)	Å
natoms	Number of atoms	-
vbm_pbe	VBM (PBE)	eV
evac	Vacuum level	eV

Table S2. CBM (eV), VBM (eV), Band Gap (eV), and Electronegativity of the 1014 Monolayer Materials.

Formula	CBM	VBM	Band gap	χ_m
CoHO ₂	-2.61	-3.61	1.00	2.88
Nb ₂ Br ₆	-3.86	-4.87	1.00	1.42
Re ₆ Te ₈ F ₂	-4.42	-5.42	1.01	2.22
In ₂ Ge ₂ Se ₂	-4.71	-5.72	1.01	2.16
Os ₂ O ₄	-5.89	-6.89	1.01	2.88
Ta ₄ Cl ₂ S ₁₂	-4.30	-5.31	1.01	2.44
Cu ₂ O ₂	-6.04	-7.05	1.01	2.71
Hf ₂ I ₄	-3.09	-4.10	1.01	2.14
Ta ₄ I ₂ Se ₁₂	-4.12	-5.13	1.01	2.24
Mo ₂ F ₆	-5.96	-6.97	1.01	3.69
Nb ₂ Te ₄ Cl ₄	-3.99	-5.01	1.02	2.07
HfI ₂	-2.15	-3.17	1.02	2.14
Hf ₂ BrI ₅	-3.43	-4.46	1.02	2.26
Ta ₄ Te ₁₂ I ₂	-3.81	-4.84	1.02	2.05
Co ₂ O ₂ Cl ₂	-5.49	-6.52	1.03	2.69
Zr ₂ Sn ₂ Te ₈	-3.70	-4.73	1.03	2.03
Zr ₂ Se ₆	-4.61	-5.64	1.03	2.25
Ag ₄ Se ₄ I ₄	-5.73	-6.76	1.03	2.24
MoCr ₃ S ₈	-2.74	-3.77	1.03	2.29
PdNiIr ₂ Se ₈	-4.71	-5.74	1.03	2.13
Nb ₄ I ₂ Se ₁₂	-4.23	-5.26	1.03	1.57
TiI ₂ Br	-2.38	-3.41	1.04	2.30
In ₂ Si ₂ Te ₂	-4.22	-5.25	1.04	1.99
ZrI ₂	-2.31	-3.35	1.04	2.16
Bi ₂ S ₃	-5.83	-6.87	1.04	2.43
LiC ₁₂	-1.93	-2.97	1.04	2.62
Bi ₂ O ₂	-3.87	-4.91	1.04	2.99

Ir_2IBrS_2	-4.46	-5.51	1.05	2.20
Rh_4Se_8	-4.94	-5.99	1.05	2.05
Fe_2Se_4	-4.69	-5.74	1.05	2.18
Zr_2ClBr_5	-3.50	-4.56	1.05	2.54
Os_3S_{12}	-4.58	-5.64	1.06	2.36
$\text{Na}_2\text{Be}_2\text{P}_2$	-1.20	-2.26	1.06	1.99
$\text{AgAlTe}_6\text{P}_2$	-4.00	-5.06	1.07	2.14
$\text{Nb}_4\text{Br}_2\text{Se}_{12}$	-4.19	-5.26	1.07	1.60
Au_2Te_2	-4.10	-5.17	1.07	2.01
$\text{Hf}_2\text{Ge}_2\text{Te}_8$	-3.73	-4.79	1.07	2.04
$\text{Ta}_4\text{Br}_2\text{Se}_{12}$	-4.04	-5.11	1.07	2.29
Ru_2Te_4	-3.92	-4.99	1.07	1.89
SiSe_2	-5.01	-6.08	1.07	2.35
$\text{Cu}_2\text{Cl}_2\text{I}_4$	-5.96	-7.04	1.07	2.42
$\text{Zr}_2\text{P}_2\text{Se}_6$	-4.29	-5.36	1.07	2.26
$\text{AgBiTe}_6\text{P}_2$	-4.22	-5.30	1.08	2.15
$\text{Nb}_4\text{Cl}_2\text{Se}_{12}$	-4.15	-5.23	1.08	1.55
$\text{Ta}_2\text{Te}_4\text{Br}_4$	-3.85	-4.93	1.08	2.30
Si_2Te_4	-3.72	-4.81	1.09	2.11
PtTeSe	-4.14	-5.23	1.09	2.02
$\text{Ta}_4\text{Te}_{12}\text{Br}_2$	-3.74	-4.83	1.09	2.09
$\text{Cu}_4\text{Te}_4\text{I}_4$	-5.32	-6.42	1.10	2.23
$\text{Hf}_2\text{Ti}_2\text{ClBr}_7$	-3.27	-4.37	1.10	2.45
$\text{Ag}_4\text{Te}_4\text{I}_4$	-5.36	-6.46	1.10	2.18
$\text{Hf}_2\text{P}_2\text{Se}_6$	-4.30	-5.39	1.10	2.26
Au_4Se_4	-4.49	-5.59	1.10	2.13
$\text{Y}_2\text{CH}_2\text{O}_2$	-1.01	-2.11	1.10	0.76
Ge_2Te_2	-3.21	-4.31	1.10	2.11
$\text{Ta}_4\text{Cl}_2\text{Se}_{12}$	-3.98	-5.09	1.10	2.31

CrMo ₃ Te ₈	-3.64	-4.74	1.11	1.96
CrW ₃ S ₈	-2.53	-3.64	1.11	2.26
MoAg ₂ Te ₄	-3.80	-4.91	1.12	2.05
Zr ₂ Ge ₂ Te ₈	-3.69	-4.81	1.12	2.05
Ag ₂ O ₂	-5.57	-6.70	1.13	2.63
CrSe ₂	-4.00	-5.13	1.13	2.19
Rh ₂ O ₂ F ₂	-6.41	-7.54	1.13	3.02
Ru ₃ S ₃ Cl ₆	-6.57	-7.70	1.13	2.45
Zr ₂ Se ₄	-4.50	-5.64	1.13	2.19
Cu ₄ Te ₄ Br ₄	-5.61	-6.75	1.14	2.33
Nb ₄ Te ₁₂ I ₂	-3.80	-4.93	1.14	1.51
Ta ₄ Te ₁₂ Cl ₂	-3.69	-4.82	1.14	2.12
RhIr ₂ GaS ₄ Br ₄	-5.16	-6.30	1.14	2.30
Au ₄ S ₂	-4.24	-5.38	1.14	2.10
Zr ₂ Br ₄	-3.35	-4.49	1.14	2.43
In ₂ TeS	-4.42	-5.56	1.14	2.20
WTe ₂	-3.36	-4.50	1.14	1.93
Y ₄ Te ₄ Br ₄	-4.91	-6.06	1.14	1.45
CrO ₂	-6.45	-7.60	1.14	3.03
AgGaCl ₂ Br ₄	-6.81	-7.95	1.15	2.58
MgGa ₂ Se ₄	-4.39	-5.53	1.15	2.30
Hf ₂ IClBr ₄	-3.43	-4.57	1.15	2.49
Zr ₂ Br ₂ Cl ₂	-3.43	-4.58	1.15	2.51
In ₂ Ge ₂ Te ₆	-4.20	-5.35	1.15	2.10
Hf ₂ I ₂ Br ₂	-3.10	-4.25	1.15	2.28
BiTeCl	-5.14	-6.29	1.15	2.43
PdNiS ₄	-5.27	-6.42	1.15	2.24
ZrTiHf ₂ Br ₈	-3.23	-4.38	1.16	2.42
HfIBr	-2.20	-3.36	1.16	2.28

Hf ₂ Si ₂ Te ₈	-3.65	-4.81	1.16	2.03
Cu ₄ S ₄ I ₄	-5.78	-6.94	1.16	2.34
Cr ₃ Se ₆	-4.11	-5.27	1.16	2.19
BiTeBr	-5.16	-6.32	1.16	2.35
Sc ₄ Se ₆	-2.29	-3.45	1.16	2.19
MgAl ₂ Te ₄	-3.44	-4.60	1.16	2.05
Rh ₄ S ₆	-5.36	-6.52	1.16	2.08
Zr ₂ Cl ₄	-3.54	-4.70	1.16	2.59
BiTeBr	-5.05	-6.21	1.16	2.35
Ag ₄ S ₄ Cl ₄	-6.43	-7.59	1.16	2.44
Ga ₂ Ge ₂ Te ₂	-4.08	-5.25	1.17	2.04
Hf ₂ I _{Br} ₃	-2.24	-3.41	1.17	2.35
W ₂ Cl ₆	-3.65	-4.82	1.17	2.60
TiBr ₂	-2.39	-3.56	1.17	2.43
Fe ₂ Te ₆ P ₂	-4.45	-5.62	1.17	2.08
ZrI _{Br}	-2.35	-3.53	1.17	2.29
Y ₄ Te ₄ Cl ₄	-4.93	-6.11	1.17	1.60
Y ₂ NH ₂ O ₂	-1.34	-2.52	1.17	2.84
Ta ₂ Te ₄ I ₄	-3.75	-4.93	1.18	2.14
BiSI	-5.19	-6.36	1.18	2.37
Ir ₂ S ₂ Br ₂	-4.66	-5.84	1.18	2.25
BiTeF	-4.38	-5.56	1.18	2.99
IrGaS ₂ I ₂	-4.45	-5.63	1.18	2.25
HfZr ₃ BrCl ₇	-3.48	-4.66	1.18	2.57
Nb ₄ Te ₁₂ Br ₂	-3.76	-4.94	1.18	1.50
Nb ₄ Te ₁₂ Cl ₂	-3.73	-4.91	1.18	1.52
In ₂ Si ₂ Te ₆	-4.23	-5.41	1.18	2.09
TiI _{Cl}	-2.45	-3.64	1.19	2.38
BiSeI	-5.11	-6.30	1.19	2.31

$\text{Bi}_2\text{Se}_2\text{Br}_2$	-5.61	-6.80	1.19	2.45
$\text{Zr}_2\text{Si}_2\text{Te}_8$	-3.63	-4.82	1.19	2.04
OsRuCl_6	-5.17	-6.37	1.20	2.54
BiTeCl	-5.19	-6.39	1.20	2.43
$\text{Nb}_2\text{Br}_2\text{Cl}_4$	-3.98	-5.18	1.20	1.98
$\text{Ir}_2\text{S}_2\text{Cl}_2$	-5.09	-6.29	1.20	2.32
ZrSe_2	-4.68	-5.89	1.20	2.19
$\text{W}_2\text{Cr}_2\text{Se}_8$	-3.87	-5.07	1.20	2.16
$\text{Co}_2\text{H}_2\text{S}_4$	-4.61	-5.82	1.20	2.29
$\text{RuNiTa}_2\text{Se}_6$	-4.49	-5.69	1.20	2.11
$\text{Mg}_2\text{Al}_2\text{Te}_5$	-3.37	-4.58	1.21	2.04
WTeO	-3.71	-4.92	1.21	2.47
$\text{Cu}_4\text{Se}_4\text{I}_4$	-5.59	-6.81	1.21	2.29
$\text{Cu}_2\text{Br}_2\text{O}_4$	-6.49	-7.70	1.21	2.87
ZrHf_2Se_6	-4.63	-5.84	1.21	2.19
$\text{Ag}_4\text{Se}_4\text{Br}_4$	-6.07	-7.28	1.21	2.34
Sc_4Te_6	-4.06	-5.28	1.21	1.96
$\text{Sc}_2\text{P}_2\text{Se}_6$	-3.77	-4.99	1.21	2.28
$\text{AgGa}_3\text{O}_4\text{Cl}_4$	-6.78	-8.00	1.22	2.93
BiSeI	-5.21	-6.42	1.22	2.31
TeGe_2S	-3.27	-4.48	1.22	2.26
HfSe_2	-4.60	-5.81	1.22	2.19
MoW_3Te_8	-3.36	-4.58	1.22	1.93
$\text{Nb}_2\text{Te}_4\text{Br}_4$	-3.83	-5.05	1.22	1.78
Ta_3TeI_7	-3.78	-5.01	1.22	2.15
HfBr_2	-2.28	-3.50	1.23	2.41
$\text{K}_2\text{C}_2\text{Se}_2\text{H}_6\text{S}_6$	-2.05	-3.28	1.23	1.28
$\text{Ta}_2\text{Rh}_2\text{S}_8$	-5.12	-6.36	1.23	2.22
Pd_2Se_4	-4.11	-5.35	1.23	2.06

Nb ₃ SI ₇	-4.10	-5.33	1.24	1.32
Nb ₃ SeI ₇	-4.04	-5.27	1.24	1.31
Zr ₂ N ₂ I ₂	-3.96	-5.20	1.24	2.41
CrMo ₃ S ₈	-2.65	-3.89	1.24	2.26
Cu ₄ O ₄ Cl ₄	-7.59	-8.82	1.24	2.75
In ₂ Al ₂ Te ₆	-4.35	-5.59	1.24	2.07
Al ₂ Ge ₂ Se ₂	-3.43	-4.67	1.24	2.14
Nb ₃ TeI ₇	-3.94	-5.19	1.24	1.30
CrSeS	-4.22	-5.46	1.24	2.25
Ag ₄ Te ₄ Cl ₄	-5.73	-6.98	1.25	2.34
MoAu ₂ Se ₄	-3.72	-4.97	1.25	2.12
Ge ₂ Te ₆ P ₂	-3.89	-5.14	1.25	2.16
Nb ₂ Ir ₂ S ₈	-5.06	-6.31	1.25	1.62
Ga ₄ Se ₆	-4.11	-5.36	1.25	2.32
Ta ₃ SeI ₇	-3.85	-5.11	1.26	2.18
Ag ₄ Te ₄ Br ₄	-5.60	-6.86	1.26	2.28
Mg ₂ Ga ₂ Se ₅	-4.27	-5.53	1.26	2.29
Au ₂ Se ₂ Br ₂	-5.41	-6.68	1.27	2.29
ZrBr ₂	-2.40	-3.68	1.28	2.43
In ₄ I ₄	-1.86	-3.14	1.28	2.20
Ag ₄ Se ₄ Cl ₄	-6.20	-7.48	1.28	2.40
W ₂ Mo ₂ Te ₈	-3.38	-4.66	1.28	1.94
Nb ₂ Te ₄ I ₄	-3.76	-5.04	1.28	1.66
Au ₄ F ₈	-6.35	-7.63	1.29	3.26
Cu ₂ Cl ₂ O ₄	-6.62	-7.91	1.29	2.91
Pd ₄ In ₂ Se ₆	-4.26	-5.55	1.29	1.99
In ₄ Te ₆	-4.22	-5.51	1.29	2.07
Zn ₂ Te ₂	-3.96	-5.25	1.29	2.48
Ta ₃ SI ₇	-3.90	-5.19	1.30	2.19

HfCl	-2.28	-3.57	1.30	2.36
Ti ₂ CO ₂	-4.80	-6.09	1.30	2.78
TiBrCl	-2.48	-3.78	1.30	2.51
K ₂ Ag ₂ Se ₂	-1.52	-2.82	1.30	1.49
CaSn ₃ S ₄ Br ₄	-5.01	-6.31	1.30	2.26
Bi ₂ P ₂ S ₆	-4.73	-6.04	1.32	2.46
ZrCl	-2.41	-3.72	1.32	2.37
Zr ₄ S ₂ Se ₄ Cl ₄	-5.93	-7.24	1.32	2.44
WAg ₂ Te ₄	-3.61	-4.93	1.32	2.05
Cr ₄ O ₁₀	-5.60	-6.92	1.32	3.12
WMo ₃ Te ₈	-3.41	-4.73	1.33	1.94
PdPt ₃ SeSCl ₆	-5.46	-6.79	1.33	2.34
Fe ₂ S ₄	-5.13	-6.46	1.33	2.28
Re ₄ Te ₈	-3.46	-4.79	1.33	1.95
Ta ₂ Ir ₂ S ₈	-5.00	-6.33	1.33	2.24
Na ₄ Ag ₄ Se ₄	-2.63	-3.96	1.33	2.17
CrW ₃ Se ₈	-3.69	-5.02	1.33	2.14
SnSe ₂	-5.12	-6.46	1.33	2.32
Hf ₂ Br ₄	-3.10	-4.44	1.33	2.41
In ₂ I ₂	-4.39	-5.72	1.34	2.19
Au ₄ S ₄	-4.54	-5.88	1.34	2.18
Cu ₄ Te ₄ Cl ₄	-5.63	-6.96	1.34	2.39
TiSeS	-4.97	-6.31	1.34	2.26
Ir ₂ O ₂ Br ₂	-3.65	-4.99	1.34	2.55
Au ₄ S ₄ I ₄	-5.17	-6.51	1.34	2.23
Hf ₄ S ₂ Se ₆	-4.67	-6.01	1.34	2.23
Sn ₂ Se ₂	-3.29	-4.63	1.35	2.24
Rh ₂ P ₂ S ₆	-4.40	-5.75	1.35	2.26
Ni ₂ SeS ₃	-4.95	-6.30	1.35	2.31

CrMo ₃ O ₈	-5.85	-7.20	1.35	3.00
Au ₂ Te ₄ I ₂	-4.26	-5.61	1.35	2.13
CrS ₂	-4.41	-5.76	1.35	2.31
Pd ₄ I ₄ Br ₄	-5.31	-6.66	1.35	2.15
HfBrCl	-2.33	-3.69	1.36	2.50
BP	-4.00	-5.36	1.36	2.19
Fe ₃ Se ₆	-4.87	-6.23	1.36	2.18
BiSeBr	-5.42	-6.78	1.36	2.45
Ir ₂ Ni ₂ S ₈	-5.01	-6.37	1.36	2.27
Al ₂ Ge ₂ Te ₂	-3.67	-5.03	1.37	2.00
MoTe ₂	-3.44	-4.81	1.37	1.94
MgIn ₂ Se ₄	-4.42	-5.80	1.38	2.28
Os ₂ Te ₄	-3.57	-4.95	1.38	1.93
Sr ₄ Bi ₄ F ₄ S ₈	-4.38	-5.76	1.38	2.27
Os ₂ S ₄	-4.67	-6.06	1.39	2.22
Ga ₂ Te ₅	-3.89	-5.28	1.39	2.11
Os ₂ Se ₄	-4.07	-5.46	1.39	2.11
Ag ₄ S ₆	-4.21	-5.60	1.39	2.31
Co ₂ O ₂ F ₂	-6.84	-8.23	1.39	3.14
Ga ₂ Al ₂ Te ₆	-4.16	-5.55	1.39	2.07
TiCl ₂	-2.59	-3.99	1.40	2.59
In ₂ P ₂ S ₆	-4.46	-5.86	1.40	2.46
Ta ₃ TeBr ₇	-3.75	-5.15	1.40	2.39
ZrBrCl	-2.48	-3.87	1.40	2.51
Cu ₂ N ₂ Cl ₂ C ₆ H ₈	-2.00	-3.40	1.40	2.56
Rh ₄ S ₈	-5.33	-6.73	1.40	2.16
GeS ₂	-5.57	-6.97	1.41	2.50
Ga ₂ Te ₂	-3.83	-5.24	1.41	2.05
Hf ₂ Br ₂ Cl ₂	-3.17	-4.58	1.41	2.50

$\text{Na}_2\text{Ag}_2\text{Te}_2$	-2.36	-3.78	1.42	2.07
Ag_2Te_3	-3.93	-5.35	1.42	2.11
$\text{Cu}_4\text{Se}_4\text{Br}_4$	-5.99	-7.41	1.42	2.39
$\text{Pd}_4\text{Te}_4\text{P}_4$	-4.42	-5.84	1.42	1.91
$\text{Bi}_2\text{GeSe}_2\text{I}_4$	-4.83	-6.25	1.42	2.31
RhSeI	-4.21	-5.63	1.43	2.05
$\text{In}_2\text{Te}_2\text{I}_2$	-4.34	-5.76	1.43	2.19
$\text{Au}_2\text{I}_2\text{S}_4$	-4.79	-6.22	1.43	2.31
CrMo_3Se_8	-3.81	-5.24	1.43	2.14
In_2Se_3	-4.83	-6.27	1.43	2.30
$\text{HfGeS}_2\text{Br}_2$	-4.44	-5.88	1.43	2.46
Nb_3TeBr_7	-3.96	-5.40	1.44	1.44
$\text{Hf}_2\text{N}_2\text{I}_2$	-3.68	-5.12	1.44	2.42
RuH_2O_2	-1.39	-2.83	1.44	2.78
$\text{Ir}_2\text{S}_2\text{F}_2$	-5.91	-7.35	1.44	2.77
$\text{Au}_4\text{S}_4\text{Br}_4\text{F}_4$	-5.55	-6.99	1.44	2.77
Nb_3OBr_7	-4.34	-5.78	1.44	1.82
$\text{Sc}_2\text{Te}_2\text{Cl}_2$	-3.71	-5.15	1.44	2.35
Ag_4Te_2	-4.41	-5.85	1.44	2.09
$\text{W}_2\text{Cr}_2\text{S}_8$	-4.29	-5.73	1.44	2.28
ZrNiF_6	-3.56	-5.00	1.44	3.70
$\text{Pd}_2\text{Se}_2\text{Cl}_4$	-5.48	-6.93	1.45	2.38
Ta_3SeBr_7	-3.84	-5.29	1.45	2.42
Ti_2S_6	-4.18	-5.63	1.45	2.40
$\text{Cu}_4\text{Se}_4\text{Cl}_4$	-6.17	-7.63	1.45	2.45
Nb_4O_8	-4.35	-5.81	1.45	1.66
$\text{Pt}_4\text{SeS}_3\text{I}_4$	-4.34	-5.79	1.46	2.13
$\text{Hf}_2\text{Te}_2\text{O}_2$	-3.79	-5.25	1.46	2.59
TiSe_2	-4.83	-6.29	1.46	2.19

