$K_3Ti_2Cl_{9-x}Br_x$: Structurally stable lead-free Perovskites as permissive absorbers for Solar Cell and Visible-Light Photocatalysis

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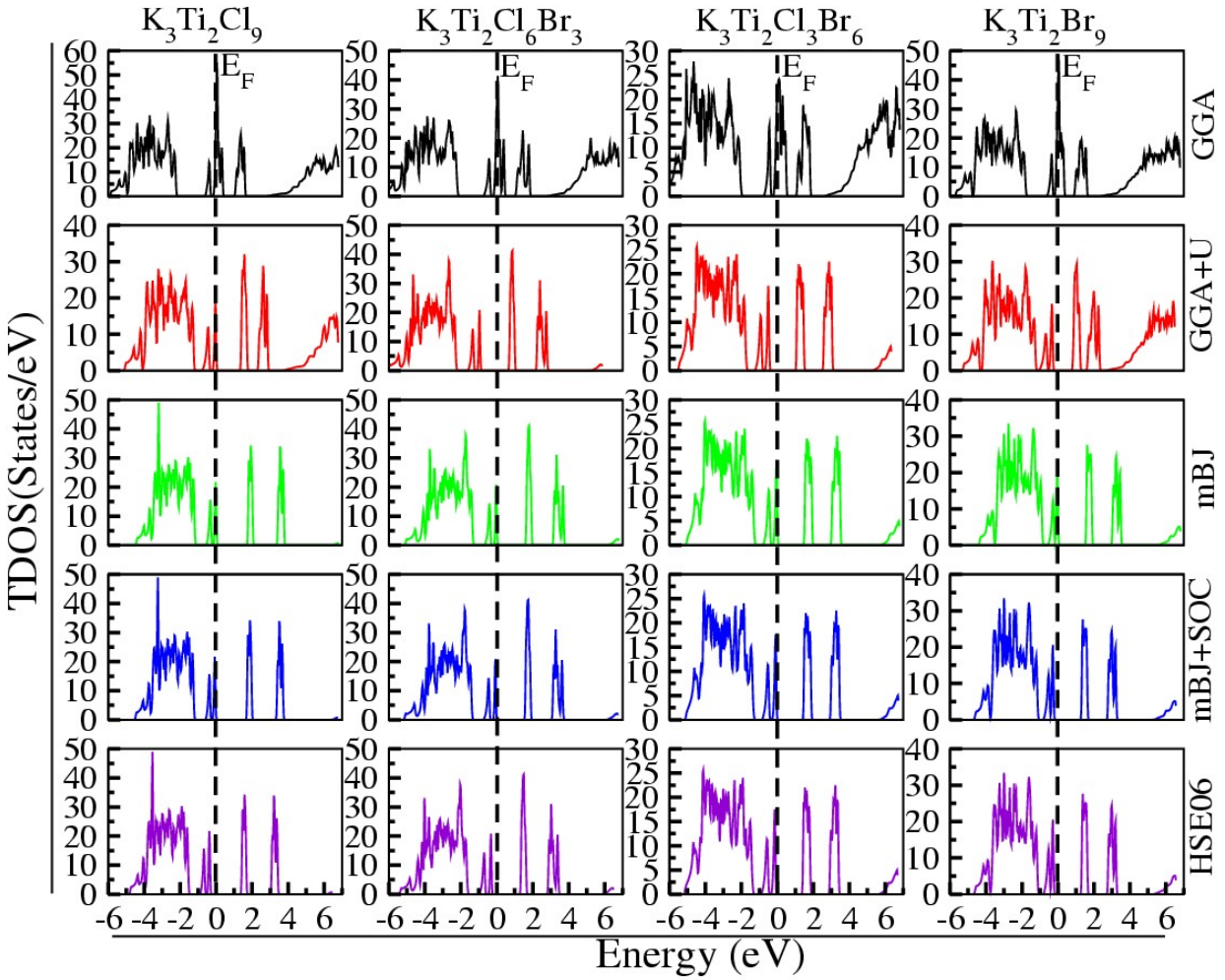

Fig. S1 TDOS of the $K_3Ti_2Cl_{9-x}Br_x$ (X = 0, 3, 6 and 9) compound.

Table S1: Input parameters for different HTLs taken in this study.

