Supplementary Information

Electrical transport properties of $TiO_2/MAPbI_3$ and $SnO_2/MAPbI_3$ heterojunction interfaces under high pressure

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Supplementary Tables

Table S1. Atomic coordinate of $\sqrt{2} \times \sqrt{2}$ supercell of (a) $TiO_2/MAPbI_3$ and (b) $SnO_2/MAPbI_3$ heterojunction interface by VASP.

(a)	x	y	z	(b)	x	y	z
Ti_1	-0.001	-0.035	-0.002	Sn_1	-0.016	-0.002	-0.002
Ti_2	0.000	-0.034	0.038	Sn_2	-0.016	-0.001	0.037
Ti_3	0.000	-0.034	0.079	Sn_3	-0.016	-0.001	0.077
Ti_4	0.000	0.034	0.119	Sn_4	-0.017	-0.001	0.117
Ti_5	0.000	-0.032	0.159	Sn_5	-0.018	-0.001	0.158
Ti_6	0.001	-0.028	0.200	Sn_6	-0.015	-0.001	0.197
Ti_7	0.500	0.466	-0.001	Sn_7	0.484	0.499	-0.003
Ti_8	0.500	0.466	0.038	Sn_8	0.484	0.499	0.037
Ti_9	0.500	0.466	0.078	Sn_9	0.483	0.499	0.077
Ti_{10}	0.500	0.466	0.119	Sn_{10}	0.482	0.499	0.117
Ti_{11}	0.500	0.463	0.159	Sn_{11}	0.481	0.499	0.157
Ti_{12}	0.500	0.447	0.198	Sn_{12}	0.475	0.500	0.196
Ti_{13}	0.000	0.466	0.016	Sn_{13}	-0.016	0.499	0.014
Ti_{14}	0.000	0.466	0.058	Sn_{14}	-0.016	0.499	0.056
Ti_{15}	0.000	0.466	0.098	Sn_{15}	-0.017	0.499	0.097
Ti_{16}	0.000	0.465	0.140	Sn_{16}	-0.019	0.499	0.138
Ti_{17}	0.000	0.476	0.182	Sn_{17}	-0.022	0.499	0.180
Ti_{18}	0.501	-0.034	0.016	Sn_{18}	0.484	-0.001	0.014
Ti_{19}	0.501	-0.034	0.059	Sn_{19}	0.484	-0.001	0.056
Ti_{20}	0.501	-0.034	0.099	Sn_{20}	0.483	-0.001	0.097
Ti_{21}	0.501	-0.035	0.140	Sn_{21}	0.483	-0.001	0.138

Ti_{22}	0.501	-0.042	0.181	Sn_{22}	0.483	0.000	0.180
O_1	0.000	0.263	-0.005	O_1	-0.015	0.295	-0.007
O_2	0.000	0.274	0.037	O_2	-0.016	0.307	0.035
O_3	0.000	0.274	0.078	O_3	-0.016	0.307	0.077
O_4	0.000	0.274	0.119	O_4	-0.017	0.307	0.117
O_5	0.000	0.276	0.160	O_5	-0.020	0.307	0.158
O_6	0.001	0.274	0.201	O_6	-0.022	0.299	0.200
O_7	0.500	0.763	-0.005	O_7	0.483	0.795	-0.007
O_8	0.499	0.774	0.037	O_8	0.483	0.807	0.035
O_9	0.499	0.774	0.078	O_9	0.483	0.807	0.077
O_{10}	0.499	0.774	0.119	O_{10}	0.483	0.807	0.117
O_{11}	0.499	0.771	0.160	O_{11}	0.483	0.808	0.159
O_{12}	0.499	0.743	0.203	O_{12}	0.481	0.794	0.201
O_{13}	-0.001	0.670	-0.005	O_{13}	-0.015	0.703	-0.007
O_{14}	0.000	0.658	0.037	O_{14}	-0.016	0.691	0.035
O_{15}	0.000	0.658	0.078	O_{15}	-0.016	0.691	0.077
O_{16}	0.000	0.658	0.119	O_{16}	-0.017	0.691	0.117
O_{17}	0.000	0.660	0.160	O_{17}	-0.020	0.691	0.158
O_{18}	0.000	0.671	0.202	O_{18}	-0.022	0.699	0.200
O_{19}	0.500	0.170	-0.005	O_{19}	0.485	0.203	-0.007
O_{20}	0.500	0.158	0.037	O_{20}	0.484	0.190	0.035
O_{21}	0.500	0.158	0.078	O_{21}	0.484	0.191	0.077
O_{22}	0.500	0.158	0.119	O_{22}	0.482	0.191	0.117
O_{23}	0.500	0.155	0.160	O_{23}	0.482	0.191	0.158
O_{24}	0.500	0.153	0.203	O_{24}	0.481	0.206	0.201
O_{25}	0.696	0.467	0.018	O_{25}	0.680	0.499	0.016