HfCl ₂	-2.41	-3.88	1.47	2.58
Pd ₂ I ₄	-4.72	-6.19	1.47	2.05
NbInBr ₆	-4.52	-6.00	1.47	2.07
BiSI	-5.21	-6.69	1.47	2.37
Hf ₂ Cl ₄	-3.28	-4.75	1.48	2.58
SnSeS	-5.10	-6.58	1.48	2.39
Al ₂ Ge ₂ Te ₆	-3.89	-5.37	1.48	2.09
Nb ₃ SeBr ₇	-4.08	-5.55	1.48	1.42
Au ₂ Cl ₂	-5.63	-7.11	1.48	2.32
Ga ₈ Te ₁₂	-3.52	-5.00	1.48	2.09
Ge ₂ Te ₂	-3.38	-4.86	1.48	2.11
Au ₄ Se ₄ I ₄	-4.98	-6.47	1.48	2.19
Ta ₄ O ₈	-4.19	-5.68	1.49	3.09
Ge ₂ H ₂	-3.73	-5.22	1.49	1.99
SnS ₂ Br ₂	-5.49	-6.98	1.49	2.57
Si ₂ F ₂	-5.50	-6.99	1.49	3.50
WTeSe	-3.30	-4.80	1.49	2.03
Zr ₂ P ₂ S ₆	-4.41	-5.91	1.50	2.38
Mg ₂ In ₂ Se ₅	-4.21	-5.71	1.50	2.28
ZrCl ₂	-2.57	-4.07	1.50	2.59
ZnGeSe ₂ Br ₂	-4.80	-6.30	1.50	2.55
BiSeCl	-5.50	-7.01	1.51	2.53
Ag ₄ S ₆	-4.82	-6.32	1.51	2.31
Ta ₃ SBr ₇	-3.89	-5.40	1.51	2.44
Ta ₃ TeCl ₇	-3.76	-5.27	1.51	2.54
P ₄	-3.89	-5.40	1.51	2.25
HfSeS	-4.62	-6.13	1.51	2.26
MoSeO	-4.07	-5.58	1.51	2.56
ZrSeS	-4.68	-6.20	1.51	2.27

Bi ₂ SeSCl ₂	-5.85	-7.37	1.52	2.56
Ir ₄ S ₈	-4.88	-6.40	1.52	2.20
Sn ₂ SeS	-3.18	-4.70	1.52	2.30
Nb ₃ SBr ₇	-4.15	-5.68	1.53	1.75
Cu ₄ S ₄ Br ₄	-6.21	-7.74	1.53	2.43
Al ₄ Te ₆	-4.14	-5.67	1.53	2.06
FeH ₂ O ₂	-2.16	-3.69	1.53	2.87
InGaTe ₂	-4.01	-5.54	1.53	2.04
Bi ₄ S ₆	-4.41	-5.95	1.54	2.43
Ir ₄ Se ₂ S ₆	-4.71	-6.24	1.54	2.18
CuGeTeBr	-3.95	-5.49	1.54	2.30
Au ₄ S ₄ Cl ₄ F ₄	-5.73	-7.27	1.54	2.82
Pd ₂ I ₂ Br ₂	-4.92	-6.46	1.54	2.15
Nb ₃ TeCl ₇	-4.00	-5.55	1.54	1.53
Ga ₄ Se ₆	-4.89	-6.44	1.55	2.32
Cu ₄ S ₄ Cl ₄	-6.44	-7.99	1.55	2.49
V ₄ O ₈	-5.33	-6.88	1.55	3.07
Au ₃ InO ₄ Br ₄	-5.58	-7.13	1.56	2.66
In ₂ TeSI ₂	-3.88	-5.44	1.56	2.28
TiPdS ₂	-4.03	-5.59	1.56	2.05
Ir ₄ Se ₃ S ₅	-4.63	-6.18	1.56	2.17
Ge ₂ Se ₂	-3.20	-4.76	1.56	2.29
Au ₂ Se ₂	-4.41	-5.97	1.56	2.13
Ge ₆ P ₈	-3.95	-5.51	1.56	2.17
InN	-4.05	-5.62	1.57	2.70
Ir ₂ O ₂ Cl ₂	-3.93	-5.50	1.57	2.62
InGaP ₂ Se ₂ S ₄	-4.18	-5.74	1.57	2.42
Ni ₂ Te ₂ S ₆	-3.87	-5.43	1.57	2.35
Ir ₄ Se ₈	-4.34	-5.90	1.57	2.10

Ta ₃ OCl ₇	-4.08	-5.65	1.57	2.68
Bi ₂ H ₂ S ₄	-4.73	-6.31	1.58	2.45
Ta ₃ SeCl ₇	-3.86	-5.44	1.58	2.56
Ru ₂ S ₄	-4.83	-6.41	1.58	2.18
MoTeS	-3.74	-5.33	1.59	2.09
In ₈ Te ₁₂	-3.54	-5.12	1.59	2.07
Au ₂ Cl ₂ Se ₄	-4.86	-6.45	1.59	2.37
Au ₂ Te ₄ Cl ₂	-4.34	-5.93	1.59	2.26
Nb ₃ OCl ₇	-4.43	-6.02	1.59	1.92
MoTeSe	-3.50	-5.09	1.59	2.03
HfGeS ₂ Cl ₂	-4.61	-6.21	1.59	2.55
Ru ₂ Se ₄	-4.19	-5.79	1.60	2.07
Cu ₁₂ S ₆	-4.54	-6.14	1.60	2.28
Rb ₄ O ₂	-1.15	-2.75	1.60	1.13
BiSBr	-5.49	-7.09	1.60	2.51
Nb ₃ SeCl ₇	-4.14	-5.74	1.60	1.50
AuBiP ₂ Se ₆	-4.52	-6.13	1.60	2.29
Hf ₂ P ₂ S ₆	-4.35	-5.96	1.61	2.39
Hf ₂ Ti ₂ Se ₈	-4.92	-6.53	1.61	2.19
Au ₂ Br ₂ S ₄	-5.05	-6.66	1.61	2.38
Hf ₂ Sn ₂ Se ₈	-3.69	-5.31	1.61	2.25
Sc ₂ Te ₂ Br ₂	-3.66	-5.28	1.62	2.26
Ba ₄ Bi ₄ F ₄ Se ₈	-4.30	-5.92	1.62	2.13
Au ₂ Te ₄ Br ₂	-4.32	-5.94	1.62	2.21
TiGeS ₂ I ₂	-3.81	-5.43	1.62	2.32
Re ₄ Se ₈	-3.74	-5.36	1.62	2.12
Cu ₂ N ₂ I ₂ C ₆ F ₈	-4.89	-6.51	1.62	3.29
PdAuSeCl	-4.45	-6.07	1.62	2.14
Y ₂ Te ₃	-4.22	-5.84	1.63	1.10

Ga_2Se_3	-3.86	-5.48	1.63	2.32
HfSe_2	-5.14	-6.77	1.63	2.19
$\text{Ti}_2\text{Te}_4\text{I}_4$	-3.65	-5.28	1.63	2.16
$\text{Ga}_2\text{Ge}_2\text{Se}_6$	-4.56	-6.19	1.63	2.32
$\text{Au}_3\text{InIBr}_3\text{O}_4$	-5.35	-6.99	1.63	2.63
$\text{Zr}_2\text{Sn}_2\text{Se}_8$	-3.68	-5.31	1.64	2.25
$\text{Ta}_2\text{O}_2\text{I}_4$	-3.67	-5.31	1.64	2.52
Ag_4F_8	-7.15	-8.79	1.64	3.31
$\text{Na}_2\text{Nb}_2\text{I}_{12}$	-4.55	-6.19	1.64	1.88
Ta_3SCl_7	-3.93	-5.57	1.64	2.58
Au_2Br_6	-5.46	-7.11	1.64	2.44
HfSeS	-5.28	-6.92	1.65	2.26
$\text{Cu}_4\text{S}_4\text{F}_4$	-6.28	-7.93	1.65	2.90
$\text{Ta}_2\text{Se}_4\text{Cl}_4$	-3.71	-5.35	1.65	2.50
AuInSI_2	-4.49	-6.14	1.65	2.24
In_2Te_5	-3.72	-5.37	1.65	2.10
MoO_2	-5.33	-6.98	1.65	2.98
$\text{Ag}_4\text{Br}_{12}$	-5.16	-6.81	1.65	2.48
Nb_3SCl_7	-4.23	-5.89	1.65	1.51
$\text{Hf}_2\text{Te}_4\text{I}_4$	-3.80	-5.46	1.66	2.16
Pt_2Br_2	-4.18	-5.84	1.66	2.12
$\text{Rh}_2\text{S}_2\text{I}_2$	-4.07	-5.73	1.67	2.10
$\text{Re}_6\text{I}_2\text{Se}_8$	-4.76	-6.42	1.67	2.09
$\text{In}_4\text{Te}_4\text{I}_4$	-4.40	-6.07	1.67	2.19
$\text{Au}_4\text{Te}_4\text{I}_4$	-4.64	-6.32	1.67	2.12
$\text{Al}_2\text{Si}_2\text{Te}_6$	-3.78	-5.45	1.67	2.08
Sn_2Te_2	-3.25	-4.92	1.67	2.05
$\text{Au}_2\text{Br}_2\text{S}_4$	-5.26	-6.94	1.68	2.38
$\text{Co}_4\text{O}_4\text{Br}_4$	-4.46	-6.14	1.68	2.63

WTeS	-3.50	-5.18	1.68	2.09
PdS ₂	-5.03	-6.72	1.68	2.15
Hf ₂ CO ₂	-4.16	-5.84	1.68	2.81
Zr ₂ Te ₄ I ₄	-3.83	-5.51	1.68	2.16
Li ₂ Nb ₂ I ₁₂	-4.52	-6.21	1.69	1.88
Pt ₄ In ₂ Se ₆	-3.88	-5.56	1.69	2.03
ZrHf ₃ Se ₈	-5.11	-6.80	1.69	2.19
V ₂ Se ₄ Cl ₄	-3.68	-5.37	1.69	2.50
Au ₄ Cu ₄ Se ₄	-4.33	-6.03	1.69	2.14
AgGaP ₂ Se ₆	-4.33	-6.02	1.69	2.31
Ta ₂ O ₂ Br ₄	-4.06	-5.76	1.70	2.72
Zr ₂ Te ₄ Cl ₄	-3.89	-5.59	1.70	2.42
Ta ₃ TeF ₇	-3.46	-5.16	1.70	3.53
Ta ₂ O ₂ Cl ₄	-4.36	-6.07	1.70	2.83
Au ₆ I ₆	-3.93	-5.63	1.70	2.12
Ni ₂ Te ₄	-4.15	-5.86	1.70	2.10
Al ₂ B ₂ S ₆	-5.24	-6.94	1.70	2.46
AgInP ₂ Se ₆	-4.29	-6.00	1.71	2.31
Ta ₂ Se ₄ I ₄	-3.59	-5.30	1.71	2.25
Hf ₂ Zr ₂ Se ₈	-5.09	-6.81	1.72	2.19
K ₂ Nb ₂ I ₁₂	-4.58	-6.29	1.72	1.61
NaCoP ₂ Se ₆	-4.67	-6.39	1.72	2.29
Rb ₂ K ₂ O ₂	-1.14	-2.85	1.72	1.09
Nb ₃ TeF ₇	-3.76	-5.48	1.72	2.14
Al ₂ Si ₂ S ₂	-3.38	-5.10	1.72	2.21
Zr ₂ S ₄	-4.65	-6.37	1.72	2.33
Hf ₂ Te ₄ Br ₄	-3.86	-5.58	1.72	2.32
Ta ₂ Se ₄ Br ₄	-3.65	-5.37	1.73	2.40
Zr ₂ CO ₂	-4.01	-5.74	1.73	2.80

WSe ₂	-3.26	-4.99	1.73	2.12
WMo ₃ O ₈	-5.19	-6.92	1.73	2.99
In ₄ Se ₆	-4.98	-6.71	1.73	2.30
Pt ₂ Te ₂ S ₆	-3.65	-5.38	1.73	2.27
Ta ₃ SeF ₇	-3.57	-5.30	1.74	3.56
AuAgBr ₄	-5.47	-7.20	1.74	2.39
Sc ₂ CBr ₂	-4.19	-5.93	1.74	2.37
Bi ₈ O ₄ Se ₈	-3.90	-5.63	1.74	2.60
Au ₂ Cl ₂ Se ₄	-4.96	-6.70	1.74	2.37
Cu ₄ Te ₂ O ₁₂	-7.66	-9.40	1.74	3.03
BiSeBr	-5.24	-6.98	1.74	2.45
Pt ₂ I ₄	-4.14	-5.88	1.74	2.09
Pd ₂ Te ₄	-3.88	-5.62	1.74	1.90
BiSCl	-5.64	-7.38	1.75	2.59
In ₂ Se ₂ Cl ₂	-4.98	-6.73	1.75	2.54
MoW ₃ Se ₈	-3.32	-5.07	1.75	2.12
Ir ₂ S ₂ I ₂	-3.67	-5.42	1.75	2.14
W ₂ Mo ₂ Se ₈	-3.41	-5.16	1.75	2.12
Sc ₂ Te ₂ I ₂	-3.57	-5.33	1.75	2.11
SnSe ₂	-4.27	-6.02	1.75	2.32
Ta ₂ I ₂ O ₄	-4.31	-6.07	1.76	2.88
Hf ₂ Ge ₂ Se ₈	-3.67	-5.43	1.76	2.26
Sn ₂ N ₂ I ₂	-4.49	-6.25	1.76	2.55
FeGa ₂ Se ₄	-3.70	-5.46	1.76	2.22
Mo ₂ Cl ₂ O ₄	-4.72	-6.48	1.76	2.96
Sc ₂ P ₂ S ₆	-3.70	-5.46	1.76	2.42
Y ₂ CCl ₂	-4.46	-6.23	1.76	1.57
Ge ₂ SeS	-3.13	-4.90	1.77	2.35
Rb ₂ K ₂ O ₂	-1.27	-3.04	1.77	1.09

InP	-3.83	-5.61	1.77	2.09
Zr ₂ Ge ₂ Se ₈	-3.68	-5.46	1.78	2.26
Ga ₂ SeSiCl	-4.55	-6.33	1.78	2.47
TiSO	-3.70	-5.47	1.78	2.74
Rb ₂ Au ₂ S ₂	-1.49	-3.27	1.78	1.49
WMo ₃ Se ₈	-3.45	-5.23	1.79	2.13
Zr ₂ Si ₂ Se ₈	-3.60	-5.39	1.79	2.26
PtPd ₃ O ₄ Cl ₄	-5.50	-7.29	1.79	2.56
PdS ₂	-4.31	-6.10	1.79	2.15
Pd ₂ F ₆	-8.17	-9.97	1.79	3.43
Zr ₂ Te ₄ Br ₄	-3.83	-5.62	1.80	2.32
Ta ₃ SF ₇	-3.65	-5.45	1.80	3.57
Pd ₂ Te ₂ O ₆	-3.57	-5.37	1.80	2.84
AgGaP ₂ S ₂ Se ₄	-4.32	-6.12	1.80	2.35
Ag ₄ Te ₂ O ₁₂	-7.26	-9.06	1.80	2.99
Al ₂ Te ₅	-3.48	-5.29	1.80	2.09
MoSe ₂	-3.51	-5.31	1.80	2.13
Nb ₃ SeF ₇	-3.91	-5.71	1.81	2.13
ScTeCl	-3.34	-5.14	1.81	2.35
Ga ₂ Si ₂ S ₂	-4.14	-5.94	1.81	2.25
Sc ₂ Se ₄ I ₄	-4.50	-6.31	1.81	2.30
Rb ₂ C ₂ Se ₂ H ₆ S ₆	-3.25	-5.06	1.81	1.28
CoTeBr	-4.20	-6.01	1.81	2.22
Nb ₂ Se ₄ I ₄	-3.64	-5.45	1.81	1.75
V ₂ Se ₄ Br ₄	-3.61	-5.42	1.81	2.41
Si ₂ Se ₂	-3.57	-5.39	1.81	2.26
Pd ₂ Te ₂ S ₆	-3.67	-5.49	1.82	2.24
IrTeI	-3.41	-5.23	1.82	2.01
Nb ₂ Se ₄ Cl ₄	-3.71	-5.53	1.82	2.14

$\text{In}_2\text{S}_2\text{I}_2$	-4.61	-6.44	1.83	2.37
$\text{Pt}_4\text{S}_3\text{Se}_5$	-4.32	-6.15	1.83	2.14
$\text{K}_2\text{Os}_2\text{C}_2\text{O}_2\text{F}_{10}$	-6.44	-8.28	1.83	3.22
MoSO	-4.30	-6.13	1.83	2.62
$\text{Li}_4\text{Ag}_4\text{Te}_4$	-2.67	-4.50	1.83	2.07
$\text{In}_2\text{IBrSe}_2$	-4.79	-6.62	1.83	2.38
K_4O_2	-1.13	-2.96	1.83	1.00
$\text{Ge}_4\text{Te}_4\text{P}_4$	-3.68	-5.51	1.84	2.16
Ga_2Te_2	-3.69	-5.53	1.84	2.05
$\text{Nb}_2\text{Se}_4\text{F}_4$	-3.59	-5.42	1.84	2.62
$\text{W}_2\text{Mo}_2\text{O}_8$	-5.02	-6.86	1.84	2.99
$\text{Ga}_2\text{Si}_2\text{Te}_2$	-3.47	-5.31	1.85	2.01
$\text{Nb}_2\text{O}_2\text{I}_4$	-3.66	-5.50	1.85	1.78
$\text{Te}_2\text{H}_2\text{P}_2\text{S}_{10}$	-4.87	-6.72	1.85	2.50
$\text{Bi}_2\text{O}_2\text{I}_2$	-4.89	-6.74	1.85	2.76
Al_2O_2	-3.53	-5.38	1.85	3.16
NaCoP_2S_6	-5.03	-6.88	1.85	2.41
$\text{Re}_6\text{Br}_2\text{Se}_8$	-4.80	-6.66	1.86	2.13
$\text{Ir}_2\text{Se}_2\text{I}_2$	-3.54	-5.40	1.86	2.10
$\text{V}_2\text{IO}_2\text{Br}_3$	-3.80	-5.66	1.86	2.66
$\text{In}_2\text{Se}_2\text{I}_2$	-4.66	-6.52	1.86	2.31
$\text{Au}_4\text{Te}_4\text{Br}_4$	-4.80	-6.66	1.86	2.23
Ga_2Te_2	-3.67	-5.53	1.86	2.05
$\text{Nb}_2\text{Se}_4\text{Br}_4$	-3.67	-5.54	1.87	1.87
$\text{Sc}_2\text{S}_4\text{I}_4$	-4.60	-6.47	1.87	2.37
Nb_3SF_7	-4.01	-5.88	1.87	2.09
$\text{In}_2\text{S}_2\text{F}_2$	-5.16	-7.04	1.87	3.23
Co_2I_6	-4.16	-6.04	1.88	2.22
$\text{In}_2\text{Ge}_2\text{Se}_6$	-4.51	-6.39	1.88	2.31

ZrNiSeS	-3.94	-5.83	1.88	2.16
K ₄ Se ₄ S ₈	-3.62	-5.50	1.88	1.90
Ga ₂ I ₆	-4.56	-6.45	1.88	2.32
WAgSeBr ₅	-4.96	-6.85	1.89	2.43
In ₂ Se ₂ Br ₂	-4.77	-6.66	1.89	2.46
ZnSnCl ₂ I ₄	-4.98	-6.87	1.89	2.52
Ag ₂ Te ₄ I ₂	-4.17	-6.05	1.89	2.18
ScInSeSI ₂	-4.55	-6.45	1.89	2.30
Re ₆ Cl ₂ Se ₈	-4.81	-6.71	1.90	2.16
Au ₄ H ₄ S ₄ Br ₄	-5.38	-7.27	1.90	2.33
In ₂ Se ₂ I ₂	-4.66	-6.57	1.90	2.31
Ni ₄ I ₈	-4.79	-6.69	1.91	2.22
In ₂ H ₂ Se ₄	-4.05	-5.96	1.91	2.32
Sc ₂ CCl ₂	-4.40	-6.31	1.91	2.49
WSeS	-3.44	-5.35	1.91	2.19
In ₂ S ₂ I ₂	-4.40	-6.31	1.91	2.37
Au ₂ Cl ₂ S ₄	-5.28	-7.19	1.91	2.43
Re ₆ I ₂ S ₈	-4.76	-6.68	1.92	2.17
K ₄ O ₂	-1.22	-3.14	1.92	1.00
Nb ₂ O ₂ Br ₄	-4.03	-5.95	1.92	1.61
Au ₄ Te ₄ Cl ₄	-4.88	-6.80	1.92	2.29
HfZrPd ₂ S ₄ I ₄	-4.43	-6.36	1.93	2.17
Au ₂ SeO ₄	-4.66	-6.58	1.93	2.81
Na ₂ Ta ₂ I ₁₂	-4.38	-6.31	1.93	2.26
Zr ₂ Sn ₂ S ₈	-3.86	-5.80	1.94	2.39
In ₆ I ₆	-3.41	-5.35	1.94	2.20
Si ₄ Te ₈	-3.46	-5.40	1.94	2.11
Ge ₂ IClO ₃	-4.15	-6.10	1.95	3.05
MoSeS	-3.72	-5.66	1.95	2.19