Parameters	**CFTS[1]**	**CuO[1]**	**CuSCn[1]**	**MoO_3[2]**	**NiO[1]**	**rGO[3]**	**PEDOT:PSS [1]**	**P3HT[1]**
Thickness (nm)	100	50	50	350	100	350	50	5
E_g (eV)	1.3	1.51	3.6	3	3.8	1.69	1.6	1.7
χ_e (eV)	3.3	4.07	1.7	2.5	1.46	3.56	3.4	3.5
ε_1(eV)	9	18.1	10^7	12.5	10.7	13.3	3	3
N_c (cm^{-3})	2.2×10^{18}	2.2×10^{19}	2.2×10^{19}	2.2×10^{18}	2.8×10^{19}	10^{18}	2.2×10^{18}	2×10^{21}
N_v (cm^{-3})	1.8×10^{19}	5.5×10^{20}	1.8×10^{18}	1.8×10^{19}	1×10^{19}	1.8×10^{19}	1.8×10^{19}	2×10^{21}
$V_{Th,e}$ (cm s^{-1})	10^7	10^7	10^7	10^7	10^7	10^7	10^7	10^7
$V_{Th,h}$ (cm s^{-1})	10^7	10^7	10^7	10^7	10^7	10^7	10^7	10^7
μ_e (cm^2Vs^{-1})	21.98	100	100	25	12	2.6×10^1	1.8×10^{-3}	4.5×10^{-2}
μ_h (cm^2Vs^{-1})	21.98	0.1	25	100	2.8	1.23×10^2	1.86×10^{-2}	4.5×10^{-2}
N_D (cm^{-3})	0	0	0	0	0	0	0	0
N_A (cm^{-3})	10^{18}	10^{18}	10^{18}	10^{18}	10^{18}	10^{18}	10^{18}	10^{18}
N_T (cm^{-3})	10^{15}	10^{15}	10^{15}	10^{15}	10^{15}	10^{15}	10^{15}	10^{15}

Table S2: Input parameters for different ETLs taken in this study.

Parameters	**TiO_2[4]**	**Li-TiO_2[4]**	**ZnO[4]**	**Al-ZnO[4]**	**C_{60}[5]**	**IGZO[5]**	**PCBM[5]**	**SnO_2[5]**
Thickness (nm)	30	100	100	100	50	30	50	100
E_g (eV)	3.2	3.15	3.28	3.1	1.7	3.05	2	3.6
χ_e (eV)	4	4	4	4	3.9	4.16	3.9	4
ε_l(eV)	9	13.6	9	9	4.2	10	3.9	9
N_c (cm^{-3})	2×10^{18}	3×10^{20}	2×10^{18}	2×10^{18}	8×10^{19}	5×10^{18}	2.5×102^{1}	2.2×10^{18}
N_v (cm^{-3})	1.8×10^{19}	2×10^{20}	1.8×10^{19}	1.8×10^{19}	8×10^{19}	5×10^{18}	2.5×10^{21}	1.8×10^{19}
$V_{Th,e}$ (cm s^{-1})	10^7	10^7	10^7	10^7	10^7	10^7	10^7	10^7
$V_{Th,h}$ (cm s^{-1})	10^7	10^7	10^7	10^7	10^7	10^7	10^7	10^7
μ_e (cm^2Vs^{-1})	20	30	43	13.84	8×10^{-2}	15	0.2	100
μ_h (cm^2Vs^{-1})	10	0.005	25	25	3.5×10^{-3}	0.1	0.2	25
N_D (cm^{-3})	9×10^{16}	8×10^{17}	2.9×10^{19}	1.2×10^{19}	10^{17}	10^{17}	10^{18}	10^{17}
N_A (cm^{-3})	0	0	0	0	0	0	0	0
N_T (cm^{-3})	10^{15}	10^{15}	10^{15}	10^{15}	10^{15}	10^{15}	10^{15}	10^{15}

Table S3: Input parameters for different Hybrid ETLs taken in this study.

Parameters	**PCBM-PCPB[6]**	**PCBM-SnS_2[7]**	**TiO_2-SnO_2[8]**
Thickness (nm)	50	45	50
E_g (eV)	2	1.57	3.3
χ_e (eV)	3.9	4	4
ε_1(eV)	3.9	4.2	9
N_c (cm^{-3})	2.5×10^{21}	2.5×10^{19}	2×10^{18}
N_v (cm^{-3})	2.5×10^{21}	2.5×10^{19}	1.8×10^{19}
$V_{Th,e}$ (cm s^{-1})	10^7	10^7	10^7
$V_{Th,h}$ (cm s^{-1})	10^7	10^7	10^7
μ_e (cm^2Vs^{-1})	5.5×10^{-4}	2.89×10^{-4}	30
μ_h (cm^2Vs^{-1})	5.5×10^{-4}	2.89×10^{-4}	15
N_D (cm^{-3})	3×10^{17}	2.4×10^{17}	2×10^{20}
N_A (cm^{-3})	0	0	0
N_T (cm^{-3})	10^{15}	10^{15}	10^{15}

Table S4: PCE verses different thickness of $K_3Ti_2Cl_9$ as absorber.