O_{26}	0.693	0.466	0.058	O_{26}	0.677	0.499	0.057
O_{27}	0.692	0.466	0.099	O_{27}	0.676	0.499	0.097
O_{28}	0.693	0.465	0.139	O_{28}	0.675	0.499	0.137
O_{29}	0.695	0.464	0.179	O_{29}	0.674	0.499	0.177
O_{30}	0.196	-0.033	0.018	O_{30}	0.181	-0.001	0.016
O_{31}	0.193	-0.034	0.058	O_{31}	0.177	-0.001	0.057
O_{32}	0.192	-0.034	0.099	O_{32}	0.176	-0.001	0.097
O_{33}	0.193	-0.034	0.139	O_{33}	0.175	-0.001	0.138
O_{34}	0.196	-0.038	0.180	O_{34}	0.179	0.000	0.178
O_{35}	0.303	0.466	0.018	O_{35}	0.288	0.499	0.016
O_{36}	0.306	0.466	0.058	O_{36}	0.291	0.499	0.057
O_{37}	0.306	0.465	0.098	O_{37}	0.290	0.499	0.097
O_{38}	0.306	0.465	0.139	O_{38}	0.288	0.499	0.137
O_{39}	0.306	0.464	0.179	O_{39}	0.282	0.499	0.177
O_{40}	0.802	-0.034	0.018	O_{40}	0.787	-0.001	0.016
O_{41}	0.807	-0.034	0.058	O_{41}	0.791	-0.001	0.057
O_{42}	0.807	-0.034	0.099	O_{42}	0.791	-0.001	0.097
O_{43}	0.807	-0.034	0.137	O_{43}	0.791	-0.001	0.138
O_{44}	0.804	-0.037	0.180	O_{44}	0.787	0.000	0.178
Pb_1	0.997	0.018	0.275	Pb_1	0.054	-0.006	0.269
Pb_2	0.003	0.992	0.350	Pb_2	0.023	-0.012	0.346
Pb_3	-0.021	0.971	0.427	Pb_3	0.012	-0.014	0.425
I_1	0.473	0.038	0.276	I_1	0.568	-0.011	0.270
I_2	0.475	0.959	0.350	I_2	0.530	-0.011	0.347
I_3	0.467	0.972	0.421	I_3	0.515	-0.020	0.423
I_4	0.950	0.539	0.275	I_4	0.052	0.491	0.273

I_5	0.951	0.499	0.349
I_6	0.949	0.481	0.424
I_7	0.002	0.042	0.234
I_8	-0.046	0.057	0.312
I_9	-0.041	0.013	0.388
I_{10}	-0.016	0.920	0.465
C_1	0.460	0.587	0.241
C_2	0.439	0.487	0.312
C_3	0.441	0.454	0.386
C_4	0.468	0.437	0.458
N_1	0.503	0.793	0.234
N_2	0.645	0.589	0.312
N_3	0.650	0.548	0.386
N_4	0.480	0.665	0.456
H_1	0.644	0.849	0.238
H_2	0.736	0.544	0.321
H_3	0.733	0.501	0.396
H_4	0.614	0.725	0.461
H_5	0.391	0.897	0.238
H_6	0.635	0.748	0.312
H_7	0.645	0.708	0.387
H_8	0.352	0.737	0.461
H_9	0.504	0.787	0.221
H_{10}	0.725	0.555	0.301
H_{11}	0.736	0.512	0.376
H_{12}	0.481	0.715	0.444

I_5	0.002	0.489	0.349
I_6	-0.022	0.487	0.423
I_7	0.147	-0.007	0.233
I_8	0.066	-0.010	0.310
I_9	0.051	-0.011	0.387
I_{10}	0.068	-0.012	0.464
C_1	0.686	0.488	0.234
C_2	0.553	0.489	0.307
C_3	0.551	0.486	0.382
C_4	0.527	0.485	0.458
N_1	0.526	0.489	0.247
N_2	0.465	0.489	0.324
N_3	0.442	0.489	0.398
N_4	0.297	0.487	0.457
H_1	0.379	0.490	0.242
H_2	0.305	0.488	0.324
H_3	0.284	0.483	0.396
H_4	0.243	0.488	0.446
H_5	0.541	0.617	0.254
H_6	0.509	0.618	0.330
H_7	0.478	0.613	0.405
H_8	0.235	0.620	0.463
H_9	0.538	0.358	0.254
H_{10}	0.509	0.359	0.330
H_{11}	0.479	0.354	0.404
H_{12}	0.233	0.355	0.463