OsH ₂ O ₂	-1.28	-3.23	1.95	2.82
Nb ₂ O ₂ Cl ₄	-4.31	-6.26	1.95	1.78
Zr ₂ Ge ₂ S ₈	-3.90	-5.86	1.95	2.40
P ₂ Se ₅	-3.79	-5.74	1.96	2.38
Si ₄ Se ₈	-3.54	-5.49	1.96	2.35
Ag ₆ I ₁₂	-4.57	-6.53	1.96	2.23
Re ₆ F ₂ Se ₈	-4.66	-6.62	1.96	2.35
MoW ₃ O ₈	-4.84	-6.80	1.96	2.99
Li ₂ Ta ₂ I ₁₂	-4.36	-6.32	1.96	2.26
Pd ₄ P ₄ Se ₄	-4.34	-6.31	1.96	2.00
In ₂ Se ₂	-4.39	-6.35	1.96	2.23
In ₈ BrClS ₄ I ₆	-4.37	-6.33	1.97	2.37
Rh ₂ I ₆	-4.10	-6.06	1.97	2.12
Y ₂ CF ₂	-2.75	-4.72	1.97	2.22
Ni ₃ P ₂ Se ₈	-4.80	-6.78	1.98	2.27
V ₂ ClO ₂ Br ₃	-3.93	-5.91	1.98	2.73
Hf ₂ Sn ₂ S ₈	-3.83	-5.81	1.98	2.39
AgBiP ₂ Se ₆	-4.24	-6.22	1.98	2.31
BiSBr	-5.32	-7.30	1.98	2.51
BiSeF	-4.83	-6.81	1.98	3.09
Na ₄ Au ₄ Se ₄	-2.29	-4.28	1.98	2.08
In ₃ I ₃	-3.24	-5.23	1.98	2.20
MgAl ₂ Se ₄	-3.44	-5.42	1.98	2.27
Sn ₂ S ₂	-3.04	-5.02	1.99	2.36
Ag ₂ F ₂ S ₄	-4.98	-6.97	1.99	2.80
Au ₄ Se ₄ Br ₄	-5.18	-7.17	1.99	2.29
BiSeCl	-5.31	-7.30	1.99	2.53
GeTe	-3.28	-5.27	1.99	2.10
Au ₄ S ₄ Br ₄	-5.40	-7.40	2.00	2.33

Pt ₂ Te ₄	-3.63	-5.63	2.00	1.93
Ga ₂ Se ₂ I ₂	-4.19	-6.19	2.00	2.32
WSeO	-3.50	-5.50	2.00	2.56
RhGaO ₂ Cl ₂	-4.61	-6.61	2.00	2.77
LiCoP ₂ Se ₆	-4.36	-6.36	2.00	2.30
Hf ₂ Ge ₂ S ₈	-3.84	-5.84	2.01	2.40
Sc ₂ CH ₂	-3.40	-5.41	2.01	1.77
Au ₂ S ₂	-4.53	-6.54	2.01	2.18
Rb ₂ Li ₂ Se ₂	-0.83	-2.84	2.01	1.10
Pd ₂ Br ₄	-5.02	-7.03	2.01	2.25
SrHOI	-2.85	-4.86	2.02	1.77
PtSeS	-4.34	-6.36	2.02	2.15
Pd ₄ I ₈	-4.67	-6.69	2.02	2.05
Ni ₄ P ₄ Se ₄	-4.67	-6.69	2.02	2.19
Sc ₂ Se ₄ Br ₄	-4.46	-6.48	2.02	2.46
Mg ₂ Al ₂ Se ₅	-3.37	-5.40	2.02	2.27
Ga ₂ Si ₂ Se ₆	-4.29	-6.32	2.03	2.32
Si ₂ Cl ₂	-4.30	-6.33	2.03	2.58
Ti ₂ Se ₄ I ₄	-3.87	-5.90	2.03	2.27
Al ₄ Se ₆	-4.47	-6.50	2.03	2.28
In ₂ Se ₃	-4.31	-6.35	2.04	2.30
Y ₂ Se ₄ Br ₄	-4.61	-6.65	2.04	1.73
Ge ₄ P ₈	-3.95	-5.99	2.04	2.19
Pd ₂ Se ₄	-4.04	-6.09	2.05	2.06
CuInP ₂ Se ₆	-4.41	-6.47	2.05	2.33
Cs ₂ Na ₂ Te ₂	-0.89	-2.94	2.05	0.99
K ₂ Ta ₂ I ₁₂	-4.41	-6.46	2.05	1.74
In ₂ Te ₂ I ₂	-4.34	-6.39	2.05	2.19
In ₂ Se ₂	-4.31	-6.37	2.06	2.23

Ag ₂ Te ₄ Br ₂	-4.16	-6.22	2.06	2.26
WS ₂	-3.61	-5.67	2.06	2.25
CuBiP ₂ Se ₆	-4.30	-6.36	2.06	2.33
W ₂ Mo ₂ S ₈	-3.77	-5.83	2.06	2.25
Ag ₂ I ₂ Br ₄	-4.81	-6.88	2.06	2.41
MoW ₃ S ₈	-3.69	-5.75	2.06	2.25
Ir ₂ S ₂ Br ₂	-3.94	-6.01	2.07	2.25
Ir ₂ Se ₂ Br ₂	-3.81	-5.88	2.07	2.20
Sc ₂ CF ₂	-3.29	-5.36	2.07	3.32
Ag ₄ Se ₂	-4.25	-6.32	2.07	2.15
WMo ₃ S ₈	-3.83	-5.91	2.08	2.25
Ga ₂ Si ₂ Se ₂	-3.86	-5.93	2.08	2.15
SiSe ₂	-3.35	-5.43	2.08	2.35
In ₈ Se ₁₂	-3.98	-6.06	2.08	2.30
Ti ₂ N ₂ Br ₂	-4.68	-6.76	2.08	2.55
Al ₂ Te ₂	-3.05	-5.14	2.09	2.04
Rb ₂ Li ₂ S ₂	-0.77	-2.86	2.09	1.18
Zr ₂ GeOI ₂ Br ₂ Se ₃	-4.93	-7.02	2.09	2.46
SnTe	-3.23	-5.32	2.09	2.05
Cs ₄ S ₂	-0.85	-2.93	2.09	0.84
Pd ₄ P ₄ S ₄	-4.46	-6.55	2.09	2.05
Ti ₂ N ₂ Cl ₂	-4.89	-6.99	2.09	2.63
Cu ₂ N ₂ Br ₂ C ₆ F ₈	-4.97	-7.06	2.09	3.33
Au ₄ H ₄ S ₄ Cl ₄	-5.51	-7.60	2.10	2.38
TiF ₂	-2.95	-5.04	2.10	3.68
Ge ₂ P ₂ S ₆	-4.06	-6.16	2.10	2.47
WO ₂	-4.64	-6.74	2.10	2.99
Ag ₂ Te ₄ Cl ₂	-4.13	-6.23	2.10	2.30
Re ₄ O ₈	-5.07	-7.17	2.10	2.94

$\text{Cu}_2\text{I}_2\text{Se}_4$	-4.62	-6.72	2.10	2.32
$\text{Ir}_2\text{S}_2\text{F}_2$	-4.32	-6.43	2.10	2.77
$\text{Al}_2\text{Si}_2\text{Te}_2$	-3.15	-5.26	2.11	1.98
AuInF_4	-4.87	-6.98	2.11	3.52
Bi_2I_6	-4.74	-6.84	2.11	2.31
Hf_2S_6	-4.41	-6.52	2.11	2.41
$\text{In}_2\text{Si}_2\text{Se}_6$	-4.31	-6.43	2.11	2.31
$\text{Rh}_2\text{Te}_2\text{F}_2$	-4.19	-6.31	2.12	2.61
$\text{In}_4\text{O}_4\text{Br}_4$	-5.68	-7.79	2.12	2.94
HfTi_3S_8	-5.23	-7.35	2.12	2.33
$\text{Ti}_2\text{BrClN}_2$	-4.77	-6.88	2.12	2.59
Pt_2Br_4	-4.35	-6.47	2.12	2.29
PtSnS_4	-4.63	-6.75	2.12	2.31
$\text{Ir}_2\text{BrClS}_2$	-3.97	-6.10	2.13	2.28
ZrHf_3S_8	-4.78	-6.91	2.13	2.34
ZrHf_3S_8	-5.39	-7.53	2.13	2.34
$\text{Rh}_2\text{S}_2\text{Br}_2$	-4.42	-6.55	2.14	2.21
$\text{Pd}_2\text{Br}_2\text{F}_2$	-5.36	-7.50	2.14	2.72
MgIn_2S_4	-4.35	-6.49	2.14	2.43
Si_2S_2	-3.64	-5.78	2.14	2.39
Bi_2Br_6	-5.44	-7.58	2.14	2.59
$\text{Rh}_2\text{Se}_2\text{Br}_2$	-4.27	-6.41	2.14	2.16
$\text{Cs}_2\text{Na}_2\text{Se}_2$	-0.83	-2.97	2.14	1.10
$\text{ZrNbSeIS}_2\text{Br}_2$	-4.66	-6.80	2.14	2.04
HfS_2	-4.74	-6.89	2.15	2.34
$\text{Hf}_2\text{Zr}_2\text{S}_8$	-5.37	-7.52	2.15	2.34
$\text{In}_2\text{Si}_2\text{Se}_2$	-3.89	-6.04	2.15	2.13
MgGa_2S_4	-4.08	-6.23	2.15	2.44
$\text{Ag}_2\text{Te}_3\text{Br}_2\text{P}_4$	-4.20	-6.35	2.15	2.26

CoSeBr	-4.24	-6.39	2.15	2.29
Zr ₂ S ₄	-5.32	-7.48	2.15	2.33
Sc ₂ P ₂ Se ₈	-4.22	-6.38	2.15	2.31
Sc ₂ Se ₂ F ₂	-3.14	-5.30	2.16	3.08
TiZr ₃ S ₈	-5.24	-7.40	2.16	2.33
Ga ₂ Te ₂ I ₂	-4.01	-6.17	2.16	2.20
HfZr ₃ S ₈	-5.35	-7.50	2.16	2.33
Pt ₂ F ₂	-5.62	-7.78	2.17	2.79
Cu ₂ Te ₄ I ₂	-4.13	-6.29	2.17	2.22
ZrS ₂	-4.81	-6.97	2.17	2.34
Au ₂ I ₂ Se ₃ P ₄	-3.81	-5.98	2.17	2.23
Ir ₂ Se ₂ F ₂	-4.03	-6.20	2.17	2.72
Ni ₄ P ₄ S ₄	-4.64	-6.82	2.17	2.24
V ₂ S ₄ Br ₄	-3.68	-5.85	2.17	2.47
Ni ₄ Br ₈	-5.09	-7.26	2.17	2.41
Rh ₂ S ₂ F ₂	-4.76	-6.93	2.18	2.72
Sn ₂ I ₄	-3.70	-5.88	2.18	2.27
Pd ₂ Se ₂ O ₆	-4.07	-6.26	2.18	2.87
Ni ₂ Se ₄	-4.26	-6.45	2.18	2.24
AlSeI	-3.96	-6.15	2.19	2.29
Al ₂ Si ₂ Se ₂	-3.27	-5.46	2.19	2.12
Pt ₂ Se ₂ O ₆	-3.22	-5.41	2.19	2.90
Ti ₂ S ₂ O ₂	-4.56	-6.75	2.19	2.75
LiGaP ₂ Se ₆	-4.24	-6.43	2.19	2.35
Pd ₂ F ₂	-6.80	-8.99	2.19	2.73
Al ₂ IBrS ₂	-3.84	-6.04	2.19	2.44
Zr ₂ S ₆	-4.33	-6.54	2.20	2.40
Ag ₂ Te ₃ Cl ₂ P ₄	-4.18	-6.38	2.20	2.30
Cu ₂ Br ₂ S ₄	-5.19	-7.39	2.20	2.47

$\text{Ir}_2\text{S}_2\text{Cl}_2$	-4.02	-6.22	2.20	2.32
$\text{In}_2\text{Si}_2\text{S}_2$	-4.21	-6.42	2.21	2.23
OsI_2	-2.66	-4.87	2.21	2.10
In_3F_3	-3.02	-5.23	2.21	3.60
Pt_4I_8	-3.99	-6.21	2.21	2.09
$\text{Bi}_8\text{O}_4\text{S}_8$	-3.75	-5.96	2.21	2.68
$\text{Zr}_2\text{Br}_2\text{S}_3$	-5.04	-7.26	2.22	2.42
AuBiP_2S_6	-4.39	-6.60	2.22	2.40
$\text{Sc}_2\text{Te}_2\text{I}_2$	-3.28	-5.50	2.22	2.11
SiS_2	-4.81	-7.03	2.22	2.49
SnO	-4.10	-6.32	2.22	3.04
TiSe_2	-4.17	-6.39	2.22	2.19
Sn_2Se_2	-3.22	-5.45	2.22	2.24
$\text{Ni}_2\text{Te}_2\text{O}_6$	-3.47	-5.69	2.22	2.95
$\text{Zn}_2\text{P}_2\text{Se}_6$	-3.90	-6.12	2.22	2.47
$\text{Ag}_2\text{I}_2\text{S}_4$	-4.31	-6.54	2.22	2.35
$\text{Al}_2\text{Se}_2\text{Cl}_2$	-3.53	-5.76	2.23	2.54
$\text{Ga}_2\text{S}_2\text{Cl}_2$	-4.78	-7.01	2.23	2.62
$\text{Au}_4\text{Se}_4\text{Cl}_4$	-5.27	-7.50	2.23	2.35
Ni_2S_4	-4.38	-6.61	2.23	2.33
Pt_2Cl_2	-4.41	-6.64	2.23	2.21
Au_6I_6	-3.61	-5.85	2.23	2.12
$\text{V}_2\text{S}_4\text{Cl}_4$	-3.65	-5.88	2.23	2.57
$\text{Ir}_2\text{Se}_2\text{Cl}_2$	-3.82	-6.06	2.24	2.27
$\text{Si}_4\text{Te}_4\text{P}_4$	-3.22	-5.46	2.24	2.15
$\text{Al}_2\text{Se}_2\text{I}_2$	-3.93	-6.17	2.24	2.29
$\text{Ag}_2\text{Br}_2\text{S}_4$	-4.79	-7.03	2.24	2.42
$\text{Zr}_2\text{Se}_4\text{I}_4$	-3.92	-6.16	2.24	2.27
ZrOBr_2	-4.53	-6.78	2.25	2.77

Mg ₂ Ga ₂ S ₅	-3.94	-6.19	2.25	2.44
Sn ₂ N ₂ Br ₂	-4.77	-7.02	2.25	2.70
In ₂ Se ₂	-3.54	-5.80	2.25	2.23
BiSF	-5.08	-7.33	2.26	3.15
Pt ₂ Br ₂ Cl ₂	-4.42	-6.68	2.26	2.35
IrSeBr	-3.47	-5.73	2.26	2.21
WSO	-3.73	-5.99	2.26	2.62
Ta ₂ S ₄ I ₄	-3.34	-5.60	2.26	2.31
Cu ₄ O ₄ F ₄	-8.13	-10.39	2.26	3.16
Ga ₂ Se ₂	-3.48	-5.73	2.26	2.26
Ag ₂ Br ₂ Se ₄	-4.57	-6.83	2.26	2.36
Ga ₂ S ₂ Br ₂	-4.73	-6.99	2.27	2.54
Ti ₂ Se ₄ Br ₄	-3.83	-6.10	2.27	2.43
Mg ₂ In ₂ S ₅	-4.10	-6.37	2.27	2.42
Rh ₂ S ₂ Cl ₂	-4.52	-6.79	2.27	2.27
Cu ₂ F ₂ Se ₄	-4.68	-6.95	2.27	2.78
Re ₆ Br ₂ S ₈	-4.87	-7.14	2.27	2.22
BiSCl	-5.42	-7.69	2.27	2.59
Rh ₂ Se ₂ Cl ₂	-4.31	-6.58	2.27	2.22
TaAgGeCl ₂ S ₄	-4.74	-7.01	2.27	2.45
In ₂ S ₂ I ₂	-4.43	-6.71	2.28	2.37
Nb ₂ S ₄ I ₄	-3.49	-5.78	2.28	1.77
AgGaP ₂ S ₆	-4.32	-6.61	2.29	2.42
In ₂ Se ₅	-3.63	-5.92	2.29	2.34
Ag ₆ I ₈	-4.24	-6.53	2.29	2.20
Li ₄ P ₄ S ₈	-3.89	-6.18	2.29	2.47
Ga ₂ Se ₂ Br ₂	-4.43	-6.73	2.29	2.47
Pd ₂ S ₂ O ₆	-4.80	-7.10	2.29	2.90
Nb ₂ I ₂ O ₄	-3.95	-6.24	2.30	2.12

Pt ₂ Se ₄	-3.77	-6.07	2.30	2.11
In ₄ SiClBr ₂ Se ₃	-4.79	-7.09	2.30	2.46
Si ₄ P ₈	-3.87	-6.16	2.30	2.19
Cu ₂ Te ₄ Br ₂	-4.14	-6.44	2.30	2.30
Cu ₂ I ₂ Se ₃ P ₄	-4.16	-6.46	2.30	2.30
Li ₂ V ₂ Au ₄ O ₁₂	-5.18	-7.48	2.30	2.89
RuI ₂	-3.08	-5.38	2.30	2.06
Pt ₄ In ₂ S ₆	-3.58	-5.89	2.31	2.12
Cu ₂ N ₂ Cl ₂ C ₆ F ₈	-5.01	-7.31	2.31	3.35
Cu ₂ Te ₄ Cl ₂	-4.15	-6.46	2.31	2.34
FeGa ₂ S ₄	-3.32	-5.63	2.31	2.34
Ba ₂ Bi ₄ S ₈	-3.31	-5.62	2.31	1.49
Re ₆ Cl ₂ S ₈	-4.93	-7.25	2.32	2.24
Al ₂ Se ₂ Br ₂	-3.63	-5.96	2.32	2.44
Cu ₆ Cl ₆	-4.80	-7.12	2.32	2.46
Pt ₂ S ₂ O ₆	-3.71	-6.03	2.32	2.93
Ti ₂ Se ₄ Cl ₄	-3.78	-6.10	2.33	2.52
Au ₄ Br ₄	-4.16	-6.49	2.33	2.25
Ta ₂ S ₄ F ₄	-3.35	-5.68	2.33	3.21
Ti ₂ N ₂ F ₂	-4.68	-7.00	2.33	3.25
Ga ₂ Ge ₂ S ₆	-4.35	-6.68	2.33	2.46
Au ₂ Ag ₂ Cl ₈	-5.63	-7.96	2.33	2.50
Hf ₂ Br ₂ S ₃	-4.93	-7.27	2.34	2.43
FeAl ₂ Se ₄	-2.74	-5.08	2.34	2.20
AgAlP ₂ Se ₆	-3.77	-6.11	2.34	2.30
Hf ₂ Se ₄ I ₄	-3.77	-6.12	2.35	2.27
W ₂ O ₄ Br ₄	-5.24	-7.59	2.35	2.87
Au ₄ S ₄ Cl ₄	-5.53	-7.88	2.35	2.39
In ₄ Br ₄	-3.22	-5.57	2.35	2.45

AgGaI ₂	-3.47	-5.83	2.35	2.20
In ₂ S ₂	-4.49	-6.84	2.35	2.37
Ba ₄ Bi ₄ F ₄ S ₈	-3.80	-6.16	2.35	2.16
Al ₂ Se ₂	-3.23	-5.59	2.36	2.24
FeAl ₂ S ₄	-2.83	-5.19	2.36	2.32
SnS ₂	-5.02	-7.38	2.36	2.47
Al ₂ Te ₂	-3.30	-5.66	2.36	2.04
Cu ₂ Cl ₂ S ₄	-5.22	-7.58	2.36	2.51
Li ₂ Au ₂ Se ₂	-3.76	-6.12	2.36	2.07
AgInP ₂ S ₆	-4.27	-6.64	2.37	2.42
IrCoClBr ₅	-4.38	-6.75	2.37	2.44
GaP	-3.43	-5.80	2.37	2.12
Pd ₄ Br ₈	-4.95	-7.32	2.37	2.25
Ga ₂ Se ₂	-3.87	-6.24	2.37	2.26
Sn ₂ N ₂ Cl ₂	-4.97	-7.34	2.37	2.79
Ge ₂ S ₂	-3.13	-5.51	2.37	2.41
Bi ₄ B ₄ S ₁₂	-3.88	-6.26	2.38	2.46
Re ₆ F ₂ S ₈	-4.88	-7.26	2.38	2.43
HfPdIClBr ₄	-4.91	-7.29	2.39	2.41
Pd ₃ P ₂ Se ₈	-4.37	-6.75	2.39	2.13
Ga ₂ S ₃	-3.77	-6.16	2.39	2.46
Sc ₂ S ₄ Cl ₄	-4.56	-6.95	2.39	2.63
Sc ₂ S ₄ Br ₄	-4.58	-6.97	2.39	2.54
LiCoP ₂ S ₆	-4.59	-6.98	2.40	2.41
In ₂ I ₆	-4.32	-6.72	2.40	2.31
Sr ₄ P ₄ F ₄ Se ₈	-3.84	-6.23	2.40	2.27
Au ₄ O ₄ F ₄	-6.65	-9.05	2.40	3.06
K ₂ Li ₂ S ₂	-0.78	-3.18	2.40	2.32
Ta ₂ S ₄ Br ₄	-3.32	-5.73	2.40	2.47