Thickness (nm)	V_{OC}	J_{SC}	FF	PCE
200	1.20	17.08	81.96	16.92
300	1.20	17.31	81.93	17.14
400	1.20	17.47	81.82	17.29
500	1.22	17.59	81.13	17.43
600	1.24	17.68	80.37	17.73
700	1.26	17.75	80.66	18.10
800	1.27	17.80	80.93	18.34
900	1.28	17.77	81.36	18.52
1000	1.28	17.76	81.68	18.67
1100	1.29	17.78	81.85	18.79
1200	1.29	17.80	81.96	18.89
1300	1.29	17.82	82.03	18.97
1400	1.30	17.83	82.08	19.05
1500	1.30	17.84	82.16	19.12
1600	1.30	17.86	82.22	19.18
1700	1.30	17.87	82.27	19.23
1800	1.31	17.88	82.31	19.28
1900	1.31	17.89	82.35	19.33
2000	1.31	17.89	82.38	19.37

Table S5: PCE verses different thickness of $K_3Ti_2Cl_6Br_3$ as absorber.

Thickness (nm)	V_{OC}	J_{SC}	FF	PCE
200	1.29	18.27	82.78	19.55
300	1.29	19.59	82.49	20.91
400	1.29	20.53	81.99	21.79
500	1.29	21.22	81.73	22.45
600	1.29	21.74	81.80	23.02
700	1.29	22.44	81.72	23.74
800	1.29	22.68	81.67	23.98
900	1.29	22.87	81.63	24.16
1000	1.29	23.02	81.60	24.31
1100	1.29	23.13	81.58	24.42
1200	1.29	23.23	81.56	24.51
1300	1.29	23.30	81.55	24.59
1400	1.29	23.37	81.54	24.65
1500	1.29	23.42	81.53	24.70
1600	1.29	23.47	81.52	24.74
1700	1.29	23.50	81.51	24.77
1800	1.29	23.53	81.51	24.80
1900	1.29	23.56	81.50	24.83
2000	1.29	23.59	81.50	24.85

Table S6: PCE verses different thickness of $K_3Ti_2Cl_3Br_6$ as absorber.

Thickness (nm)	V_{OC}	J_{SC}	FF	PCE
200	1.27	21.01	80.82	21.67
300	1.27	22.32	80.09	22.75
400	1.26	23.25	79.82	23.55
500	1.26	23.93	79.73	24.15
600	1.26	24.42	79.69	24.57
700	1.25	24.79	79.69	24.88
800	1.25	25.07	79.73	25.09
900	1.25	25.29	79.76	25.25
1000	1.24	25.45	79.78	25.36
1100	1.24	25.58	79.80	25.44
1200	1.24	25.68	79.82	25.50
1300	1.24	25.76	79.84	25.54
1400	1.23	25.83	79.87	25.56
1500	1.23	25.88	79.92	25.58
1600	1.23	25.92	79.95	25.58
1700	1.23	25.96	79.97	25.58
1800	1.23	25.98	79.99	25.58
1900	1.22	26.01	80.00	25.57
2000	1.22	26.03	80.01	25.56

Table S7: PCE verses different thickness of $K_3Ti_2Br_9$ as absorber.

Thickness (nm)	V_{OC}	J_{SC}	FF	PCE
200	1.36	22.04	82.24	24.78
300	1.36	23.59	81.54	26.30
400	1.36	24.68	80.99	27.31
500	1.36	25.46	80.57	27.99
600	1.36	26.03	80.25	28.47
700	1.36	26.44	80.00	28.81
800	1.35	26.76	79.80	29.04
900	1.35	27.00	79.66	29.20
1000	1.35	27.18	79.55	29.32
1100	1.35	27.33	79.48	29.41
1200	1.35	27.44	79.40	29.46
1300	1.35	27.54	79.34	29.50
1400	1.34	27.61	79.28	29.52
1500	1.34	27.67	79.24	29.54
1600	1.34	27.73	79.20	29.54
1700	1.34	27.77	79.18	29.54
1800	1.34	27.81	79.15	29.53
1900	1.34	27.84	79.15	29.53
2000	1.33	27.86	79.17	29.52

Table S8: PCE verses different thickness of $K_3Ti_2Cl_9$ as absorber.