H_{15}	0.361	0.510	0.375	H_{15}	0.505	0.625	0.375
H_{16}	0.326	0.384	0.452	H_{16}	0.586	0.624	0.452
H_{17}	0.453	0.597	0.255	H_{17}	0.664	0.350	0.226
H_{18}	0.363	0.528	0.324	H_{18}	0.501	0.350	0.301
H_{19}	0.356	0.497	0.397	H_{19}	0.507	0.348	0.375
H_{20}	0.466	0.394	0.471	H_{20}	0.583	0.348	0.452
H_{21}	0.583	0.480	0.238	H_{21}	0.838	0.482	0.239
H_{22}	0.461	0.321	0.311	H_{22}	0.721	0.489	0.308
H_{23}	0.458	0.286	0.385	H_{23}	0.717	0.487	0.384
H24	0.603	0.375	0.455	H24	0.573	0.482	0.469

Table S2. Atomic coordinate of $\sqrt{2} \times \sqrt{2}$ supercell of (a) $TiO_2/MAPbI_3$ and (b) $SnO_2/MAPbI_3$ heterojunction interfaces by MS (Materials Studio).

(a)	x	y	z	(b)	x	y	z
Ti_1	-0.001	-0.035	-0.002	Sn_1	-0.015	-0.002	-0.002
Ti_2	0.000	-0.034	0.038	Sn_2	-0.015	-0.001	0.036
Ti_3	0.000	-0.034	0.079	Sn_3	-0.015	-0.001	0.078
Ti_4	0.000	0.034	0.119	Sn_4	-0.017	-0.001	0.117
Ti_5	0.000	-0.032	0.159	Sn_5	-0.018	-0.001	0.158
Ti_6	0.001	-0.028	0.200	Sn_6	-0.015	-0.001	0.197
Ti_7	0.501	0.467	-0.001	Sn_7	0.484	0.498	-0.003

Ti_8	0.501	0.467	0.038	Sn_8	0.484	0.498	0.037
Ti_9	0.501	0.467	0.078	Sn_9	0.483	0.498	0.077
Ti_{10}	0.500	0.466	0.119	Sn_{10}	0.482	0.499	0.117
Ti_{11}	0.500	0.463	0.159	Sn_{11}	0.481	0.499	0.157
Ti_{12}	0.500	0.447	0.198	Sn_{12}	0.475	0.500	0.196
Ti_{13}	0.000	0.466	0.016	Sn_{13}	-0.016	0.499	0.014
Ti_{14}	0.000	0.466	0.058	Sn_{14}	-0.016	0.499	0.056
Ti_{15}	0.000	0.466	0.098	Sn_{15}	-0.017	0.499	0.097
Ti_{16}	0.000	0.465	0.140	Sn_{16}	-0.019	0.499	0.138
Ti_{17}	0.000	0.476	0.182	Sn_{17}	-0.022	0.499	0.180
Ti_{18}	0.500	-0.034	0.016	Sn_{18}	0.485	-0.001	0.014
Ti_{19}	0.500	-0.034	0.059	Sn_{19}	0.485	-0.001	0.056
Ti_{20}	0.500	-0.034	0.099	Sn_{20}	0.483	-0.001	0.097
Ti_{21}	0.500	-0.035	0.140	Sn_{21}	0.483	-0.001	0.138
Ti_{22}	0.500	-0.042	0.181	Sn_{22}	0.483	0.000	0.180
O_1	0.000	0.263	-0.005	O_1	-0.015	0.295	-0.007
O_2	0.000	0.274	0.037	O_2	-0.016	0.307	0.035
O_3	0.000	0.274	0.078	O_3	-0.016	0.307	0.077
O_4	0.000	0.274	0.119	O_4	-0.017	0.307	0.117
O_5	0.000	0.276	0.160	O_5	-0.020	0.307	0.158
O_6	0.001	0.274	0.201	O_6	-0.022	0.299	0.200
O_7	0.500	0.763	-0.005	O_7	0.483	0.795	-0.007
O_8	0.499	0.774	0.037	O_8	0.483	0.807	0.035
O_9	0.499	0.774	0.078	O_9	0.483	0.807	0.077
O_{10}	0.499	0.774	0.119	O_{10}	0.483	0.807	0.117
O_{11}	0.499	0.771	0.160	O_{11}	0.483	0.808	0.159