$\text{Al}_2\text{Ge}_2\text{Se}_6$	-3.96	-6.37	2.41	2.30
$\text{NaGaP}_2\text{Se}_6$	-4.08	-6.49	2.41	2.35
$\text{Li}_2\text{Cu}_2\text{Se}_2$	-2.24	-4.65	2.42	2.24
$\text{Ag}_2\text{Cl}_2\text{Se}_4$	-4.60	-7.02	2.42	2.41
$\text{Ta}_2\text{S}_4\text{Cl}_4$	-3.34	-5.76	2.42	2.56
Ga_2O_2	-5.38	-7.80	2.42	3.16
$\text{Cu}_2\text{Cl}_2\text{Se}_4$	-4.75	-7.17	2.42	2.45
OsBr_2	-2.63	-5.06	2.42	2.31
$\text{In}_2\text{Al}_2\text{Se}_6$	-4.08	-6.50	2.42	2.29
$\text{Y}_2\text{S}_4\text{Cl}_4$	-4.68	-7.11	2.43	1.94
Sn_4S_4	-2.90	-5.33	2.43	2.36
$\text{In}_2\text{Ge}_2\text{S}_6$	-4.46	-6.89	2.43	2.45
$\text{Y}_2\text{Se}_2\text{F}_2$	-4.42	-6.85	2.43	2.09
In_2S_2	-4.43	-6.86	2.43	2.37
$\text{Ga}_4\text{Te}_4\text{I}_4$	-3.82	-6.25	2.43	2.20
$\text{Ge}_4\text{P}_4\text{Se}_4$	-3.75	-6.18	2.43	2.28
$\text{Al}_2\text{S}_2\text{I}_2$	-3.63	-6.07	2.43	2.37
GeS_2	-3.99	-6.43	2.43	2.50
$\text{Pt}_4\text{P}_4\text{Se}_4$	-3.85	-6.29	2.44	2.04
Ge_2Se_2	-3.24	-5.67	2.44	2.29
Ga_2ICl	-2.60	-5.04	2.44	2.42
$\text{Al}_2\text{S}_2\text{I}_2$	-4.05	-6.49	2.44	2.37
$\text{Al}_8\text{Te}_{12}$	-2.89	-5.34	2.44	2.06
$\text{Ag}_2\text{F}_2\text{Se}_4$	-4.16	-6.60	2.44	2.74
$\text{Y}_2\text{S}_4\text{Br}_4$	-4.67	-7.11	2.44	1.77
$\text{In}_4\text{Te}_4\text{I}_4$	-3.96	-6.40	2.44	2.19
PdPt_3O_8	-5.68	-8.13	2.45	2.78
Ir_2I_6	-3.44	-5.89	2.45	2.15
$\text{Zr}_2\text{Se}_4\text{Br}_4$	-3.86	-6.31	2.45	2.43

LiInP ₂ Se ₆	-4.02	-6.47	2.45	2.35
Al ₄ Se ₆	-3.26	-5.72	2.46	2.28
Nb ₂ S ₄ Br ₄	-3.48	-5.94	2.47	1.58
Au ₄ Te ₂ O ₁₂	-6.33	-8.79	2.47	2.96
Ga ₂ O ₂	-5.32	-7.80	2.47	3.16
In ₂ Te ₂ Br ₂	-4.51	-6.98	2.47	2.34
Co ₂ F ₂ O ₄	-6.52	-9.00	2.47	3.22
Ti ₂ S ₄ Br ₄	-4.08	-6.56	2.48	2.50
PtS ₂	-4.39	-6.87	2.49	2.20
Ge ₂ S ₂	-3.28	-5.76	2.49	2.41
SnI ₂	-3.83	-6.32	2.49	2.28
Nb ₂ S ₄ F ₄	-3.38	-5.87	2.50	2.69
Ag ₆ I ₆	-3.73	-6.22	2.50	2.18
Cu ₂ N ₂ I ₂ C ₆ H ₈	-3.27	-5.77	2.50	2.46
SnI ₂	-3.79	-6.30	2.50	2.28
IrSCl	-3.70	-6.20	2.51	2.32
Be ₄ Te ₄	-2.44	-4.95	2.51	2.03
Ga ₂ Se ₂	-3.76	-6.26	2.51	2.26
ZrSe ₂	-4.08	-6.59	2.51	2.19
SnS ₂	-4.37	-6.88	2.51	2.47
Pd ₂ Te ₂ O ₆	-3.50	-6.01	2.51	2.84
In ₄ S ₆	-4.75	-7.26	2.51	2.44
Zr ₂ S ₄ I ₄	-4.05	-6.56	2.51	2.34
Sn ₂ S ₂	-2.99	-5.51	2.52	2.36
Hf ₂ Se ₄ Br ₄	-3.75	-6.27	2.52	2.43
Ti ₂ S ₄ Cl ₄	-4.06	-6.58	2.52	2.59
ZnGeSBr ₂	-4.04	-6.57	2.52	2.59
Nb ₂ S ₄ Cl ₄	-3.45	-5.98	2.53	2.17
Cu ₂ N ₂ Br ₂ H ₄ C ₄	-3.56	-6.09	2.53	2.53

Ag ₄ S ₆	-3.28	-5.81	2.53	2.31
Pt ₄ Br ₈	-4.21	-6.75	2.54	2.29
Hf ₂ Se ₄ Cl ₄	-3.79	-6.32	2.54	2.53
Ge ₂ N ₂ Br ₂	-4.66	-7.20	2.54	2.73
Zr ₂ Se ₄ Cl ₄	-3.82	-6.36	2.54	2.53
K ₂ Au ₂ Se ₂	-1.39	-3.93	2.54	1.44
RuBr ₂	-3.11	-5.65	2.54	2.28
Ba ₄ P ₄ F ₄ Se ₈	-3.75	-6.30	2.55	2.18
Ni ₂ Se ₂ O ₆	-3.83	-6.39	2.55	2.98
Cu ₂ Br ₂ Se ₃ P ₄	-4.28	-6.83	2.56	2.36
In ₂ S ₅	-3.65	-6.20	2.56	2.49
Zn ₂ Te ₂ N ₄ H ₈	-0.79	-3.36	2.57	2.63
InGaS ₂	-4.29	-6.86	2.57	2.38
Ga ₄ S ₆	-4.68	-7.25	2.57	2.46
FeAl ₂ S ₄	-2.57	-5.14	2.58	2.32
In ₄ S ₆	-4.83	-7.41	2.58	2.44
AuInS ₂ Cl ₂	-4.91	-7.50	2.58	2.48
Au ₂ I ₂	-2.62	-5.21	2.59	2.12
K ₄ Cu ₄ Te ₄	-1.95	-4.54	2.59	1.48
Sn ₂ I ₂ Br ₂	-3.66	-6.25	2.59	2.41
CuBiP ₂ S ₆	-4.36	-6.95	2.59	2.44
ZnI ₂	-3.84	-6.44	2.60	2.49
Co ₂ H ₂ O ₄	-3.53	-6.13	2.60	2.88
Al ₂ Te ₂	-3.04	-5.63	2.60	2.04
ZrFeI ₆	-3.60	-6.20	2.60	2.22
Ba ₄ Bi ₄ Cl ₄ S ₈	-3.35	-5.95	2.60	1.88
In ₄ Se ₄ I ₄	-4.16	-6.76	2.60	2.30
Pd ₂ F ₄	-5.76	-8.36	2.61	3.19
Mo ₂ F ₆	-4.57	-7.18	2.61	3.69

NaInP ₂ Se ₆	-3.90	-6.51	2.61	2.35
Sn ₄ O ₄	-2.72	-5.33	2.61	3.05
MoCu ₂ S ₄	-4.23	-6.84	2.62	2.30
Ag ₄ S ₂	-3.96	-6.58	2.62	2.19
Ga ₈ Se ₁₂	-3.41	-6.03	2.62	2.32
In ₂ Te ₂ Cl ₂	-4.55	-7.17	2.62	2.43
Sc ₂ I ₆	-3.46	-6.09	2.63	2.25
Zn ₂ Se ₂	-3.77	-6.40	2.63	2.57
HfSe ₂	-4.03	-6.66	2.63	2.19
P ₈ S ₁₂	-3.52	-6.17	2.64	2.49
In ₂ Te ₂ F ₂	-4.10	-6.74	2.65	3.06
In ₂ S ₂ Cl ₂	-4.69	-7.34	2.65	2.61
Ag ₂ Br ₂ Se ₃ P ₄	-4.13	-6.78	2.65	2.33
Pt ₄ P ₄ S ₄	-3.88	-6.53	2.65	2.10
In ₂ Si ₂ S ₆	-4.27	-6.93	2.66	2.46
Pd ₂ Se ₂ O ₆	-3.94	-6.60	2.66	2.87
Hf ₂ N ₂ I ₂	-3.55	-6.22	2.66	2.42
In ₂ S ₂	-3.53	-6.19	2.66	2.37
GeI ₂	-3.63	-6.30	2.67	2.30
CoSCl	-4.54	-7.21	2.67	2.40
Cu ₂ Cl ₂ Se ₃ P ₄	-4.32	-7.00	2.68	2.40
Mo ₂ O ₄ Br ₄	-5.00	-7.68	2.68	2.86
Ag ₂ Cl ₂ Br ₄	-4.88	-7.57	2.68	2.52
In ₂ BrClS ₂	-4.61	-7.29	2.69	2.57
In ₄ S ₆	-3.94	-6.63	2.69	2.44
In ₈ S ₁₂	-4.12	-6.82	2.69	2.44
Cu ₂ I ₂ S ₃ P ₄	-3.93	-6.62	2.69	2.34
P ₄ S ₆	-3.69	-6.39	2.70	2.49
Ge ₂ BrClSe ₂	-4.00	-6.69	2.70	2.51

P_4Se_6	-3.17	-5.87	2.70	2.37
$Sc_2Se_2I_2$	-3.59	-6.29	2.70	2.22
$Sc_2Se_2Cl_2$	-3.79	-6.49	2.70	2.46
$In_2Se_2Br_2$	-4.97	-7.68	2.70	2.46
Sn_6O_6	-2.61	-5.32	2.71	3.05
Al_2S_2	-3.23	-5.94	2.71	2.37
$Na_2PdH_6S_6$	-3.41	-6.12	2.71	2.35
$OsCl_2$	-2.59	-5.30	2.71	2.44
$IrInI_3Br_3$	-3.86	-6.58	2.72	2.36
$In_2H_2S_4$	-3.81	-6.53	2.72	2.46
Zn_2S_4	-2.97	-5.69	2.72	2.61
Al_2Se_2	-3.59	-6.31	2.72	2.24
$In_2S_2Br_2$	-4.51	-7.23	2.73	2.52
$Ga_2Al_2Se_6$	-3.85	-6.58	2.73	2.30
$Zr_2S_4Br_4$	-4.01	-6.74	2.73	2.50
$Pt_2Se_2O_6$	-3.12	-5.85	2.73	2.90
$Pd_2I_4O_{12}$	-4.36	-7.09	2.73	3.04
P_2	-3.92	-6.65	2.73	2.25
$InGaS_2Br_2$	-4.47	-7.21	2.74	2.53
$Ga_2Te_2Br_2$	-4.09	-6.83	2.74	2.36
Al_2SeSBr_2	-3.56	-6.29	2.74	2.48
TiS_2	-4.41	-7.15	2.74	2.33
Rh_2Br_6	-4.30	-7.04	2.74	2.36
Ga_2S_5	-3.54	-6.28	2.74	2.50
$Ga_4Te_4Br_4$	-3.97	-6.72	2.75	2.36
$K_4Se_4O_8$	-2.32	-5.07	2.75	2.37
$Sn_4I_4F_4$	-3.71	-6.47	2.75	3.05
$Zr_2N_2Br_2$	-4.21	-6.97	2.76	2.56
Ga_2S_2	-3.39	-6.14	2.76	2.40

Zn ₂ P ₄ S ₈	-3.72	-6.48	2.76	2.54
In ₄ Te ₄ Br ₄	-4.06	-6.82	2.76	2.34
GaAlSe ₂	-3.50	-6.27	2.77	2.23
Sc ₂ SeSI ₂	-3.68	-6.45	2.77	2.26
ScAgP ₂ Se ₆	-3.55	-6.32	2.78	2.29
Pt ₂ F ₄	-4.68	-7.46	2.78	3.22
Ag ₂ I ₂	-3.38	-6.16	2.78	2.18
Pt ₂ S ₄	-3.56	-6.35	2.79	2.20
SnSe	-3.38	-6.17	2.79	2.23
Ge ₄ P ₄ S ₄	-3.79	-6.58	2.79	2.36
In ₄ S ₄ I ₄	-4.07	-6.86	2.79	2.38
SiS ₂	-3.51	-6.30	2.79	2.49
Zr ₂ S ₄ Cl ₄	-3.99	-6.79	2.79	2.60
HfFeI ₆	-3.37	-6.17	2.80	2.22
K ₂ PdH ₆ S ₆	-3.30	-6.09	2.80	1.22
Cs ₂ C ₆ N ₆ Se ₆	-3.39	-6.20	2.81	2.28
GeO	-4.27	-7.08	2.81	3.10
Ni ₂ Se ₂ O ₆	-3.74	-6.56	2.82	2.98
Sc ₂ Se ₂ Br ₂	-3.72	-6.54	2.82	2.37
Ga ₄ Se ₄ I ₄	-3.69	-6.52	2.82	2.32
Bi ₂ Br ₆	-5.00	-7.82	2.82	2.59
RuCl ₂	-3.12	-5.94	2.82	2.41
Ga ₂ Te ₂ F ₂	-3.98	-6.81	2.83	3.07
CuInP ₂ S ₆	-4.19	-7.02	2.83	2.44
Si ₄ P ₄ Se ₄	-3.28	-6.11	2.83	2.28
Ga ₄ Se ₄ Br ₄	-4.56	-7.39	2.83	2.47
Al ₂ Se ₂ I ₂	-3.45	-6.28	2.83	2.29
In ₂ Ga ₂ S ₆	-4.60	-7.43	2.83	2.45
Zr ₂ N ₂ Br ₂	-4.98	-7.82	2.83	2.56

In ₂ S ₂ Br ₂	-5.00	-7.83	2.83	2.52
Y ₂ O ₂ I ₂	-3.10	-5.93	2.83	1.68
In ₄ Te ₄ Cl ₄	-4.40	-7.24	2.84	2.44
Ag ₅ I ₅	-3.33	-6.17	2.84	2.18
Pd ₂ S ₂ O ₆	-4.47	-7.32	2.85	2.90
Si ₂ H ₂	-2.71	-5.57	2.86	1.84
W ₂ O ₆	-6.91	-9.78	2.87	3.18
Al ₂ Se ₂	-3.42	-6.28	2.87	2.24
Ga ₄ Te ₄ Cl ₄	-4.16	-7.03	2.87	2.45
PdO ₂	-5.93	-8.80	2.88	2.75
Pd ₃ P ₂ S ₈	-4.53	-7.41	2.88	2.23
Hf ₂ S ₄ Br ₄	-3.82	-6.70	2.88	2.51
Al ₂ S ₂	-3.87	-6.75	2.88	2.37
In ₄ Cl ₈	-4.58	-7.47	2.88	2.74
Zn ₂ I ₂	-3.11	-5.99	2.88	2.55
Hf ₂ SeSI ₄	-3.67	-6.56	2.88	2.26
Ni ₃ P ₂ S ₈	-4.69	-7.58	2.89	2.36
Ga ₄ Te ₄ Cl ₄	-3.99	-6.88	2.89	2.45
Ga ₂ Te ₂ Cl ₂	-4.16	-7.05	2.89	2.45
Ir ₂ Br ₆	-3.55	-6.44	2.89	2.39
P ₄ Se ₆	-3.29	-6.18	2.90	2.37
In ₃ SeSBr ₅	-4.76	-7.66	2.90	2.54
In ₂ Te ₂ H ₂ S ₈	-3.66	-6.56	2.90	2.46
Ag ₄ S ₂	-3.63	-6.54	2.91	2.19
Ag ₂ Ge ₂ I ₆	-3.47	-6.38	2.91	2.24
Al ₂ Ge ₂ S ₆	-3.73	-6.64	2.91	2.44
Na ₂ Nb ₂ Br ₁₂	-4.63	-7.55	2.91	2.12
GeSe	-3.31	-6.22	2.92	2.28
In ₄ Te ₄ Cl ₄	-4.01	-6.92	2.92	2.44

Sc ₂ SeSCl ₂	-3.92	-6.84	2.92	2.50
LiAlP ₂ Se ₆	-3.56	-6.48	2.92	2.34
Li ₂ S ₂ F ₂	-3.06	-5.99	2.92	3.40
Au ₂ Br ₂	-2.97	-5.90	2.93	2.25
Cs ₄ Cu ₄ Se ₄	-1.14	-4.07	2.93	1.55
Al ₂ H ₂ S ₄	-3.13	-6.06	2.93	2.45
Sr ₄ P ₄ F ₄ S ₈	-3.63	-6.56	2.94	2.34
LiNbBr ₆	-4.84	-7.78	2.94	1.90
Al ₂ Te ₂ I ₂	-3.42	-6.36	2.94	2.18
Sc ₄ S ₆	-2.96	-5.90	2.94	2.33
Al ₂ S ₂	-3.77	-6.71	2.95	2.37
Hf ₂ S ₄ Cl ₄	-3.80	-6.75	2.95	2.60
Ge ₂ N ₂ Cl ₂	-4.44	-7.39	2.95	2.82
Al ₂ I ₆	-3.49	-6.44	2.96	2.30
K ₂ Cu ₂ Se ₂	-1.50	-4.45	2.96	1.54
Ba ₄ P ₄ F ₄ S ₈	-3.64	-6.60	2.96	2.25
Ag ₂ Br ₂	-4.27	-7.23	2.96	2.31
Mg ₂ P ₂ Se ₆	-3.56	-6.53	2.96	2.34
MgK ₂ Se ₂ H ₄ S ₈	-2.95	-5.91	2.97	1.48
Sr ₂ I ₄ O ₈	-2.00	-4.96	2.97	2.10
Ga ₄ S ₄ I ₄	-3.52	-6.49	2.97	2.39
Ag ₈ S ₄	-3.66	-6.63	2.97	2.19
Pt ₂ S ₂ O ₆	-3.43	-6.41	2.98	2.93
SnS	-3.58	-6.56	2.98	2.34
Cu ₂ Br ₂ S ₃ P ₄	-4.01	-7.00	2.99	2.41
Ag ₂ Cl ₂ Se ₃ P ₄	-4.10	-7.09	2.99	2.37
Al ₂ Si ₂ Se ₆	-3.50	-6.49	2.99	2.30
Li ₆ Te ₂ H ₂ S ₈	-2.91	-5.90	2.99	2.45
Fe ₂ Cu ₂ I ₆	-2.90	-5.90	2.99	2.20

LiGaP ₂ S ₆	-4.13	-7.13	3.00	2.49
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Table S3. Distribution statistics of the screening results based on ΔV (eV) and $\Delta\chi_m$.

Predict Type (Z- scheme)	$\Delta V > 0$	$\Delta V > 0.3$	$\Delta V > 0.6$	$\Delta V > 0.9$	$\Delta V > 1.2$	$\Delta V > 1.5$	$\Delta V > 1.8$	$\Delta V > 2.1$
$\Delta\chi_m > 0$	24471	18834	13562	9069	5444	3150	1643	754
$\Delta\chi_m > 0.1$	18652	14398	10400	6984	4194	2484	1325	612
$\Delta\chi_m > 0.2$	13781	10732	7842	5317	3215	1938	1050	482
$\Delta\chi_m > 0.3$	10093	7974	5887	4068	2504	1511	840	389
$\Delta\chi_m > 0.4$	7412	5935	4450	3138	1994	1226	685	321
$\Delta\chi_m > 0.5$	5489	4426	3351	2409	1558	974	547	262
$\Delta\chi_m > 0.6$	4239	3423	2607	1862	1208	762	429	208
$\Delta\chi_m > 0.7$	3084	2501	1901	1360	881	562	308	140
$\Delta\chi_m > 0.8$	2194	1778	1359	982	637	402	220	103
$\Delta\chi_m > 0.9$	1484	1212	923	656	416	258	128	58
$\Delta\chi_m > 1.0$	954	791	609	437	262	161	78	27
$\Delta\chi_m > 1.1$	643	542	421	311	191	117	59	21
$\Delta\chi_m > 1.2$	411	335	247	180	105	69	38	11
$\Delta\chi_m > 1.3$	264	208	154	110	65	46	23	5
$\Delta\chi_m > 1.4$	151	114	82	60	41	28	15	5
$\Delta\chi_m > 1.5$	87	62	48	37	27	19	10	3

Table S4. 46 potential Z-scheme heterostructure photocatalysts identified through high-throughput screening.