N_A	V_{OC}	J_{SC}	FF	PCE
1×10^{10}	1.20	17.84	81.73	17.64
1×10^{11}	1.20	17.84	81.73	17.64
1×10^{12}	1.20	17.84	81.73	17.64
1×10^{13}	1.20	17.84	81.73	17.64
1×10^{14}	1.21	17.84	81.63	17.63
1×10^{15}	1.28	17.77	81.36	18.52
1×10^{16}	1.37	17.56	83.26	20.08
1×10^{17}	1.44	17.46	84.26	21.30
1×10^{18}	1.56	17.42	85.02	22.32
1×10^{19}	1.61	17.52	84.33	23.28
1×10^{20}	1.67	17.52	83.83	24.65
N_t				
1×10^{10}	1.28	17.77	81.42	18.54
1×10^{11}	1.28	17.77	81.42	18.54
1×10^{12}	1.28	17.77	81.42	18.54
1×10^{13}	1.28	17.77	81.42	18.54
1×10^{14}	1.28	17.77	82.36	18.52
1×10^{15}	1.28	17.76	80.83	18.39
1×10^{16}	1.27	17.72	77.61	17.58
1×10^{17}	1.23	17.60	72.25	15.71

Table S9: PCE verses different thickness of $K_3Ti_2Cl_6Br_3$ as absorber.

N_A	V_{OC}	J_{SC}	FF	PCE
1×10^{10}	1.28	23.64	78.88	23.99
1×10^{11}	1.28	23.64	78.88	23.99
1×10^{12}	1.28	23.64	78.86	23.98
1×10^{13}	1.28	23.64	78.64	23.91
1×10^{14}	1.28	23.64	79.39	24.11
1×10^{15}	1.29	23.59	81.50	24.85
1×10^{16}	1.32	23.08	81.94	24.99
1×10^{17}	1.36	22.52	82.86	25.56
1×10^{18}	1.41	22.34	83.44	26.39
1×10^{19}	1.38	22.29	79.24	24.43
1×10^{20}	1.51	22.28	86.49	29.29
N_t				
1×10^{10}	1.30	23.61	82.18	25.28
1×10^{11}	1.30	23.61	82.18	25.28
1×10^{12}	1.30	23.61	82.18	25.28
1×10^{13}	1.30	23.60	82.08	25.23
1×10^{14}	1.29	23.59	81.50	24.85
1×10^{15}	1.25	23.45	79.52	23.40
1×10^{16}	1.20	23.06	75.71	20.98
1×10^{17}	1.11	22.42	71.47	17.92

Table S10: PCE verses different thickness of $K_3Ti_2Cl_3Br_6$ as absorber.

N_A	V_{OC}	J_{SC}	FF	PCE
1×10^{10}	1.25	25.29	77.75	24.69
1×10^{11}	1.25	25.29	77.75	24.69
1×10^{12}	1.25	25.29	77.75	24.69
1×10^{13}	1.25	25.29	77.61	24.68
1×10^{14}	1.25	25.29	79.47	24.61
1×10^{15}	1.25	25.29	79.76	25.25
1×10^{16}	1.27	25.68	81.41	26.18
1×10^{17}	1.28	24.96	81.83	26.31
1×10^{18}	1.30	23.75	82.18	25.53
1×10^{19}	1.29	22.96	77.72	23.06
1×10^{20}	1.42	22.81	83.70	27.14
N_t				
1×10^{10}	1.28	25.29	82.08	26.70
1×10^{11}	1.28	25.29	82.08	26.70
1×10^{12}	1.28	25.29	81.99	26.66
1×10^{13}	1.28	25.29	81.33	26.39
1×10^{14}	1.25	25.29	79.76	25.25
1×10^{15}	1.17	25.28	78.41	23.38
1×10^{16}	1.10	25.22	74.94	20.92
1×10^{17}	1.02	24.75	69.53	17.57

Table S11: PCE verses different thickness of $K_3Ti_2Br_9$ as absorber.

N_A	V_{OC}	J_{SC}	FF	PCE
1×10^{10}	1.36	22.04	82.37	24.82
1×10^{11}	1.36	22.04	82.37	24.82
1×10^{12}	1.36	22.04	82.35	24.82
1×10^{13}	1.36	22.04	82.35	24.82
1×10^{14}	1.36	22.04	82.24	24.78
1×10^{15}	1.36	22.04	82.41	24.85
1×10^{16}	1.37	22.04	82.77	24.93
1×10^{17}	1.38	22.04	83.17	25.08
1×10^{18}	1.40	22.02	82.98	24.91
1×10^{19}	1.44	21.78	78.48	22.69
1×10^{20}	1.48	19.49	83.42	22.25
N_t				
1×10^{10}	1.37	22.04	83.33	25.17
1×10^{11}	1.37	22.04	83.33	25.17
1×10^{12}	1.37	22.04	83.33	25.17
1×10^{13}	1.36	22.04	82.23	24.78
1×10^{14}	1.34	22.04	79.15	23.53
1×10^{15}	1.33	22.04	79.17	23.37
1×10^{16}	1.24	22.04	77.75	21.37
1×10^{17}	1.15	22.04	75.73	19.23

Table S12: PCE verses different thickness of $K_3Ti_2Cl_9$ as absorber.