O_{12}	0.499	0.743	0.203	O_{12}	0.483	0.794	0.201
O_{13}	-0.001	0.670	-0.005	O_{13}	-0.015	0.703	-0.007
O_{14}	0.000	0.658	0.037	O_{14}	-0.016	0.691	0.035
O_{15}	0.000	0.658	0.078	O_{15}	-0.016	0.691	0.077
O_{16}	0.000	0.658	0.119	O_{16}	-0.017	0.691	0.117
O_{17}	0.000	0.660	0.160	O_{17}	-0.020	0.691	0.158
O_{18}	0.000	0.671	0.202	O_{18}	-0.022	0.699	0.200
O_{19}	0.500	0.170	-0.005	O_{19}	0.485	0.203	-0.007
O_{20}	0.500	0.158	0.037	O_{20}	0.484	0.190	0.035
O_{21}	0.500	0.158	0.078	O_{21}	0.484	0.191	0.077
O_{22}	0.500	0.158	0.119	O_{22}	0.482	0.191	0.117
O_{23}	0.500	0.155	0.160	O_{23}	0.482	0.191	0.158
O_{24}	0.500	0.153	0.203	O_{24}	0.481	0.206	0.201
O_{25}	0.696	0.467	0.018	O_{25}	0.680	0.498	0.016
O_{26}	0.693	0.466	0.058	O_{26}	0.677	0.498	0.057
O_{27}	0.692	0.466	0.099	O_{27}	0.676	0.498	0.097
O_{28}	0.693	0.465	0.139	O_{28}	0.675	0.498	0.137
O_{29}	0.695	0.464	0.179	O_{29}	0.675	0.498	0.177
O_{30}	0.196	-0.033	0.018	O_{30}	0.181	-0.001	0.016
O_{31}	0.193	-0.034	0.058	O_{31}	0.177	-0.001	0.057
O_{32}	0.192	-0.034	0.099	O_{32}	0.176	-0.001	0.097
O_{33}	0.193	-0.034	0.139	O_{33}	0.175	-0.001	0.138
O_{34}	0.196	-0.038	0.180	O_{34}	0.179	0.000	0.178
O_{35}	0.303	0.466	0.018	O_{35}	0.288	0.498	0.016
O_{36}	0.306	0.466	0.058	O_{36}	0.291	0.498	0.057
O_{37}	0.306	0.466	0.098	O_{37}	0.290	0.498	0.097

O_{38}	0.306	0.466	0.139	O_{38}	0.288	0.498	0.137
O_{39}	0.306	0.466	0.179	O_{39}	0.282	0.498	0.177
O_{40}	0.802	-0.034	0.018	O_{40}	0.787	-0.001	0.016
O_{41}	0.807	-0.034	0.058	O_{41}	0.791	-0.001	0.057
O_{42}	0.807	-0.034	0.099	O_{42}	0.791	-0.001	0.097
O_{43}	0.807	-0.034	0.137	O_{43}	0.791	-0.001	0.138
O_{44}	0.804	-0.037	0.180	O_{44}	0.787	0.000	0.178
Pb_1	0.997	0.018	0.275	Pb_1	0.054	-0.006	0.269
Pb_2	0.003	0.992	0.350	Pb_2	0.023	-0.012	0.346
Pb_3	-0.021	0.971	0.427	Pb_3	0.012	-0.014	0.425
I_1	0.473	0.038	0.276	I_1	0.568	-0.011	0.270
I_2	0.475	0.959	0.350	I_2	0.530	-0.011	0.347
I_3	0.467	0.972	0.421	I_3	0.515	-0.020	0.423
I_4	0.950	0.539	0.275	I_4	0.052	0.491	0.273
I_5	0.951	0.499	0.349	I_5	0.002	0.489	0.349
I_6	0.949	0.481	0.424	I_6	-0.022	0.487	0.423
I_7	0.002	0.042	0.234	I_7	0.147	-0.007	0.233
I_8	-0.046	0.057	0.312	I_8	0.066	-0.010	0.310
I_9	-0.041	0.013	0.388	I_9	0.051	-0.011	0.387
I_{10}	-0.016	0.920	0.465	I_{10}	0.068	-0.012	0.464
C_1	0.460	0.587	0.241	C_1	0.686	0.488	0.234
C_2	0.439	0.487	0.312	C_2	0.553	0.488	0.307
C_3	0.441	0.454	0.386	C_3	0.551	0.486	0.382
C_4	0.467	0.437	0.458	C_4	0.527	0.485	0.458
N_1	0.501	0.793	0.234	N_1	0.526	0.488	0.247
N_2	0.645	0.589	0.312	N_2	0.465	0.488	0.324