Heterostructure	CBM_A (eV)	VBM_A (eV)	CBM_B (eV)	VBM_B (eV)	ΔV (eV)	$\Delta\chi_m$
Ta ₃ SF ₇ /K ₂ Au ₂ Se ₂	-3.65	-5.45	-1.39	-3.93	1.99	2.13
Ta ₃ SF ₇ /Cs ₄ Cu ₄ Se ₄	-3.65	-5.45	-1.14	-4.07	2.09	2.03
Ta ₃ SeF ₇ /K ₂ Au ₂ Se ₂	-3.57	-5.30	-1.39	-3.93	1.82	2.11
Ta ₃ SeF ₇ /Cs ₄ Cu ₄ Se ₄	-3.57	-5.30	-1.14	-4.07	1.92	2.01
Ta ₃ TeF ₇ /K ₂ Au ₂ Se ₂	-3.46	-5.16	-1.39	-3.93	1.60	2.09
Ta ₃ TeF ₇ /Cs ₄ Cu ₄ Se ₄	-3.46	-5.16	-1.14	-4.07	1.70	1.98
CrMo ₃ O ₈ /Nb ₂ O ₂ Br ₄	-5.85	-7.20	-4.03	-5.95	1.73	1.38
MoCr ₃ S ₈ /Cs ₂ Na ₂ Te ₂	-2.74	-3.77	-0.89	-2.94	1.65	1.31
BiSF/Si ₂ H ₂	-5.08	-7.33	-2.71	-5.57	1.87	1.31
BiSeF/SrHOI	-4.83	-6.81	-2.85	-4.86	1.94	1.32
BiTeF/K ₂ Cu ₂ Se ₂	-4.38	-5.56	-1.50	-4.45	2.81	1.45
TiSeS/In ₃ F ₃	-4.97	-6.31	-3.02	-5.23	1.68	1.34
Rh ₄ S ₆ /Li ₂ S ₂ F ₂	-5.36	-6.52	-3.06	-5.99	1.68	1.32
Sc ₄ S ₆ /K ₄ O ₂	-2.96	-5.90	-1.22	-3.14	1.57	1.33
Cr ₄ O ₁₀ /Nb ₂ S ₄ Br ₄	-5.60	-6.92	-3.48	-5.94	1.79	1.54
Cr ₄ O ₁₀ /Nb ₂ S ₄ I ₄	-5.60	-6.92	-3.49	-5.78	1.93	1.35
Cr ₄ O ₁₀ /MgK ₂ Se ₂ H ₄ S ₈	-5.60	-6.92	-2.95	-5.91	2.35	1.63
Cr ₄ O ₁₀ /Ba ₂ Bi ₄ S ₈	-5.60	-6.92	-3.31	-5.62	2.27	1.63
Cr ₄ O ₁₀ /K ₂ PdH ₆ S ₆	-5.60	-6.92	-3.30	-6.09	1.81	1.90
In ₂ S ₂ F ₂ /Si ₂ H ₂	-5.16	-7.04	-2.71	-5.57	2.04	1.39
Au ₄ O ₄ F ₄ /Y ₂ Se ₄ Br ₄	-6.65	-9.05	-4.61	-6.65	2.03	1.33
In ₄ O ₄ Br ₄ /Nb ₂ S ₄ Br ₄	-5.68	-7.79	-3.48	-5.94	1.94	1.36
Y ₄ Te ₄ Br ₄ /Sn ₄ O ₄	-4.91	-6.06	-2.72	-5.33	1.78	1.60
Si ₂ F ₂ /Ga ₂ Te ₂	-5.50	-6.99	-3.67	-5.53	1.80	1.44
Si ₂ F ₂ /Ga ₂ Te ₂	-5.50	-6.99	-3.69	-5.53	1.79	1.44
Si ₂ F ₂ /Si ₂ H ₂	-5.50	-6.99	-2.71	-5.57	2.72	1.66

$Y_4Te_4Cl_4/Sn_4O_4$	-4.93	-6.11	-2.72	-5.33	1.82	1.45
Ga_2O_2/Sc_2CH_2	-5.32	-7.80	-3.40	-5.41	1.84	1.39
Ga_2O_2/Sc_2CH_2	-5.38	-7.80	-3.40	-5.41	1.95	1.39
Sn_2S_2/K_4O_2	-2.99	-5.51	-1.22	-3.14	1.62	1.35
$Ag_2F_2S_4/Rb_2C_2Se_2H_6S_6$	-4.98	-6.97	-3.25	-5.06	1.66	1.51
Sn_4O_4/Rb_4O_2	-2.72	-5.33	-1.15	-2.75	1.53	1.92
Sn_4O_4/Cs_4S_2	-2.72	-5.33	-0.85	-2.93	1.65	2.21
Sn_4S_4/K_4O_2	-2.90	-5.33	-1.13	-2.96	1.72	1.35
$Pt_2F_4/SrHOI$	-4.68	-7.46	-2.85	-4.86	1.65	1.46
$Ag_4F_8/LiNbBr_6$	-7.15	-8.79	-4.84	-7.78	1.69	1.41
$Au_4F_8/K_2Ta_2I_{12}$	-6.35	-7.63	-4.41	-6.46	1.83	1.51
$Li_2V_2Au_4O_{12}/MgK_2Se_2H_4S_8$	-5.18	-7.48	-2.95	-5.91	1.50	1.41
$Mo_2O_4Br_4/Rb_2C_2Se_2H_6S_6$	-5.00	-7.68	-3.25	-5.06	1.69	1.57
$W_2O_4Br_4/MgK_2Se_2H_4S_8$	-5.24	-7.59	-2.95	-5.91	1.63	1.38
$AuInF_4/Sr_2I_4O_8$	-4.87	-6.98	-2.00	-4.96	2.79	1.41
$Au_4S_4Br_4F_4/K_2PdH_6S_6$	-5.55	-6.99	-3.30	-6.09	1.72	1.55
$Au_4S_4Cl_4F_4/K_2PdH_6S_6$	-5.73	-7.27	-3.30	-6.09	2.07	1.60
$Bi_2Br_6/Rb_2C_2Se_2H_6S_6$	-5.00	-7.82	-3.25	-5.06	1.69	1.31
$Mo_2F_6/Ir_2S_2Cl_2$	-5.96	-6.97	-4.02	-6.22	1.68	1.37
$Mo_2F_6/Ir_2Se_2Cl_2$	-5.96	-6.97	-3.82	-6.06	2.04	1.42

Table S5. 279 screened potential solar cell candidates.

Heterostructures	CBM_A (eV)	VBM_A (eV)	CBM_B (eV)	VBM_B (eV)	PCE (%)
Zr ₂ Se ₆ /HfSeS	-4.61	-5.64	-4.62	-6.13	20.55
Zr ₂ Se ₆ /Ir ₂ S ₂ Br ₂	-4.61	-5.64	-4.66	-5.84	20.01
P ₄ /Bi ₂ O ₂	-3.89	-5.40	-3.87	-4.91	20.29
Re ₆ Te ₈ F ₂ /Fe ₂ Te ₆ P ₂	-4.42	-5.42	-4.45	-5.62	20.36
Re ₆ Te ₈ F ₂ /In ₂ P ₂ S ₆	-4.42	-5.42	-4.46	-5.86	20.30
CaSn ₃ S ₄ Br ₄ /Rh ₄ Se ₈	-5.01	-6.31	-4.94	-5.99	20.01
CaSn ₃ S ₄ Br ₄ /Ir ₂ Ni ₂ S ₈	-5.01	-6.31	-5.01	-6.37	21.19
Pt ₄ SeS ₃ I ₄ /In ₂ Te ₂ I ₂	-4.34	-5.79	-4.34	-5.76	20.90
Pt ₄ SeS ₃ I ₄ /Au ₂ Te ₄ Cl ₂	-4.34	-5.79	-4.34	-5.93	20.06
Pt ₄ SeS ₃ I ₄ /Hf ₂ P ₂ Se ₆	-4.34	-5.79	-4.30	-5.39	20.19
Pt ₄ SeS ₃ I ₄ /Zr ₂ P ₂ Se ₆	-4.34	-5.79	-4.29	-5.36	20.06
Nb ₃ OBr ₇ /In ₂ Te ₂ I ₂	-4.34	-5.78	-4.34	-5.76	20.88
Nb ₃ OBr ₇ /Au ₂ Te ₄ Cl ₂	-4.34	-5.78	-4.34	-5.93	20.10
Nb ₃ OBr ₇ /Hf ₂ P ₂ Se ₆	-4.34	-5.78	-4.30	-5.39	20.17
Nb ₃ OBr ₇ /Zr ₂ P ₂ Se ₆	-4.34	-5.78	-4.29	-5.36	20.04
Ta ₃ OCl ₇ /Sc ₄ Te ₆	-4.08	-5.65	-4.06	-5.28	20.04
Nb ₃ SI ₇ /Sc ₄ Te ₆	-4.10	-5.33	-4.06	-5.28	20.49
Nb ₃ SI ₇ /Pd ₂ Se ₄	-4.10	-5.33	-4.11	-5.35	21.01
Ta ₃ SBr ₇ /Ga ₂ Te ₅	-3.89	-5.40	-3.89	-5.28	20.61
Ta ₃ SBr ₇ /Ge ₂ Te ₆ P ₂	-3.89	-5.40	-3.89	-5.14	20.57
Ta ₃ SBr ₇ /W ₂ Cr ₂ Se ₈	-3.89	-5.40	-3.87	-5.07	20.25
Ta ₃ SI ₇ /Ta ₃ SeI ₇	-3.90	-5.19	-3.85	-5.11	20.35
Ta ₃ SI ₇ /Ge ₂ Te ₆ P ₂	-3.90	-5.19	-3.89	-5.14	21.15
Ta ₃ SI ₇ /W ₂ Cr ₂ Se ₈	-3.90	-5.19	-3.87	-5.07	20.74
Nb ₃ SeBr ₇ /Nb ₃ SeI ₇	-4.08	-5.55	-4.04	-5.27	20.11
Nb ₃ SeI ₇ /Sc ₄ Te ₆	-4.04	-5.27	-4.06	-5.28	20.76
Ta ₃ SeBr ₇ /CrMo ₃ Se ₈	-3.84	-5.29	-3.81	-5.24	20.46

Ta ₃ SeBr ₇ /Nb ₂ Te ₄ Br ₄	-3.84	-5.29	-3.83	-5.05	20.81
Ta ₃ SeBr ₇ /MoAg ₂ Te ₄	-3.84	-5.29	-3.80	-4.91	20.21
Ta ₃ SeCl ₇ /Ta ₂ Te ₄ Br ₄	-3.86	-5.44	-3.85	-4.93	20.04
Ta ₃ SeI ₇ /Ga ₂ Te ₅	-3.85	-5.11	-3.89	-5.28	20.39
Ta ₃ SeI ₇ /Ge ₂ Te ₆ P ₂	-3.85	-5.11	-3.89	-5.14	20.54
Ta ₃ SeI ₇ /MoAg ₂ Te ₄	-3.85	-5.11	-3.80	-4.91	20.13
Nb ₃ TeBr ₇ /Nb ₃ TeI ₇	-3.96	-5.40	-3.94	-5.19	20.63
Nb ₃ TeCl ₇ /AgAlTe ₆ P ₂	-4.00	-5.55	-4.00	-5.06	20.33
Nb ₃ TeCl ₇ /Nb ₂ Te ₄ Cl ₄	-4.00	-5.55	-3.99	-5.01	20.28
Nb ₃ TeI ₇ /Ge ₆ P ₈	-3.94	-5.19	-3.95	-5.51	20.24
Ta ₃ TeBr ₇ /Ta ₃ TeCl ₇	-3.75	-5.15	-3.76	-5.27	20.45
Ta ₃ TeBr ₇ /Si ₂ Te ₄	-3.75	-5.15	-3.72	-4.81	20.53
Ta ₃ TeBr ₇ /Hf ₂ Ge ₂ Te ₈	-3.75	-5.15	-3.73	-4.79	20.61
Ta ₃ TeBr ₇ /Zr ₂ Sn ₂ Te ₈	-3.75	-5.15	-3.70	-4.73	20.13
Ta ₃ TeBr ₇ /MoAu ₂ Se ₄	-3.75	-5.15	-3.72	-4.97	20.55
Ta ₃ TeCl ₇ /Nb ₂ Te ₄ I ₄	-3.76	-5.27	-3.76	-5.04	20.56
Ta ₃ TeCl ₇ /Ta ₂ Te ₄ I ₄	-3.76	-5.27	-3.75	-4.93	20.47
Ta ₃ TeI ₇ /CrMo ₃ Se ₈	-3.78	-5.01	-3.81	-5.24	20.50
Ta ₃ TeI ₇ /Ta ₂ Te ₄ I ₄	-3.78	-5.01	-3.75	-4.93	20.65
CrMo ₃ O ₈ /Bi ₂ S ₃	-5.85	-7.20	-5.83	-6.87	20.73
CrMo ₃ Se ₈ /Nb ₂ Te ₄ I ₄	-3.81	-5.24	-3.76	-5.04	20.05
CrMo ₃ Se ₈ /Sc ₂ P ₂ Se ₆	-3.81	-5.24	-3.77	-4.99	20.35
CrMo ₃ Se ₈ /MoAg ₂ Te ₄	-3.81	-5.24	-3.80	-4.91	20.74
CrMo ₃ Te ₈ /CrW ₃ Se ₈	-3.64	-4.74	-3.69	-5.02	20.15
CrMo ₃ Te ₈ /Hf ₂ Si ₂ Te ₈	-3.64	-4.74	-3.65	-4.81	20.72
CrMo ₃ Te ₈ /W ₂ Cl ₆	-3.64	-4.74	-3.65	-4.82	20.74
CrW ₃ Se ₈ /Hf ₂ Si ₂ Te ₈	-3.69	-5.02	-3.65	-4.81	20.50
CrW ₃ Se ₈ /W ₂ Cl ₆	-3.69	-5.02	-3.65	-4.82	20.52
MoW ₃ Te ₈ /WMo ₃ Te ₈	-3.36	-4.58	-3.41	-4.73	20.32

MoW ₃ Te ₈ /Zr ₂ Br ₄	-3.36	-4.58	-3.35	-4.49	21.05
MoW ₃ Te ₈ /W ₂ Mo ₂ Te ₈	-3.36	-4.58	-3.38	-4.66	20.83
WMo ₃ Te ₈ /Zr ₂ Br ₄	-3.41	-4.73	-3.35	-4.49	20.07
WMo ₃ Te ₈ /Re ₄ Te ₈	-3.41	-4.73	-3.46	-4.79	20.14
WMo ₃ Te ₈ /W ₂ Mo ₂ Te ₈	-3.41	-4.73	-3.38	-4.66	20.82
BiSBr/Co ₂ O ₂ Cl ₂	-5.49	-7.09	-5.49	-6.52	20.01
BiSeBr/Au ₂ Se ₂ Br ₂	-5.42	-6.78	-5.41	-6.68	21.05
BiSeBr/Rh ₄ S ₆	-5.42	-6.78	-5.36	-6.52	20.05
BiTeBr/BiTeCl	-5.16	-6.32	-5.19	-6.39	20.46
BiTeBr/BiTeCl	-5.16	-6.32	-5.14	-6.29	20.56
BiTeBr/BiSI	-5.16	-6.32	-5.19	-6.36	20.59
BiTeBr/BiSeI	-5.16	-6.32	-5.21	-6.42	20.19
BiTeBr/Ir ₂ S ₂ Cl ₂	-5.05	-6.21	-5.09	-6.29	20.44
BiSeCl/Co ₂ O ₂ Cl ₂	-5.50	-7.01	-5.49	-6.52	20.40
BiSeCl/Si ₂ F ₂	-5.50	-7.01	-5.50	-6.99	20.62
BiSeCl/SnS ₂ Br ₂	-5.50	-7.01	-5.49	-6.98	20.33
BiTeCl/BiSI	-5.19	-6.39	-5.21	-6.69	20.51
BiTeCl/BiSI	-5.19	-6.39	-5.19	-6.36	21.07
BiTeCl/BiSeI	-5.19	-6.39	-5.21	-6.42	20.98
BiTeCl/BiSI	-5.14	-6.29	-5.19	-6.36	20.01
BiTeF/In ₂ TeS	-4.38	-5.56	-4.42	-5.56	20.13
BiTeF/MgIn ₂ Se ₄	-4.38	-5.56	-4.42	-5.80	20.25
BiSI/BiSI	-5.21	-6.69	-5.19	-6.36	20.37
BiSI/BiSeI	-5.21	-6.69	-5.21	-6.42	20.76
BiSI/BiSeI	-5.19	-6.36	-5.21	-6.42	20.80
BiSeI/Ir ₂ S ₂ Cl ₂	-5.11	-6.30	-5.09	-6.29	20.84
BiSeI/Fe ₂ S ₄	-5.11	-6.30	-5.13	-6.46	20.76
HfBrCl/HfClCl	-2.33	-3.69	-2.28	-3.57	20.12
HfBrCl/HfBr ₂	-2.33	-3.69	-2.28	-3.50	20.06

TiBrCl/TiCl	-2.48	-3.78	-2.45	-3.64	20.65
ZrBrCl/TiCl	-2.48	-3.87	-2.45	-3.64	20.59
TiBr/ZrCl	-2.38	-3.41	-2.41	-3.72	20.71
TiBr/TiBr ₂	-2.38	-3.41	-2.39	-3.56	20.77
TiBr/ZrBr ₂	-2.38	-3.41	-2.40	-3.68	20.86
ZrBr/ZrCl	-2.35	-3.53	-2.41	-3.72	20.16
ZrBr/TiBr ₂	-2.35	-3.53	-2.39	-3.56	20.17
ZrBr/ZrBr ₂	-2.35	-3.53	-2.40	-3.68	20.29
ZrBr/ZrI ₂	-2.35	-3.53	-2.31	-3.35	20.22
HfCl/HfBr ₂	-2.28	-3.57	-2.28	-3.50	21.29
ZrCl/TiBr ₂	-2.41	-3.72	-2.39	-3.56	21.06
ZrCl/ZrBr ₂	-2.41	-3.72	-2.40	-3.68	21.17
Mg ₂ Al ₂ Te ₅ /Ge ₂ Te ₂	-3.37	-4.58	-3.38	-4.86	20.63
Mg ₂ Al ₂ Te ₅ /Zr ₂ Br ₄	-3.37	-4.58	-3.35	-4.49	20.76
HfSeS/Co ₂ H ₂ S ₄	-4.62	-6.13	-4.61	-5.82	20.57
HfSeS/HfSe ₂	-4.62	-6.13	-4.60	-5.81	20.28
RhSeI/Ti ₂ S ₆	-4.21	-5.63	-4.18	-5.63	20.37
Mg ₂ Ga ₂ Se ₅ /In ₂ Si ₂ Te ₂	-4.27	-5.53	-4.22	-5.25	20.08
Mg ₂ In ₂ Se ₅ /Ti ₂ S ₆	-4.21	-5.71	-4.18	-5.63	20.07
PtTeSe/Ti ₂ S ₆	-4.14	-5.23	-4.18	-5.63	20.24
SnSeS/Ir ₂ S ₂ Cl ₂	-5.10	-6.58	-5.09	-6.29	20.56
ZrSeS/Ir ₂ S ₂ Br ₂	-4.68	-6.20	-4.66	-5.84	20.23
WTeSe/TeGe ₂ S	-3.30	-4.80	-3.27	-4.48	20.11
WTeSe/Sn ₂ Se ₂	-3.30	-4.80	-3.29	-4.63	20.46
Ag ₂ Te ₃ /Ga ₂ Te ₅	-3.93	-5.35	-3.89	-5.28	20.33
Ag ₂ Te ₃ /Ru ₂ Te ₄	-3.93	-5.35	-3.92	-4.99	20.82
Bi ₂ S ₃ /Bi ₂ SeSCl ₂	-5.83	-6.87	-5.85	-7.37	20.17
Al ₂ Ge ₂ Te ₂ /Ir ₂ O ₂ Br ₂	-3.67	-5.03	-3.65	-4.99	20.85
Al ₂ Ge ₂ Te ₂ /Sc ₂ Te ₂ Cl ₂	-3.67	-5.03	-3.71	-5.15	20.15

$\text{Au}_2\text{Se}_2\text{Br}_2/\text{Rh}_4\text{S}_6$	-5.41	-6.68	-5.36	-6.52	20.25
$\text{Ag}_4\text{S}_6/\text{Au}_2\text{I}_2\text{S}_4$	-4.82	-6.32	-4.79	-6.22	20.20
$\text{Ag}_4\text{S}_6/\text{ZnGeSe}_2\text{Br}_2$	-4.82	-6.32	-4.80	-6.30	20.40
$\text{Ag}_4\text{S}_6/\text{Au}_2\text{Te}_4\text{I}_2$	-4.21	-5.60	-4.26	-5.61	20.13
$\text{Ag}_4\text{S}_6/\text{Nb}_4\text{Br}_2\text{Se}_{12}$	-4.21	-5.60	-4.19	-5.26	20.73
$\text{Al}_4\text{Te}_6/\text{Pd}_2\text{Se}_4$	-4.14	-5.67	-4.11	-5.35	20.08
$\text{Al}_4\text{Te}_6/\text{Cr}_3\text{Se}_6$	-4.14	-5.67	-4.11	-5.27	20.06
$\text{Ga}_4\text{Se}_6/\text{Fe}_3\text{Se}_6$	-4.89	-6.44	-4.87	-6.23	20.02
$\text{Ga}_4\text{Se}_6/\text{Ir}_4\text{S}_8$	-4.89	-6.44	-4.88	-6.40	20.23
$\text{Ga}_4\text{Se}_6/\text{Sc}_4\text{Te}_6$	-4.11	-5.36	-4.06	-5.28	20.34
$\text{Bi}_2\text{Se}_2\text{Br}_2/\text{Au}_2\text{Cl}_2$	-5.61	-6.80	-5.63	-7.11	20.45
$\text{In}_4\text{Te}_6/\text{Au}_2\text{Te}_4\text{I}_2$	-4.22	-5.51	-4.26	-5.61	20.28
$\text{Sc}_4\text{Se}_6/\text{Hf}_2\text{IBr}_3$	-2.29	-3.45	-2.24	-3.41	20.09
$\text{Sc}_4\text{Te}_6/\text{Os}_2\text{Se}_4$	-4.06	-5.28	-4.07	-5.46	20.98
$\text{Sc}_4\text{Te}_6/\text{Pd}_2\text{Se}_4$	-4.06	-5.28	-4.11	-5.35	20.17
$\text{Hf}_2\text{Br}_2\text{Cl}_2/\text{Sn}_2\text{SeS}$	-3.17	-4.58	-3.18	-4.70	20.36
$\text{Zr}_2\text{Br}_2\text{Cl}_2/\text{Hf}_2\text{IClBr}_4$	-3.43	-4.58	-3.43	-4.57	21.00
$\text{Zr}_2\text{Br}_2\text{Cl}_2/\text{MgAl}_2\text{Te}_4$	-3.43	-4.58	-3.44	-4.60	20.91
$\text{HfI}_2\text{Br}_2/\text{Hf}_2\text{I}_4$	-3.10	-4.25	-3.09	-4.10	20.73
$\text{Ir}_2\text{O}_2\text{Br}_2/\text{Hf}_2\text{N}_2\text{I}_2$	-3.65	-4.99	-3.68	-5.12	20.33
$\text{Ir}_2\text{S}_2\text{Br}_2/\text{Co}_2\text{H}_2\text{S}_4$	-4.66	-5.84	-4.61	-5.82	20.13
$\text{Ir}_2\text{S}_2\text{Br}_2/\text{ZrSe}_2$	-4.66	-5.84	-4.68	-5.89	20.74
$\text{Ir}_2\text{S}_2\text{Br}_2/\text{Os}_2\text{S}_4$	-4.66	-5.84	-4.67	-6.06	20.91
$\text{Co}_2\text{O}_2\text{Cl}_2/\text{Si}_2\text{F}_2$	-5.49	-6.52	-5.50	-6.99	20.49
$\text{Ga}_2\text{Te}_5/\text{Al}_2\text{Ge}_2\text{Te}_6$	-3.89	-5.28	-3.89	-5.37	20.77
$\text{Ga}_2\text{Te}_5/\text{Ge}_2\text{Te}_6\text{P}_2$	-3.89	-5.28	-3.89	-5.14	21.11
$\text{Ga}_2\text{Te}_5/\text{Ta}_2\text{Te}_4\text{Br}_4$	-3.89	-5.28	-3.85	-4.93	20.36
$\text{Ga}_2\text{Te}_5/\text{W}_2\text{Cr}_2\text{Se}_8$	-3.89	-5.28	-3.87	-5.07	20.74
$\text{Ga}_2\text{Te}_5/\text{Nb}_2\text{Br}_6$	-3.89	-5.28	-3.86	-4.87	20.63