R_s	V_{OC}	J_{SC}	FF	PCE
0	1.30	17.84	82.16	19.12
1	1.30	17.84	80.87	18.82
2	1.30	17.84	79.59	18.52
3	1.30	17.84	78.30	18.22
4	1.30	17.84	77.02	17.92
5	1.30	17.77	75.74	17.62
6	1.30	17.56	74.46	17.32
7	1.30	17.46	73.23	17.04
8	1.30	17.42	71.94	16.74
9	1.30	17.52	70.71	16.45
10	1.30	17.52	69.45	16.15
R_{sh}				
10^1	0.17	16.99	25.00	0.76
10^2	1.18	17.76	37.33	7.86
10^3	1.26	17.84	78.56	17.77
10^4	1.29	17.84	81.39	18.85
10^5	1.30	17.84	81.50	18.96
10^6	1.30	17.84	81.51	18.97
10^7	1.30	17.84	81.51	18.97
10^8	1.30	17.84	81.51	18.97

Table S13: PCE verses different thickness of $K_3Ti_2Cl_6Br_3$ as absorber.

R_s	V_{OC}	J_{SC}	FF	PCE
0	1.29	23.42	81.53	24.70
1	1.29	23.42	79.82	24.18
2	1.29	23.42	78.11	23.67
3	1.29	23.42	76.41	23.15
4	1.29	23.42	74.74	22.64
5	1.29	23.42	73.06	22.13
6	1.29	23.42	69.71	21.12
7	1.29	23.42	68.04	20.61
8	1.29	23.42	66.37	20.11
9	1.29	23.42	64.72	19.61
10	1.29	23.42	63.06	19.11
R_{sh}				
10^1	0.23	22.31	22.00	1.31
10^2	1.20	23.36	47.96	13.27
10^3	1.28	23.38	81.42	18.54
10^4	1.28	23.40	81.42	18.54
10^5	1.28	23.42	82.36	18.52
10^6	1.28	23.42	82.83	18.39
10^7	1.28	23.42	82.83	17.58
10^8	1.28	23.42	82.83	15.71

Table S14: PCE verses different thickness of $K_3Ti_2Cl_3Br_6$ as absorber.

Rs	V_{OC}	J_{SC}	FF	PCE
0	1.23	25.88	79.92	25.58
1	1.23	25.88	77.95	24.95
2	1.23	25.88	75.98	24.32
3	1.23	25.88	74.02	23.69
4	1.23	25.88	72.07	23.07
5	1.23	25.88	70.12	22.44
6	1.23	25.88	68.17	21.82
7	1.23	25.88	66.31	21.23
8	1.23	25.88	64.40	20.62
9	1.23	25.88	62.51	20.01
10	1.23	25.88	60.62	19.41
R_{sh}				
10^1	0.25	24.65	28.00	1.60
10^2	1.13	25.75	52.93	15.41
10^3	1.20	25.87	77.96	24.25
10^4	1.23	25.88	79.00	25.16
10^5	1.23	25.88	78.94	25.25
10^6	1.23	25.88	78.93	25.26
10^7	1.23	25.88	78.93	25.26
10^8	1.23	25.88	78.93	25.26

Table S15: PCE verses different thickness of $K_3Ti_2Br_9$ as absorber.

Rs	V_{OC}	J_{SC}	FF	PCE
0	1.34	27.67	79.24	29.54
1	1.34	27.67	77.30	28.81
2	1.34	27.67	75.36	28.09
3	1.34	27.67	73.43	27.37
4	1.34	27.67	71.51	26.66
5	1.34	27.67	69.58	25.94
6	1.34	27.67	67.67	25.23
7	1.34	27.67	65.81	24.53
8	1.34	27.67	63.93	23.84
9	1.34	27.67	62.07	23.14
10	1.34	27.67	60.21	22.45
R_{sh}				
10^1	0.27	27.37	29	1.71
10^2	1.11	27.48	72.25	17.58
10^3	1.20	27.59	77.61	18.39
10^4	1.20	27.67	80.83	18.52
10^5	1.20	27.67	81.36	18.54
10^6	1.20	27.67	81.42	18.54
10^7	1.20	27.67	81.42	18.54
10^8	1.20	27.67	81.42	18.54

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