N_3	0.650	0.548	0.386	N_3	0.442	0.488	0.398
N_4	0.480	0.665	0.456	N_4	0.297	0.488	0.457
H_1	0.644	0.849	0.238	H_1	0.379	0.490	0.242
H_2	0.736	0.544	0.321	H_2	0.305	0.488	0.324
H_3	0.733	0.501	0.396	H_3	0.284	0.483	0.396
H_4	0.614	0.725	0.461	H_4	0.243	0.488	0.446
H_5	0.391	0.897	0.238	H_5	0.541	0.617	0.254
H_6	0.635	0.748	0.312	H_6	0.509	0.617	0.330
H_7	0.645	0.708	0.387	H_7	0.478	0.613	0.405
H_8	0.352	0.737	0.461	H_8	0.235	0.620	0.463
H_9	0.504	0.787	0.221	H_9	0.538	0.358	0.254
H_{10}	0.725	0.555	0.301	H_{10}	0.509	0.359	0.330
H_{11}	0.736	0.512	0.376	H_{11}	0.479	0.354	0.404
H_{12}	0.481	0.715	0.444	H_{12}	0.233	0.355	0.463
H_{15}	0.360	0.510	0.375	H_{15}	0.505	0.625	0.375
H_{16}	0.325	0.384	0.452	H_{16}	0.586	0.624	0.452
H_{17}	0.455	0.596	0.255	H_{17}	0.664	0.350	0.226
H_{18}	0.365	0.528	0.324	H_{18}	0.501	0.350	0.301
H_{19}	0.356	0.497	0.397	H_{19}	0.507	0.348	0.375
H_{20}	0.466	0.394	0.471	H_{20}	0.583	0.349	0.452
H_{21}	0.585	0.480	0.238	H_{21}	0.838	0.480	0.239
H_{22}	0.461	0.320	0.311	H_{22}	0.721	0.489	0.308
H_{23}	0.455	0.285	0.385	H_{23}	0.717	0.487	0.384
H24	0.600	0.375	0.455	H24	0.572	0.482	0.469

Table S3.The interface model parameters of SnO_2 (TiO_2)/$MAPbI_3$ heterojunction.

Optimized heterojunction interface models	Atomic bond	Atomic bond length (Å)	Interface binding energy (eV/nm^2)
TiO_2/$MAPbI_3$	Pb-O I-Ti	2.80 2.90	-6.75
SnO_2/$MAPbI_3$	Pb-O I-Sn	1.78 1.89	-1.02

Table S4.The binding energy of SnO_2 (TiO_2)/$MAPbI_3$ heterojunction interfaces system under ambient conditions.

Heterojunction interfaces	E(eV)	E_{MAPbI3}(eV)	$E_{SnO2\ (TiO2)}$(eV)	ΔE(eV)	ΔE_{unit}(eV/nm^2)
SnO_2 /$MAPbI_3$	-1044.88	-330.25	-715.52	-0.89	-1.02
TiO_2/$MAPbI_3$	-976.38	-330.05	-652.20	-5.87	-6.75

Table S5.The interface binding energy of SnO_2 (TiO_2)/$MAPbI_3$ heterojunction up to 20 GPa.

Pressure (GPa)	Heterojunction interface models	Interface binding energy (eV/nm^2)
0 GPa	TiO_2/$MAPbI_3$	-6.75
	SnO_2/$MAPbI_3$	-1.02
5 GPa	TiO_2/$MAPbI_3$	-6.61
	SnO_2/$MAPbI_3$	-0.92
10 GPa	TiO_2/$MAPbI_3$	-6.41
	SnO_2/$MAPbI_3$	-0.84
15 GPa	TiO_2/$MAPbI_3$	-6.15
	SnO_2/$MAPbI_3$	-0.77
20 GPa	TiO_2/$MAPbI_3$	-5.85
	SnO_2/$MAPbI_3$	-0.72

Table S6. The charge transport driving force of SnO_2 (TiO_2)/$MAPbI_3$ heterojunction interfaces up to 20 GPa.

Heterojunction interfaces	E_d(eV)	ΔE_d(eV)	Pressure(GPa)
TiO_2/$MAPbI_3$	0.75	0.70	0
SnO_2/$MAPbI_3$	1.45		
TiO_2/$MAPbI_3$	0.82	0.84	5
SnO_2/$MAPbI_3$	1.66		
TiO_2/$MAPbI_3$	0.94	0.99	10
SnO_2/$MAPbI_3$	1.93		
TiO_2/$MAPbI_3$	1.09	1.25	15
SnO_2/$MAPbI_3$	2.34		
TiO_2/$MAPbI_3$	1.26	1.62	20
SnO_2/$MAPbI_3$	2.88		

Table S7. Binding energy (BE) of the SnO_2/$MAPbI_3$ and TiO_2/$MAPbI_3$ interfaces on MA orientation [001] [011] and [111] under ambient conditions.