$\text{Cr}_4\text{O}_{10}/\text{Ag}_4\text{Te}_4\text{Br}_4$	-5.60	-6.92	-5.60	-6.86	21.28
$\text{Cr}_4\text{O}_{10}/\text{Cu}_4\text{Se}_4\text{I}_4$	-5.60	-6.92	-5.59	-6.81	21.17
$\text{Ir}_2\text{S}_2\text{Cl}_2/\text{SnSe}_2$	-5.09	-6.29	-5.12	-6.46	20.59
$\text{Ir}_2\text{S}_2\text{Cl}_2/\text{Fe}_2\text{S}_4$	-5.09	-6.29	-5.13	-6.46	20.37
$\text{Sc}_2\text{Te}_2\text{Cl}_2/\text{Ge}_2\text{H}_2$	-3.71	-5.15	-3.73	-5.22	20.44
$\text{Ir}_4\text{Se}_3\text{S}_5/\text{ZrHf}_2\text{Se}_6$	-4.63	-6.18	-4.63	-5.84	20.31
$\text{Ir}_2\text{S}_2\text{F}_2/\text{Os}_2\text{O}_4$	-5.91	-7.35	-5.89	-6.89	20.55
$\text{InN}/\text{TiPdS}_2$	-4.05	-5.62	-4.03	-5.59	20.02
$\text{Au}_2\text{Te}_2/\text{Pd}_2\text{Se}_4$	-4.10	-5.17	-4.11	-5.35	21.10
$\text{Au}_2\text{Te}_2/\text{Cr}_3\text{Se}_6$	-4.10	-5.17	-4.11	-5.27	20.92
$\text{Au}_2\text{Te}_2/\text{Ga}_2\text{Al}_2\text{Te}_6$	-4.10	-5.17	-4.16	-5.55	20.11
$\text{In}_2\text{Te}_2\text{I}_2/\text{Nb}_4\text{O}_8$	-4.34	-5.76	-4.35	-5.81	20.62
$\text{In}_2\text{Te}_2\text{I}_2/\text{Hf}_2\text{P}_2\text{Se}_6$	-4.34	-5.76	-4.30	-5.39	20.30
$\text{In}_2\text{Te}_2\text{I}_2/\text{Zr}_2\text{P}_2\text{Se}_6$	-4.34	-5.76	-4.29	-5.36	20.17
$\text{In}_2\text{Te}_2\text{I}_2/\text{W}_2\text{Cr}_2\text{S}_8$	-4.34	-5.76	-4.29	-5.73	20.04
$\text{Ag}_4\text{Te}_4\text{Br}_4/\text{Cu}_4\text{Te}_4\text{Cl}_4$	-5.60	-6.86	-5.63	-6.96	20.74
$\text{Ag}_4\text{Te}_4\text{Cl}_4/\text{Au}_4\text{S}_4\text{Cl}_4\text{F}_4$	-5.73	-6.98	-5.73	-7.27	20.38
$\text{Ag}_4\text{Se}_4\text{I}_4/\text{Au}_4\text{S}_4\text{Cl}_4\text{F}_4$	-5.73	-6.76	-5.73	-7.27	20.38
$\text{Au}_4\text{S}_4\text{I}_4/\text{Ta}_2\text{Rh}_2\text{S}_8$	-5.17	-6.51	-5.12	-6.36	20.31
$\text{Au}_4\text{S}_4\text{I}_4/\text{OsRuCl}_6$	-5.17	-6.51	-5.17	-6.37	21.27
$\text{Cu}_4\text{Se}_4\text{Br}_4/\text{Cu}_2\text{Cl}_2\text{I}_4$	-5.99	-7.41	-5.96	-7.04	20.56
$\text{Cu}_4\text{Te}_4\text{Br}_4/\text{Cu}_4\text{Te}_4\text{Cl}_4$	-5.61	-6.75	-5.63	-6.96	20.96
$\text{Pd}_4\text{I}_4\text{Br}_4/\text{Rh}_4\text{S}_8$	-5.31	-6.66	-5.33	-6.73	20.60
$\text{Y}_4\text{Te}_4\text{Br}_4/\text{Y}_4\text{Te}_4\text{Cl}_4$	-4.91	-6.06	-4.93	-6.11	20.73
$\text{Cu}_4\text{Te}_4\text{Cl}_4/\text{Cu}_4\text{Se}_4\text{I}_4$	-5.63	-6.96	-5.59	-6.81	20.64
$\text{Cu}_4\text{Te}_4\text{I}_4/\text{Rh}_4\text{S}_8$	-5.32	-6.42	-5.33	-6.73	20.85
$\text{Ge}_2\text{Se}_2/\text{Sn}_2\text{SeS}$	-3.20	-4.76	-3.18	-4.70	20.01
$\text{Ge}_2\text{Te}_2/\text{Zr}_2\text{Br}_4$	-3.38	-4.86	-3.35	-4.49	20.22
$\text{Pd}_4\text{Te}_4\text{P}_4/\text{In}_2\text{P}_2\text{S}_6$	-4.42	-5.84	-4.46	-5.86	20.31

$\text{Pd}_4\text{Te}_4\text{P}_4/\text{Sr}_4\text{Bi}_4\text{F}_4\text{S}_8$	-4.42	-5.84	-4.38	-5.76	20.24
$\text{In}_2\text{I}_2/\text{HfGeS}_2\text{Br}_2$	-4.39	-5.72	-4.44	-5.88	20.04
$\text{In}_2\text{I}_2/\text{In}_2\text{Al}_2\text{Te}_6$	-4.39	-5.72	-4.35	-5.59	20.45
$\text{TeGe}_2\text{S}/\text{Sn}_2\text{Se}_2$	-3.27	-4.48	-3.29	-4.63	20.88
$\text{TeGe}_2\text{S}/\text{Hf}_2\text{Cl}_4$	-3.27	-4.48	-3.28	-4.75	20.68
$\text{In}_2\text{TeS}/\text{IrGaS}_2\text{I}_2$	-4.42	-5.56	-4.45	-5.63	20.59
$\text{In}_2\text{TeS}/\text{HfGeS}_2\text{Br}_2$	-4.42	-5.56	-4.44	-5.88	20.63
$\text{In}_2\text{TeS}/\text{MgGa}_2\text{Se}_4$	-4.42	-5.56	-4.39	-5.53	20.24
$\text{In}_2\text{TeS}/\text{MgIn}_2\text{Se}_4$	-4.42	-5.56	-4.42	-5.80	21.14
$\text{Au}_2\text{Te}_4\text{Cl}_2/\text{Ir}_4\text{Se}_8$	-4.34	-5.93	-4.34	-5.90	20.03
$\text{Au}_2\text{I}_2\text{S}_4/\text{Bi}_2\text{GeSe}_2\text{I}_4$	-4.79	-6.22	-4.83	-6.25	20.34
$\text{Au}_2\text{Te}_4\text{I}_2/\text{AgBiTe}_6\text{P}_2$	-4.26	-5.61	-4.22	-5.30	20.44
$\text{Au}_2\text{Te}_4\text{I}_2/\text{Au}_4\text{S}_2$	-4.26	-5.61	-4.24	-5.38	20.75
$\text{Au}_2\text{Te}_4\text{I}_2/\text{In}_2\text{Si}_2\text{Te}_6$	-4.26	-5.61	-4.23	-5.41	20.57
$\text{Au}_2\text{Te}_4\text{I}_2/\text{Pd}_4\text{In}_2\text{Se}_6$	-4.26	-5.61	-4.26	-5.55	21.17
$\text{Au}_2\text{Te}_4\text{I}_2/\text{Nb}_4\text{I}_2\text{Se}_{12}$	-4.26	-5.61	-4.23	-5.26	20.52
$\text{Bi}_2\text{H}_2\text{S}_4/\text{Bi}_2\text{P}_2\text{S}_6$	-4.73	-6.31	-4.73	-6.04	20.12
$\text{Zn}_2\text{Te}_2/\text{Ru}_2\text{Te}_4$	-3.96	-5.25	-3.92	-4.99	20.43
$\text{Cu}_2\text{Cl}_2\text{O}_4/\text{Ru}_3\text{S}_3\text{Cl}_6$	-6.62	-7.91	-6.57	-7.70	20.27
$\text{Co}_2\text{H}_2\text{S}_4/\text{HfSe}_2$	-4.61	-5.82	-4.60	-5.81	20.93
$\text{Au}_4\text{S}_4/\text{RuNiTa}_2\text{Se}_6$	-4.54	-5.88	-4.49	-5.69	20.27
$\text{Au}_4\text{S}_4/\text{Cu}_{12}\text{S}_6$	-4.54	-5.88	-4.54	-6.14	20.03
$\text{Au}_4\text{Se}_4/\text{Zr}_2\text{Se}_4$	-4.49	-5.59	-4.50	-5.64	20.71
$\text{Pd}_2\text{Se}_2\text{Cl}_4/\text{PdPt}_3\text{SeSCl}_6$	-5.48	-6.93	-5.46	-6.79	20.48
$\text{HfGeS}_2\text{Br}_2/\text{Rh}_2\text{P}_2\text{S}_6$	-4.44	-5.88	-4.40	-5.75	20.26
$\text{HfGeS}_2\text{Br}_2/\text{MgIn}_2\text{Se}_4$	-4.44	-5.88	-4.42	-5.80	20.68
$\text{HfCl}_2/\text{TiBr}_2$	-2.41	-3.88	-2.39	-3.56	20.60
$\text{HfCl}_2/\text{ZrBr}_2$	-2.41	-3.88	-2.40	-3.68	20.69
$\text{In}_2\text{TeSI}_2/\text{Ni}_2\text{Te}_2\text{S}_6$	-3.88	-5.44	-3.87	-5.43	20.01

$\text{In}_2\text{TeSI}_2/\text{W}_2\text{Cr}_2\text{Se}_8$	-3.88	-5.44	-3.87	-5.07	20.10
$\text{In}_2\text{TeSI}_2/\text{Nb}_2\text{Br}_6$	-3.88	-5.44	-3.86	-4.87	20.00
$\text{Hf}_2\text{IClBr}_4/\text{Re}_4\text{Te}_8$	-3.43	-4.57	-3.46	-4.79	20.54
$\text{SnSe}_2/\text{Fe}_2\text{S}_4$	-5.12	-6.46	-5.13	-6.46	21.10
$\text{TiBr}_2/\text{ZrBr}_2$	-2.39	-3.56	-2.40	-3.68	21.23
$\text{TiSe}_2/\text{Ru}_2\text{S}_4$	-4.83	-6.29	-4.83	-6.41	20.12
$\text{RhIr}_2\text{GaS}_4\text{Br}_4/\text{OsRuCl}_6$	-5.16	-6.30	-5.17	-6.37	21.08
$\text{AgAlTe}_6\text{P}_2/\text{Nb}_2\text{Te}_4\text{Cl}_4$	-4.00	-5.06	-3.99	-5.01	20.57
$\text{AgBiTe}_6\text{P}_2/\text{Au}_4\text{S}_2$	-4.22	-5.30	-4.24	-5.38	20.69
$\text{AgBiTe}_6\text{P}_2/\text{In}_2\text{Si}_2\text{Te}_6$	-4.22	-5.30	-4.23	-5.41	21.10
$\text{AgBiTe}_6\text{P}_2/\text{Pd}_4\text{In}_2\text{Se}_6$	-4.22	-5.30	-4.26	-5.55	20.58
$\text{Hf}_2\text{Br}_4/\text{Hf}_2\text{I}_4$	-3.10	-4.44	-3.09	-4.10	20.96
$\text{Os}_2\text{Te}_4/\text{Zr}_2\text{Cl}_4$	-3.57	-4.95	-3.54	-4.70	20.63
$\text{Pd}_2\text{I}_4/\text{PdNiIr}_2\text{Se}_8$	-4.72	-6.19	-4.71	-5.74	20.59
$\text{Pd}_2\text{Se}_4/\text{Cr}_3\text{Se}_6$	-4.11	-5.35	-4.11	-5.27	21.31
$\text{Pd}_2\text{Se}_4/\text{Ga}_2\text{Al}_2\text{Te}_6$	-4.11	-5.35	-4.16	-5.55	20.30
$\text{Au}_4\text{S}_2/\text{In}_2\text{Ge}_2\text{Te}_6$	-4.24	-5.38	-4.20	-5.35	20.20
$\text{Au}_4\text{S}_2/\text{W}_2\text{Cr}_2\text{S}_8$	-4.24	-5.38	-4.29	-5.73	20.09
$\text{Si}_2\text{Te}_4/\text{MoAu}_2\text{Se}_4$	-3.72	-4.81	-3.72	-4.97	21.33
$\text{Ag}_4\text{Te}_2/\text{In}_2\text{P}_2\text{S}_6$	-4.41	-5.85	-4.46	-5.86	20.07
$\text{Ag}_4\text{Te}_2/\text{Rh}_2\text{P}_2\text{S}_6$	-4.41	-5.85	-4.40	-5.75	20.79
$\text{Ag}_4\text{Te}_2/\text{Zr}_2\text{P}_2\text{S}_6$	-4.41	-5.85	-4.41	-5.91	20.67
$\text{Ag}_4\text{Te}_2/\text{Sr}_4\text{Bi}_4\text{F}_4\text{S}_8$	-4.41	-5.85	-4.38	-5.76	20.33
$\text{Zr}_2\text{Br}_4/\text{W}_2\text{Mo}_2\text{Te}_8$	-3.35	-4.49	-3.38	-4.66	20.57
$\text{Zr}_2\text{Cl}_4/\text{ZrNiF}_6$	-3.54	-4.70	-3.56	-5.00	20.66
$\text{Zr}_2\text{Cl}_4/\text{Zr}_2\text{ClBr}_5$	-3.54	-4.70	-3.50	-4.56	20.29
$\text{RuNiTa}_2\text{Se}_6/\text{Fe}_2\text{Te}_6\text{P}_2$	-4.49	-5.69	-4.45	-5.62	20.36
$\text{Cr}_3\text{Se}_6/\text{Ga}_2\text{Al}_2\text{Te}_6$	-4.11	-5.27	-4.16	-5.55	20.28
$\text{Nb}_4\text{O}_8/\text{In}_2\text{Al}_2\text{Te}_6$	-4.35	-5.81	-4.35	-5.59	20.86

Re ₄ Te ₈ /Hf ₂ BrI ₅	-3.46	-4.79	-3.43	-4.46	20.68
PdNiIr ₂ Se ₈ /Bi ₂ P ₂ S ₆	-4.71	-5.74	-4.73	-6.04	20.85
PdNiIr ₂ Se ₈ /Ir ₄ Se ₂ S ₆	-4.71	-5.74	-4.71	-6.24	20.45
Rh ₄ Se ₈ /Ta ₂ Ir ₂ S ₈	-4.94	-5.99	-5.00	-6.33	20.08
Rh ₄ Se ₈ /Ni ₂ SeS ₃	-4.94	-5.99	-4.95	-6.30	21.08
Ta ₄ O ₈ /Ga ₂ Al ₂ Te ₆	-4.19	-5.68	-4.16	-5.55	20.21
Al ₂ Ge ₂ Te ₆ /Ge ₂ Te ₆ P ₂	-3.89	-5.37	-3.89	-5.14	20.74
Al ₂ Ge ₂ Te ₆ /Ta ₂ Te ₄ Br ₄	-3.89	-5.37	-3.85	-4.93	20.05
Al ₂ Ge ₂ Te ₆ /W ₂ Cr ₂ Se ₈	-3.89	-5.37	-3.87	-5.07	20.40
Al ₂ Ge ₂ Te ₆ /Nb ₂ Br ₆	-3.89	-5.37	-3.86	-4.87	20.29
In ₂ Al ₂ Te ₆ /Rh ₂ P ₂ S ₆	-4.35	-5.59	-4.40	-5.75	20.18
In ₂ Al ₂ Te ₆ /Sr ₄ Bi ₄ F ₄ S ₈	-4.35	-5.59	-4.38	-5.76	20.62
Bi ₂ P ₂ S ₆ /Hf ₄ S ₂ Se ₆	-4.73	-6.04	-4.67	-6.01	20.04
Fe ₂ Te ₆ P ₂ /In ₂ P ₂ S ₆	-4.45	-5.62	-4.46	-5.86	20.95
In ₂ Ge ₂ Te ₆ /In ₂ Si ₂ Te ₆	-4.20	-5.35	-4.23	-5.41	20.57
In ₂ Ge ₂ Te ₆ /Pd ₄ In ₂ Se ₆	-4.20	-5.35	-4.26	-5.55	20.11
Ge ₂ Te ₆ P ₂ /Nb ₂ Te ₄ Br ₄	-3.89	-5.14	-3.83	-5.05	20.01
Ge ₂ Te ₆ P ₂ /Ta ₂ Te ₄ Br ₄	-3.89	-5.14	-3.85	-4.93	20.46
Ge ₂ Te ₆ P ₂ /W ₂ Cr ₂ Se ₈	-3.89	-5.14	-3.87	-5.07	20.91
Hf ₂ P ₂ Se ₆ /Zr ₂ P ₂ Se ₆	-4.30	-5.39	-4.29	-5.36	20.68
RuH ₂ O ₂ /Y ₂ NH ₂ O ₂	-1.39	-2.83	-1.34	-2.52	20.18
In ₂ Si ₂ Te ₆ /Pd ₄ In ₂ Se ₆	-4.23	-5.41	-4.26	-5.55	20.71
Ni ₂ Te ₂ S ₆ /Nb ₂ Br ₆	-3.87	-5.43	-3.86	-4.87	20.25
Nb ₂ Te ₄ Br ₄ /Sc ₂ P ₂ Se ₆	-3.83	-5.05	-3.77	-4.99	20.07
Nb ₂ Te ₄ Br ₄ /W ₂ Cr ₂ Se ₈	-3.83	-5.05	-3.87	-5.07	20.40
Nb ₂ Te ₄ Br ₄ /MoAg ₇ Te ₄	-3.83	-5.05	-3.80	-4.91	20.56
Rh ₂ P ₂ S ₆ /Zr ₂ P ₂ S ₆	-4.40	-5.75	-4.41	-5.91	20.49
Nb ₂ Te ₄ I ₄ /Ta ₂ Te ₄ I ₄	-3.76	-5.04	-3.75	-4.93	21.24
Nb ₂ Te ₄ I ₄ /Hf ₂ Ge ₂ Te ₈	-3.76	-5.04	-3.73	-4.79	20.63

$\text{Nb}_2\text{Te}_4\text{I}_4/\text{Zr}_2\text{Sn}_2\text{Te}_8$	-3.76	-5.04	-3.70	-4.73	20.09
$\text{Nb}_2\text{Te}_4\text{I}_4/\text{MoAu}_2\text{Se}_4$	-3.76	-5.04	-3.72	-4.97	20.57
$\text{Ta}_2\text{Te}_4\text{Br}_4/\text{W}_2\text{Cr}_2\text{Se}_8$	-3.85	-4.93	-3.87	-5.07	20.81
$\text{Sc}_2\text{P}_2\text{Se}_6/\text{MoAu}_2\text{Se}_4$	-3.77	-4.99	-3.72	-4.97	20.18
$\text{Ta}_2\text{Te}_4\text{I}_4/\text{Hf}_2\text{Ge}_2\text{Te}_8$	-3.75	-4.93	-3.73	-4.79	20.54
$\text{Zr}_2\text{P}_2\text{S}_6/\text{Sr}_4\text{Bi}_4\text{F}_4\text{S}_8$	-4.41	-5.91	-4.38	-5.76	20.06
$\text{HfZr}_3\text{BrCl}_7/\text{Hf}_2\text{BrI}_5$	-3.48	-4.66	-3.43	-4.46	20.04
$\text{W}_2\text{Cr}_2\text{Se}_8/\text{Nb}_2\text{Br}_6$	-3.87	-5.07	-3.86	-4.87	21.14
$\text{Hf}_2\text{Ge}_2\text{Te}_8/\text{Nb}_4\text{Te}_{12}\text{Br}_2$	-3.73	-4.79	-3.76	-4.94	20.43
$\text{Hf}_2\text{Ge}_2\text{Te}_8/\text{Ta}_4\text{Te}_{12}\text{Br}_2$	-3.73	-4.79	-3.74	-4.83	20.44
$\text{Hf}_2\text{Ge}_2\text{Te}_8/\text{Nb}_4\text{Te}_{12}\text{Cl}_2$	-3.73	-4.79	-3.73	-4.91	21.13
$\text{Zr}_2\text{Ge}_2\text{Te}_8/\text{Nb}_4\text{Te}_{12}\text{Cl}_2$	-3.69	-4.81	-3.73	-4.91	20.26
$\text{Hf}_2\text{Si}_2\text{Te}_8/\text{W}_2\text{Cl}_6$	-3.65	-4.81	-3.65	-4.82	21.16
$\text{Ir}_2\text{Ni}_2\text{S}_8/\text{Ta}_2\text{Ir}_2\text{S}_8$	-5.01	-6.37	-5.00	-6.33	21.13
$\text{Ta}_2\text{Rh}_2\text{S}_8/\text{OsRuCl}_6$	-5.12	-6.36	-5.17	-6.37	20.26
$\text{Zr}_2\text{Si}_2\text{Te}_8/\text{W}_2\text{Cl}_6$	-3.63	-4.82	-3.65	-4.82	20.60
$\text{MgGa}_2\text{Se}_4/\text{MgIn}_2\text{Se}_4$	-4.39	-5.53	-4.42	-5.80	20.47
$\text{Nb}_4\text{Te}_{12}\text{Br}_2/\text{Ta}_4\text{Te}_{12}\text{Br}_2$	-3.76	-4.94	-3.74	-4.83	20.79
$\text{Nb}_4\text{Te}_{12}\text{Br}_2/\text{Nb}_4\text{Te}_{12}\text{Cl}_2$	-3.76	-4.94	-3.73	-4.91	20.52
$\text{Nb}_4\text{Te}_{12}\text{Cl}_2/\text{Ta}_4\text{Te}_{12}\text{Cl}_2$	-3.73	-4.91	-3.69	-4.82	20.21

Table S6. Calculated formation energies (E_f , in meV) and binding energies (E_b , in $meV/\text{\AA}^2$) for four representative heterostructures: $\text{Si}_2\text{F}_2/\text{Ga}_2\text{Te}_2$, $\text{Si}_2\text{F}_2/\text{Si}_2\text{H}_2$, $\text{HfBr}_2/\text{HfCl}$, $\text{ZrBr}_2/\text{ZrCl}$.