MA orientation	Interface binding energy (eV/nm^2)			
	SnO_2/$MAPbI_3$		TiO_2/$MAPbI_3$	
	MAI-termination	PbI_2-termination	MAI-termination	PbI_2-termination
[001]	0.84	2.98	0.86	2.36
[011]	0.86	2.84	0.94	2.42
[111]	1.51	2.72	1.22	2.32

Table S8. Binding energy (BE) of the SnO_2/$MAPbI_3$ and TiO_2/$MAPbI_3$ interfaces on MA orientation [001] [011] and [111] at 5 GPa.

MA orientation	Interface binding energy (eV/nm^2)			
	SnO_2/$MAPbI_3$		TiO_2/$MAPbI_3$	
	MAI-termination	PbI_2-termination	MAI-termination	PbI_2-termination

[001]	0.92	3.12	0.97	3.34
[011]	0.94	3.44	1.02	3.02
[111]	1.71	3.32	1.40	2.94

Table S9.Binding energy (BE) of the $SnO_2/MAPbI_3$ and $TiO_2/MAPbI_3$ interfaces on MA orientation [001] [011] and [111] at 10 GPa.

MA orientation	Interface binding energy (eV/nm^2)			
	$SnO_2/MAPbI_3$		$TiO_2/MAPbI_3$	
	MAI-termination	PbI_2-termination	MAI-termination	PbI_2-termination
[001]	1.24	3.25	1.27	3.42
[011]	1.27	3.78	1.34	3.36
[111]	1.95	3.79	1.61	3.49

Table S10.Binding energy (BE) of the $SnO_2/MAPbI_3$ and $TiO_2/MAPbI_3$ interfaces on MA orientation [001] [011] and [111] at 15 GPa.

MA orientation	Interface binding energy (eV/nm^2)			
	$SnO_2/MAPbI_3$		$TiO_2/MAPbI_3$	
	MAI-termination	PbI_2-termination	MAI-termination	PbI_2-termination
[001]	1.47	3.45	1.52	3.64
[011]	1.52	3.94	1.61	3.54
[111]	2.08	3.99	1.74	3.69

Supplementary Figures

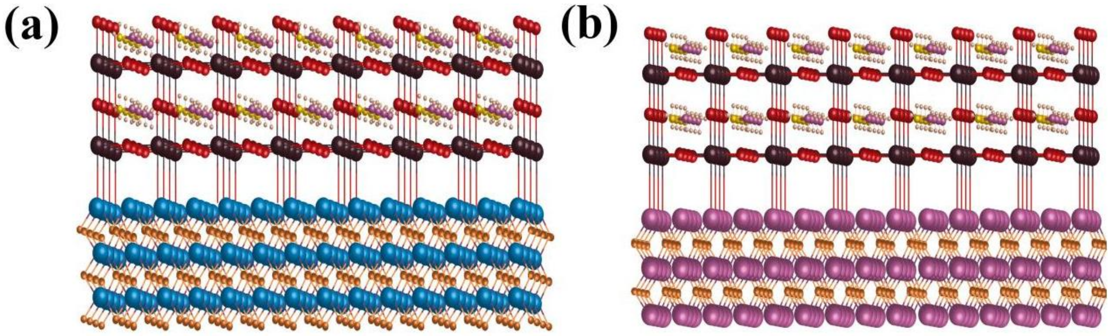

Fig. S1 Initial geometry of TiO_2/$MAPbI_3$ and SnO_2/$MAPbI_3$ heterojunction interfaces.