	E_f (meV)	E_b ($meV/\text{\AA}^2$)
$\text{Si}_2\text{F}_2/\text{Si}_2\text{H}_2$	-114.26	-9.23
$\text{Si}_2\text{F}_2/\text{Ga}_2\text{Te}_2$	-285.37	-25.33
$\text{HfBr}_2/\text{HfCl}$	-57.10	-11.69
$\text{ZrBr}_2/\text{ZrCl}$	-205.86	-20.16

Table S7. Bader charge variations for the top layer (Q_T), the bottom layer (Q_B) in representative heterostructures. The values represent net charge deviations with respect to neutral atoms (in units of e). Positive values indicate electron accumulation, and negative values indicate electron depletion.

	$Q_T (e)$	$Q_B (e)$
$\text{Si}_2\text{F}_2/\text{Si}_2\text{H}_2$	0.0361	-0.0361
$\text{Si}_2\text{F}_2/\text{Ga}_2\text{Te}_2$	0.1800	-0.1800
$\text{HfBr}_2/\text{HfICl}$	0.0025	-0.0025
$\text{ZrBr}_2/\text{ZrICl}$	0.0108	-0.0108

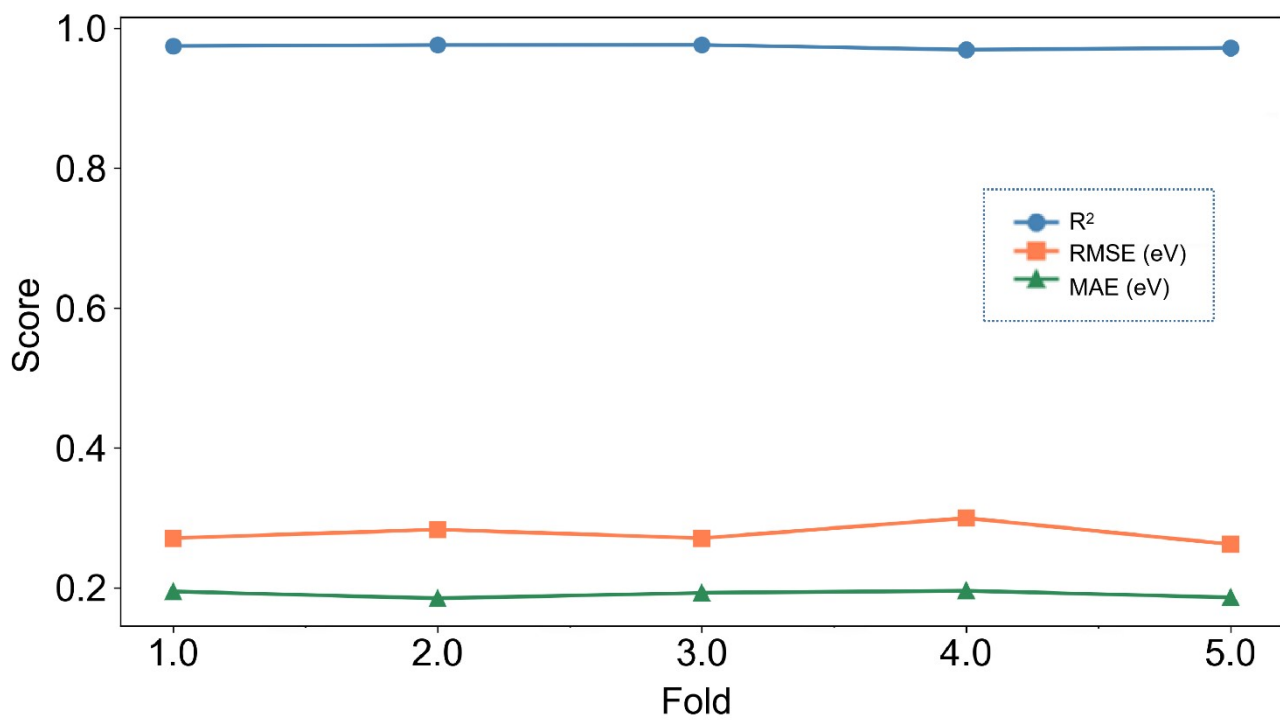


Figure S1. Five-fold cross-validation performance of the XGBoost model.

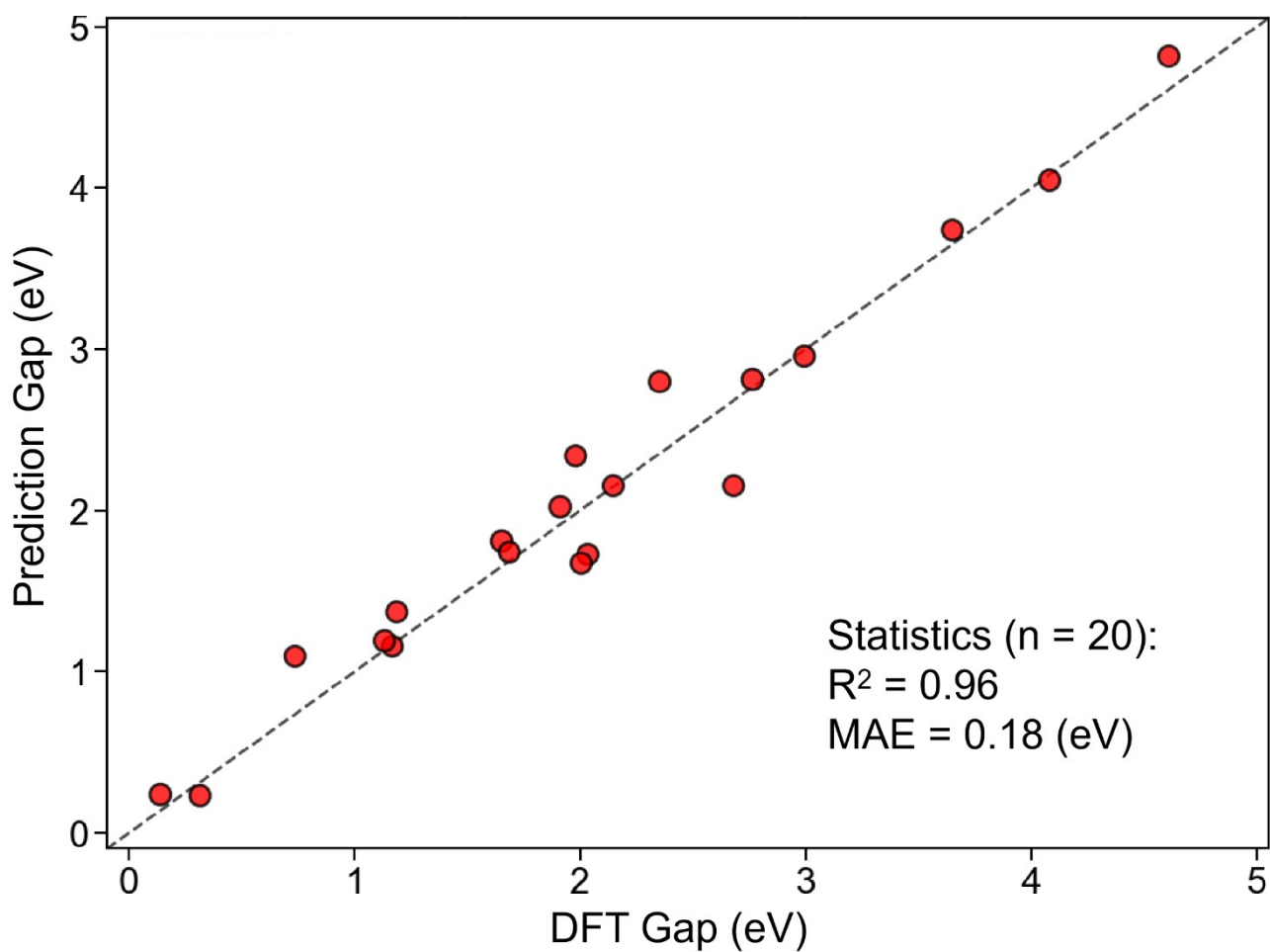


Figure S2. Prediction performance of the optimal XGBoost model on an independent test set consisting of 20 held-out samples.

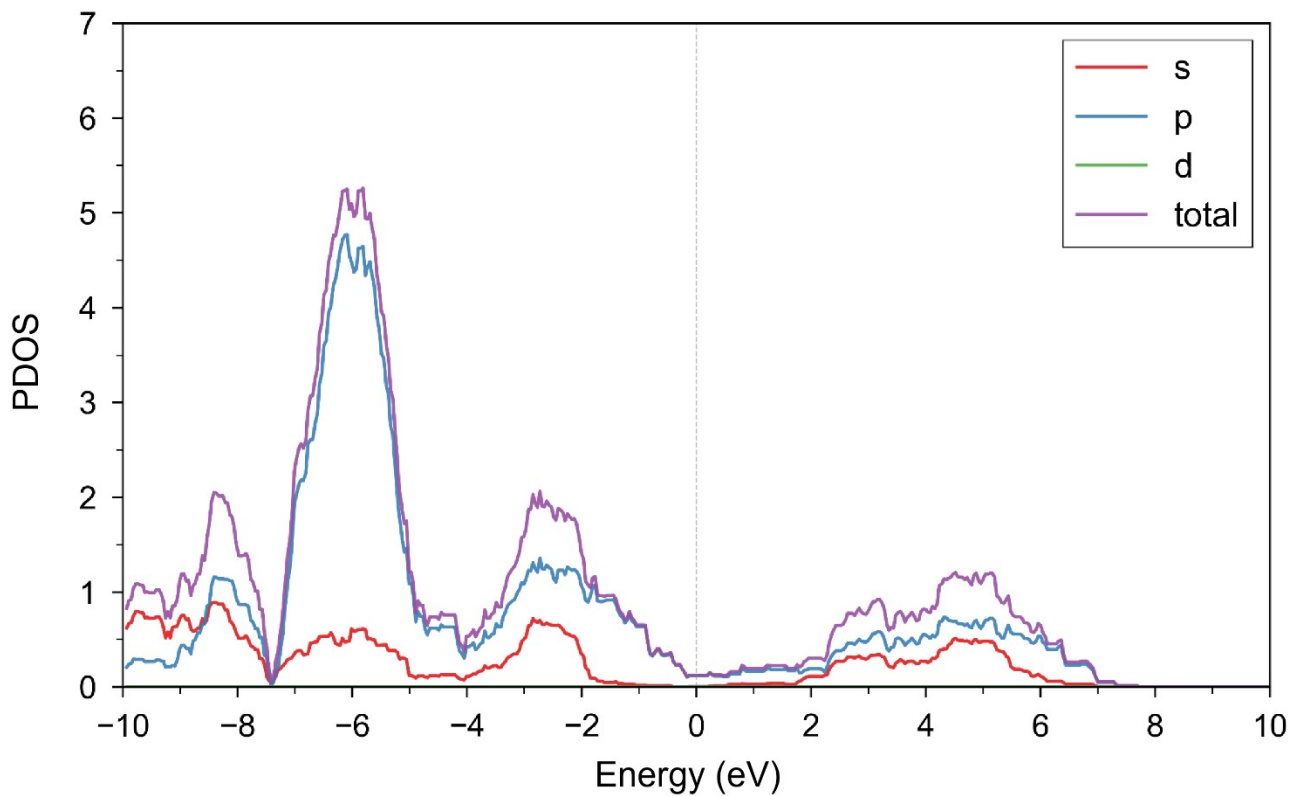


Figure S3. Partial density of states (PDOS) of the Si₂F₂/Si₂H₂ heterostructure, showing the orbital contributions from Si, F, and H atoms near the band edges.

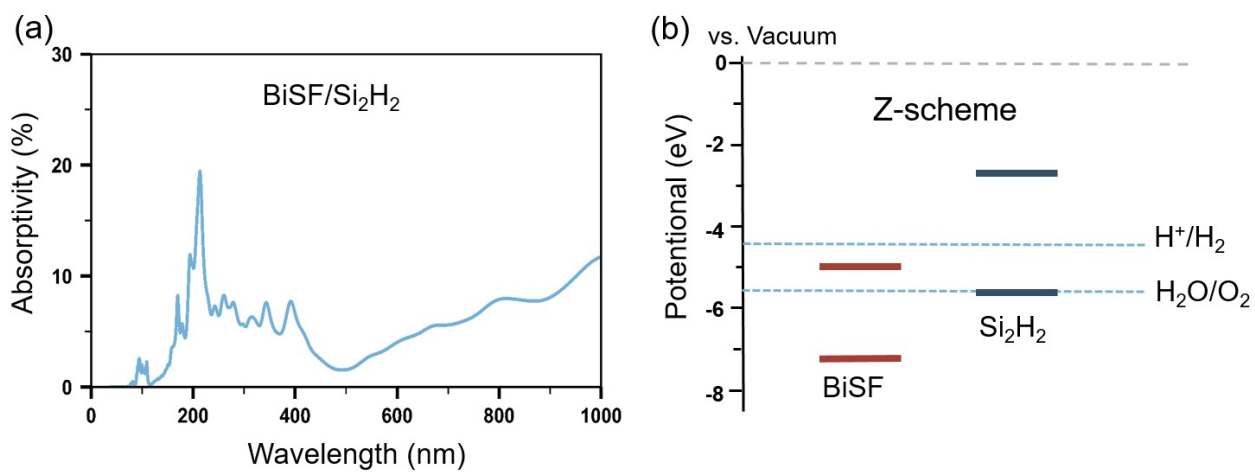


Figure S4. Optical absorption spectrum and electronic band structure of the BiSF/Si₂H₂ heterostructure.

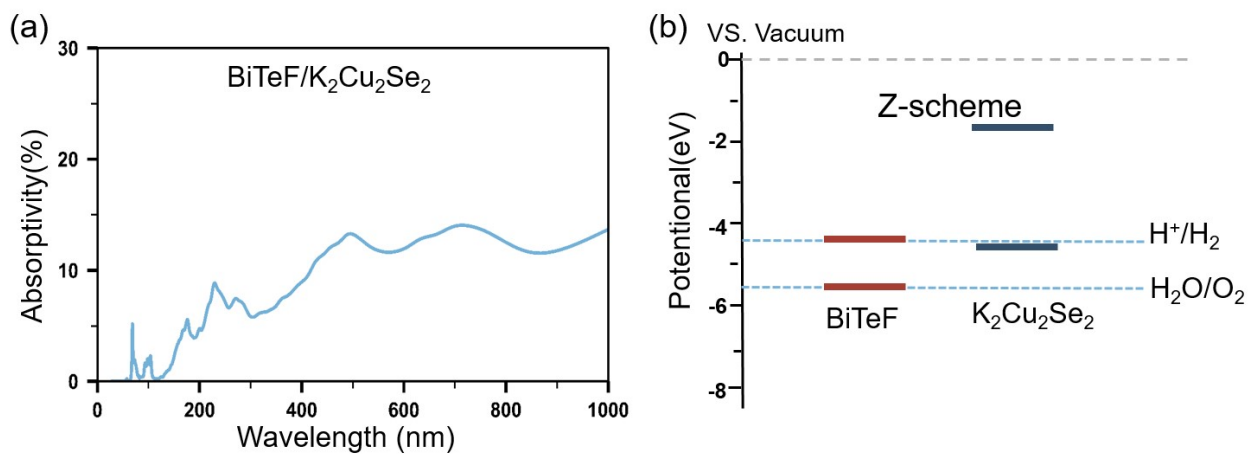


Figure S5. Optical absorption spectrum and electronic band structure of the BiTeF/K₂Cu₂Se₂ heterostructure.

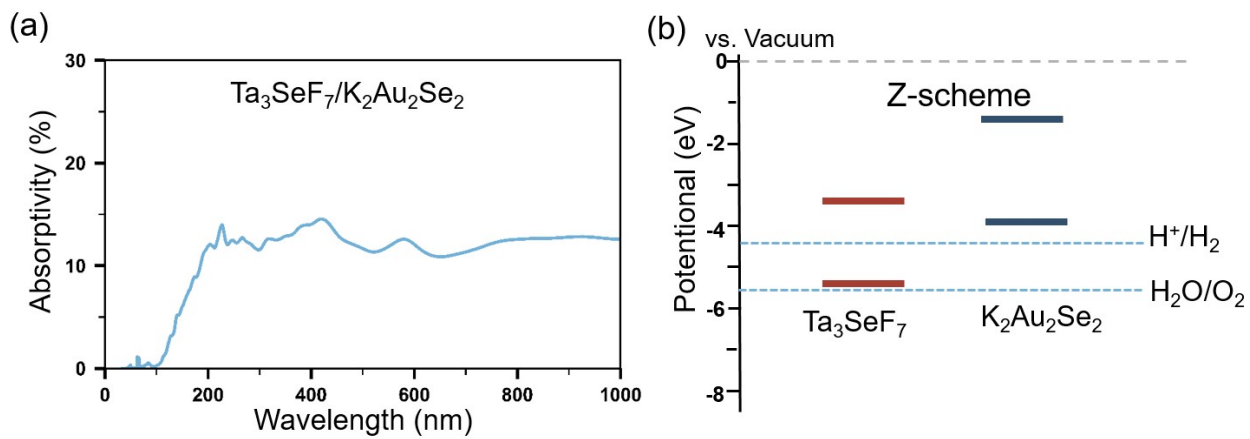


Figure S6. Optical absorption spectrum and electronic band structure of the $\text{Ta}_3\text{SeF}_7/\text{K}_2\text{Au}_2\text{Se}_2$ heterostructure.

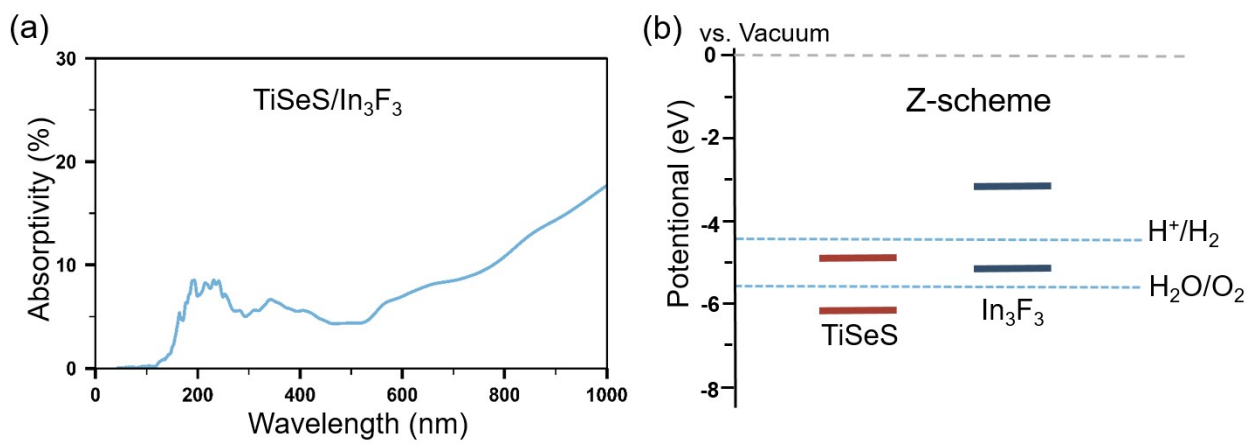


Figure S7. Optical absorption spectrum and electronic band structure of the TiSeS/In₃F₃ heterostructure.