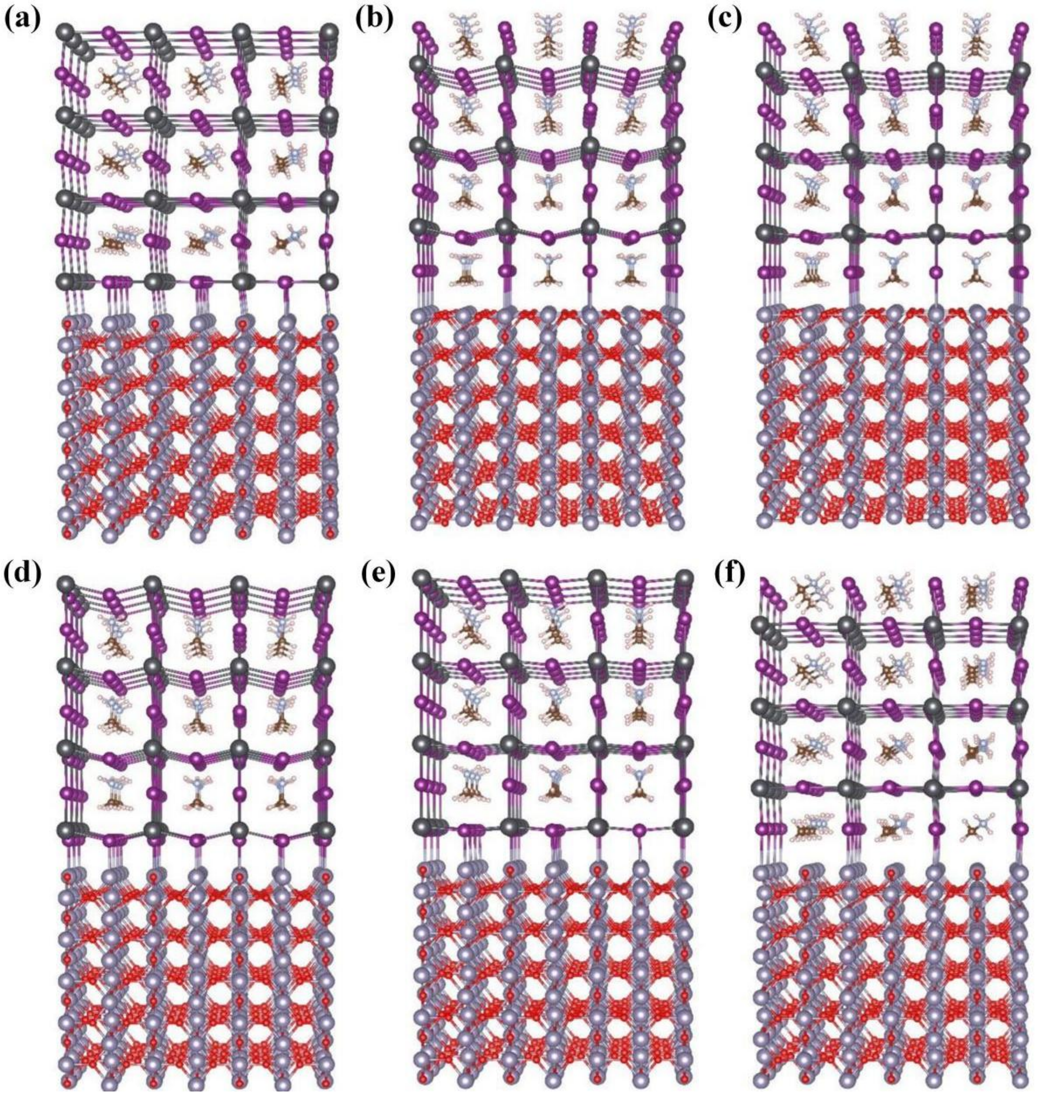

Fig. S2 Initial geometry of SnO_2 (TiO_2)/$MAPbI_3$ interfaces of (a-c) MAI-termination with (a) [001], (b) [011], and (c) [111] direction of MA and at (d-f) PbI_2-termination with (d) [001], (e) [011], and (f) [111] direction of MA. [Pb (black), I (purple), C (brown) N (light blue), H (white), Sn (dark blue), and O (red)].

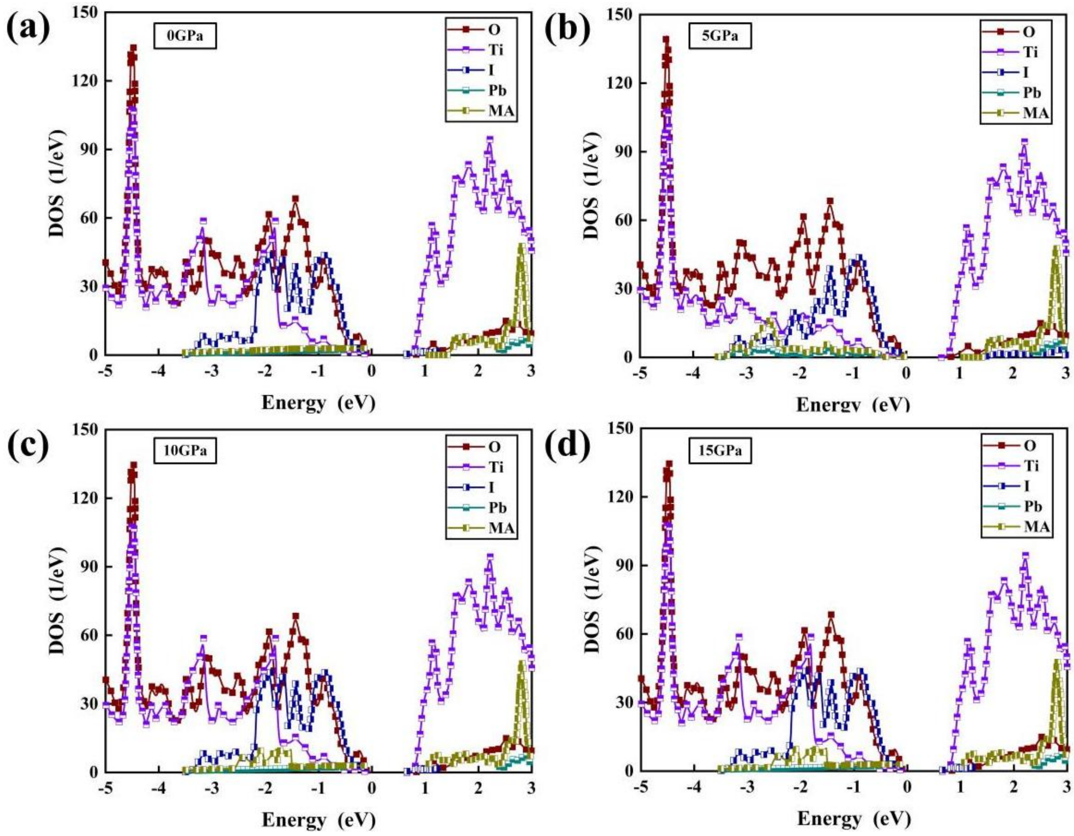

Fig. S3 PDOS of MA, Pb, I, Ti, O at (a) 0 GPa, (b) 5 GPa, (c) 10 GPa, (d) 15 GPa.

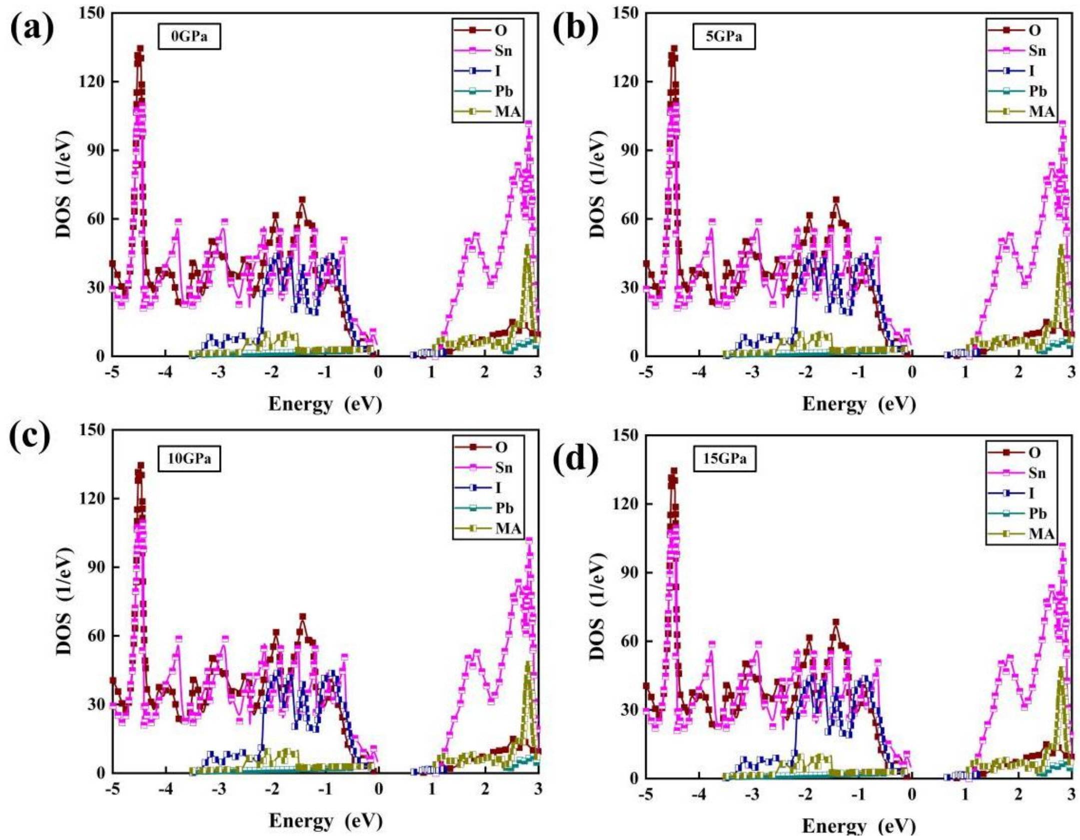

Fig. S4 PDOS of MA, Pb, I, Sn, O at (a) 0 GPa, (b) 5 GPa, (c) 10 GPa, (d) 15 GPa.