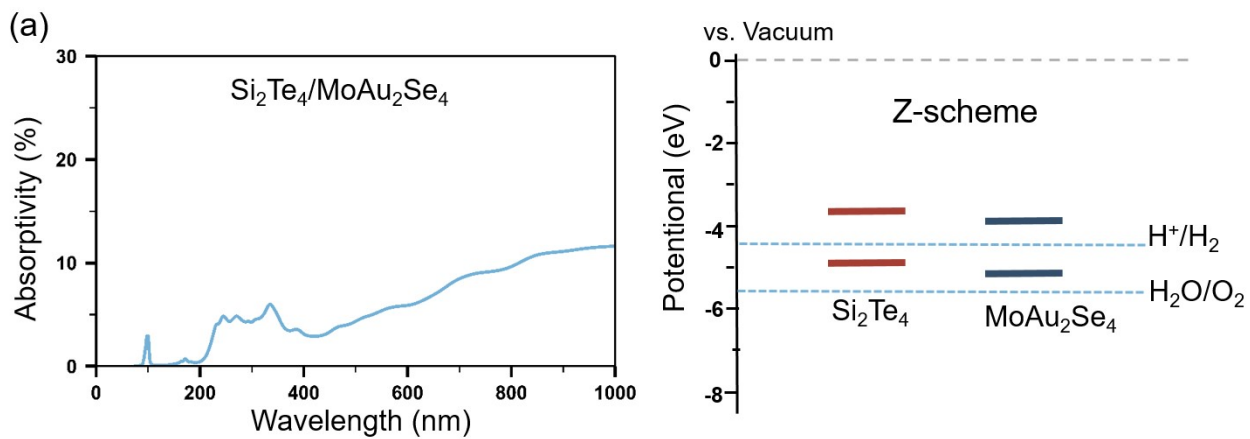


Figure S8. Optical absorption spectrum and electronic band structure of the $\text{Si}_2\text{Te}_4/\text{MoAu}_2\text{Se}_4$ heterostructure.

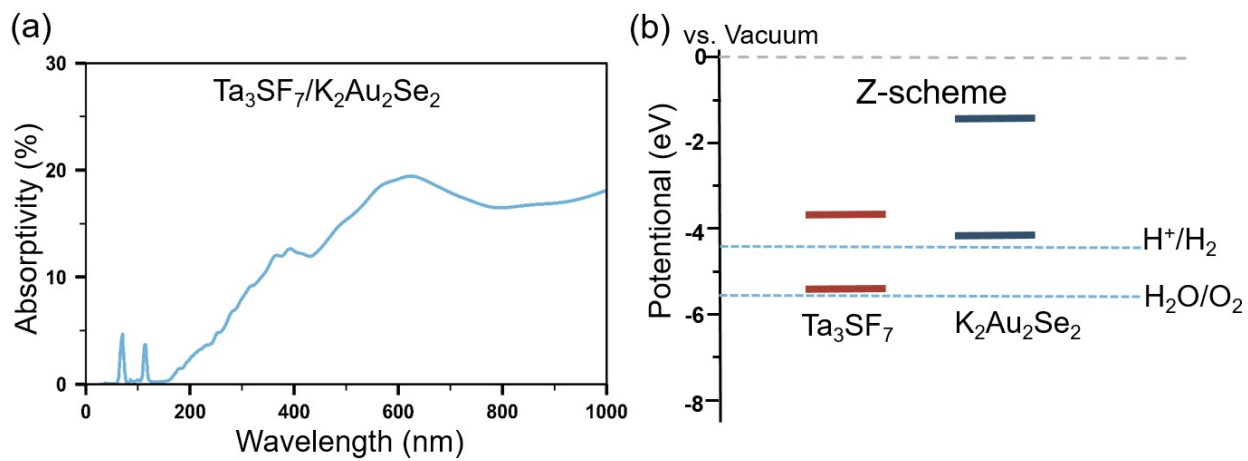


Figure S9. Optical absorption spectrum and electronic band structure of the $\text{Ta}_3\text{SF}_7/\text{K}_2\text{Au}_2\text{Se}_2$ heterostructure.

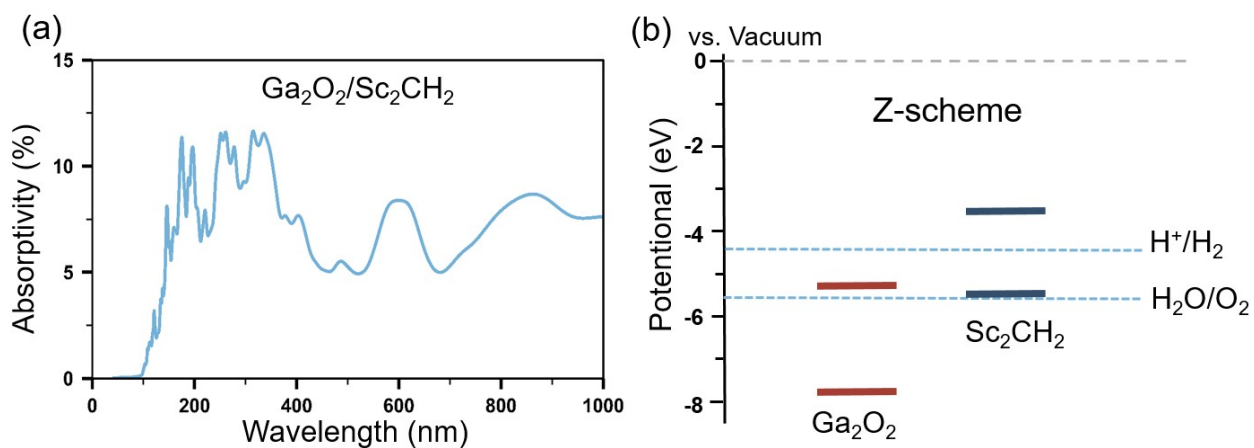


Figure S10. Optical absorption spectrum and electronic band structure of the Ga₂O₂/Sc₂CH₂ heterostructure.

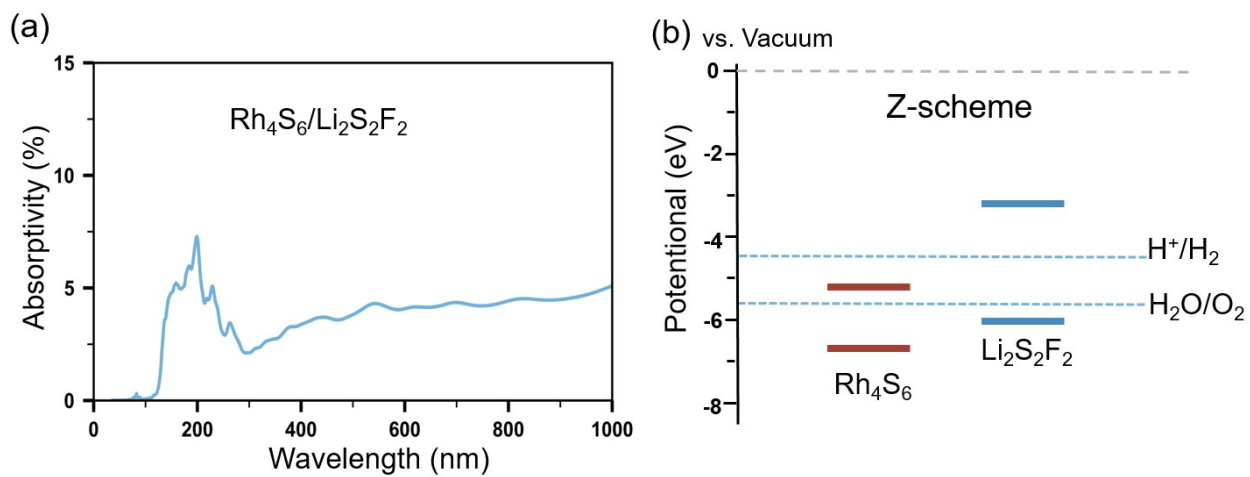


Figure S11. Optical absorption spectrum and electronic band structure of the $\text{Rh}_4\text{S}_6/\text{Li}_2\text{S}_2\text{F}_2$ heterostructure.

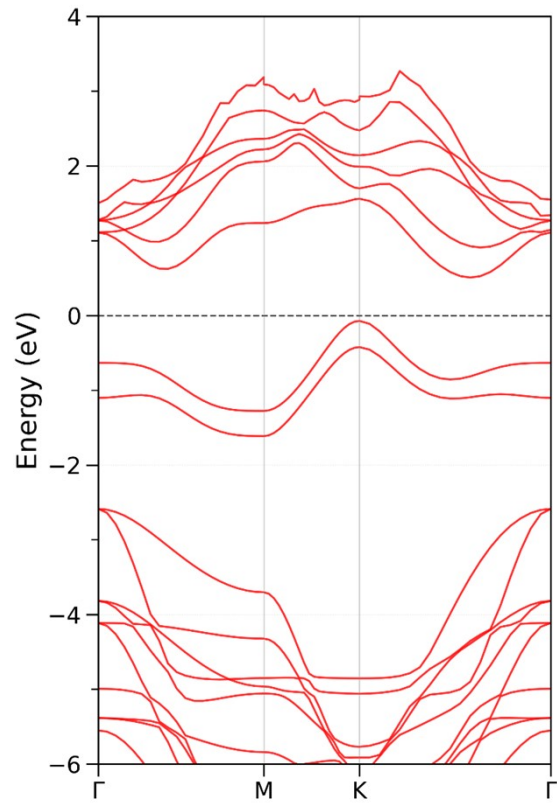


Figure S12. Band structure of the representative heterostructure HfBr₂/HfICl.

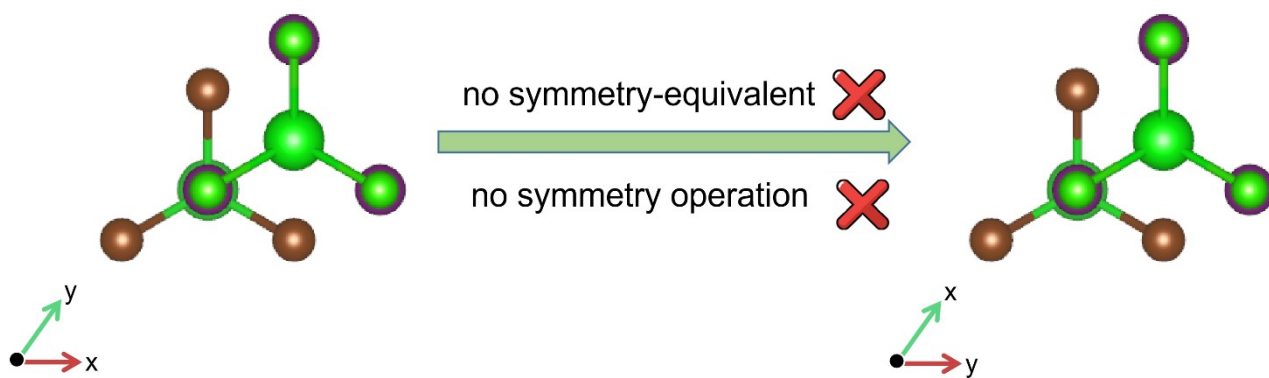


Figure S13. The representative heterostructures exhibits no symmetry operations, and therefore no symmetric equivalents exist.

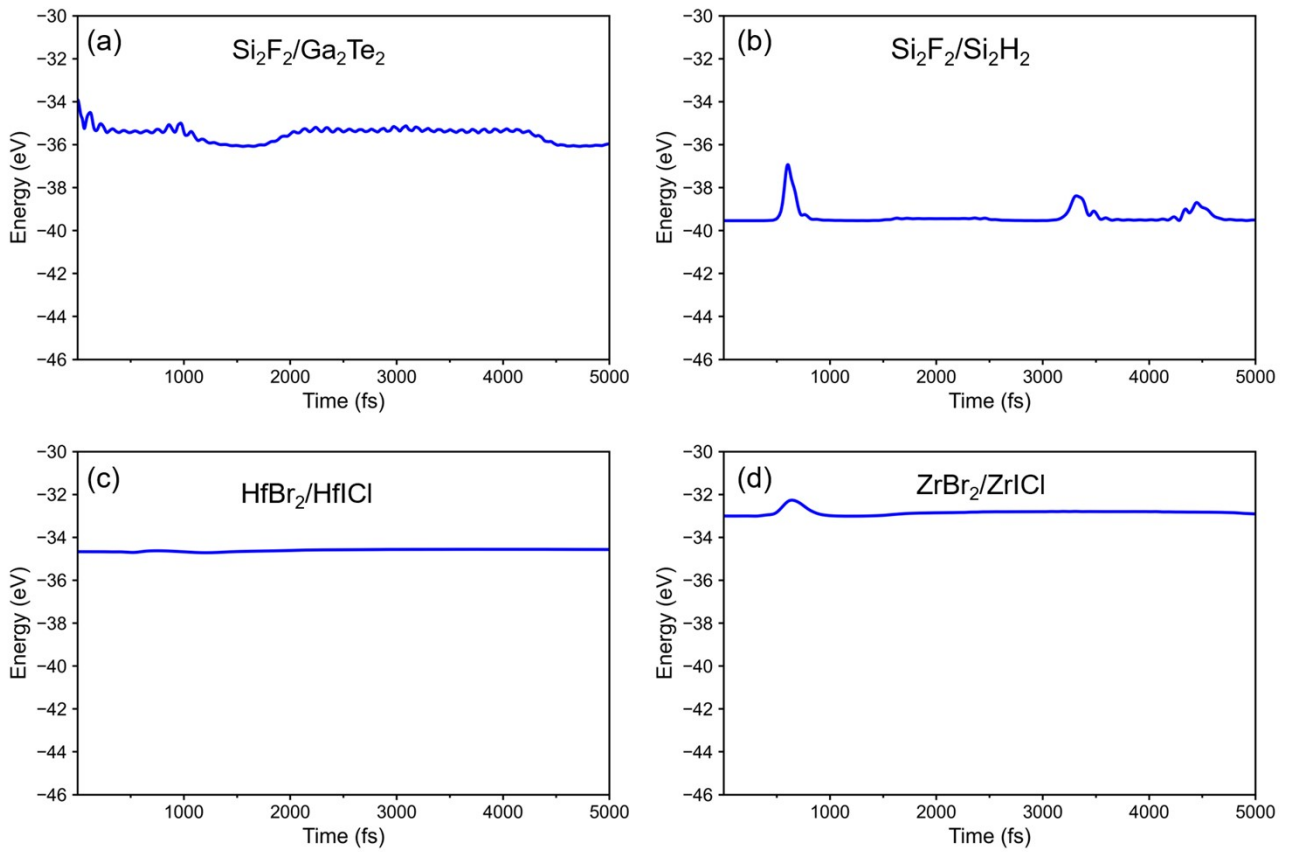


Figure S14. Time evolution of the total energy during ab initio molecular dynamics (AIMD) simulations performed in the NVT ensemble at 300 K for four representative heterostructures: (a) $\text{Si}_2\text{F}_2/\text{Ga}_2\text{Te}_2$, (b) $\text{Si}_2\text{F}_2/\text{Si}_2\text{H}_2$, (c) $\text{HfBr}_2/\text{HfCl}$, (d) $\text{ZrBr}_2/\text{ZrCl}$.

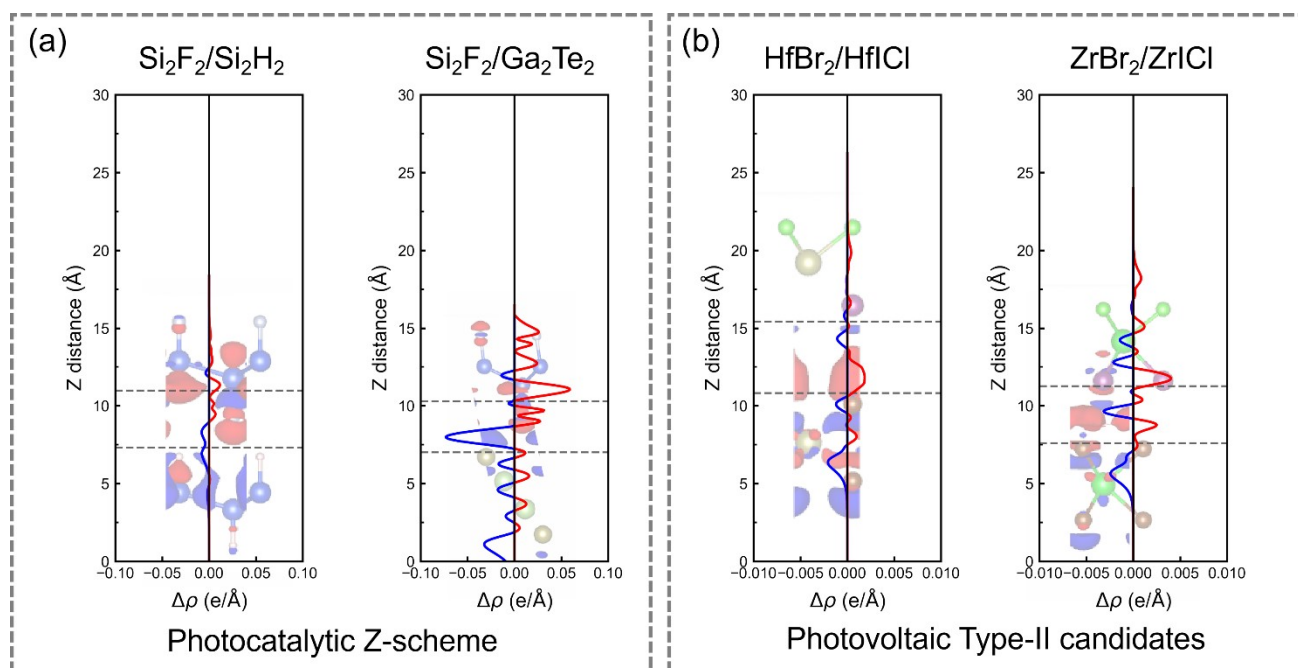


Figure S15. Charge density difference (CDD) and planar-averaged charge density difference profiles ($\Delta\rho(z)$) for four representative heterostructures: (a) $\text{Si}_2\text{F}_2/\text{Si}_2\text{H}_2$ and $\text{Si}_2\text{F}_2/\text{Ga}_2\text{Te}_2$, (b) $\text{HfBr}_2/\text{HfCl}$ and $\text{ZrBr}_2/\text{ZrCl}$. The blue and red regions in the CDD plots indicate electron accumulation and depletion, respectively.

To further assess the structural stability of the screened heterostructures, we performed additional energetic and finite-temperature analyses on several representative systems. Four heterostructures, $\text{Si}_2\text{F}_2/\text{Si}_2\text{H}_2$, $\text{Si}_2\text{F}_2/\text{Ga}_2\text{Te}_2$, $\text{HfBr}_2/\text{HfCl}$, and $\text{ZrBr}_2/\text{ZrCl}$, were selected as prototypical examples, as they span both photocatalytic and photovoltaic candidates identified in our screening workflow and cover a range of chemical compositions, band alignments, and interfacial interaction strengths. The calculated formation energies (E_f) and binding energies (E_b) for these systems (see Table S6) are all negative, indicating thermodynamically favorable formation and stable interlayer coupling. To further evaluate their thermal stability, ab initio molecular dynamics (AIMD) simulations were carried out at ambient conditions. As shown in Fig. S14, all four systems exhibit small and well-bounded total energy fluctuations during the simulations. No noticeable structural distortion, bond breaking and interlayer delamination is observed, and the lattice frameworks remain intact throughout the simulation time. These results confirm that the heterostructures possess good thermodynamic stability at finite temperature.

Further insight into the interfacial charge redistribution was obtained from charge density difference (CDD), planar-averaged charge density difference ($\Delta\rho(z)$), and Bader charge analyses for four representative

heterostructures, namely $\text{Si}_2\text{F}_2/\text{Si}_2\text{H}_2$, $\text{Si}_2\text{F}_2/\text{Ga}_2\text{Te}_2$, $\text{HfBr}_2/\text{HfCl}$, and $\text{ZrBr}_2/\text{ZrCl}$. These systems were selected to represent both photocatalytic Z-scheme and photovoltaic type-II candidates identified in this work. As shown in Fig. S15, the CDD isosurfaces reveal pronounced charge redistribution localized at the van der Waals interfaces, characterized by electron accumulation and depletion on opposite sides of the interface. The corresponding $\Delta\rho(z)$ profiles exhibit clear asymmetry along the out-of-plane direction, indicating the formation of interfacial dipoles and associated built-in electric fields. The Bader charge analysis further quantifies the interlayer charge transfer (see Table S7). Among the four systems, $\text{Si}_2\text{F}_2/\text{Ga}_2\text{Te}_2$ exhibits the largest charge transfer (± 0.1800 e), suggesting a strong interfacial polarization. In comparison, $\text{Si}_2\text{F}_2/\text{Si}_2\text{H}_2$ shows a moderate charge transfer (± 0.0361 e), while $\text{HfBr}_2/\text{HfCl}$, and $\text{ZrBr}_2/\text{ZrCl}$ display much smaller values of ± 0.0025 e and ± 0.0108 e, respectively, indicative of relatively weak interfacial polarization. These results provide direct microscopic evidence for the interfacial charge separation mechanism proposed for both photocatalytic and photovoltaic applications.