Table 3 . Input Parameters of Interface Defect and Absorber Defect.

Parameters and units	Cs2TiBr6	ETL/Cs2TiBr6 interface	Cs2TiBr6 / HTL interface
DEFECT TYPE	NEUTRAL	Acceptor	Acceptor
Capture cross section for electron and holes (cm2)	$2.0X10^{-14}$, $2X10^{-14}$	$1.0X10^{-17}$, $1X10^{-18}$	$1.0X10^{-18}$, $1X10^{-19}$
Energetic distribution	GAUSSIAN	SINGLE	SINGLE
Energy level with respect to EV (above EV , eV)	0.6	0.6	0.6
Characteristics energy (eV)	0.1	-	-
Total Density (cm-3)	$1.0 X 10^{13}$	$1.0 X 10^{10}$ - $1.0 X 10^{12}$	$1.0 X 10^{10}$ - $1.0 X 10^{12}$

TABLE 2 INPUT PARAMETERS OF HTLs.

PARAMETERS	Cu20	CuAlO2	CuSbS2	CuSCN	MoO3	Spiro-OMeTAD	P3HT	PEDOT:PSS	Cs2TiBr6
Thickness (nm)	30	30	30	30	30	30	30	30	900
BandGap , Eg(eV)	2.17	3.46	1.58	3.2	3	3	1.85	2.2	1.6
Electrno affinity X (eV)	3.2	2.5	4.2	1.9	2.5	2.45	3.1	2.9	4.47
Realtive Dielectric Permittivity	7.1	60	14.6	10	12.5	3	3.4	3	10
CB , Effective density of states Nc (cm-3)	$2.02x10^{17}$	$2.2X10^{18}$	$2X10^{18}$	$2.2X10^{19}$	$2.2X10^{18}$	$1X10^{19}$	$1E^{+22}$	$2.2E^{+15}$	$1E^{19}$
VB , effective density of states Nv (cm-3)	$1.1x10^{19}$	$1.8X10^{19}$	$1X10^{-4}$	$1.8X10^{19}$	$1.8X10^{19}$	$1X10^{19}$	$1E^{+22}$	$2.2E^{+17}$	$1E^{19}$
Electron mobility (cm2v-1s-1)	200	2	49	$1X10^{-4}$	100	$2X10^{-4}$	$1E^{-4}$	$2X10^{-3}$	4.4
Hole mobility (cm2v-1s-1)	80	8.6	49	$1X10^{-1}$	25	$2X10^{-4}$	$1E^{-4}$	$2X10^{-3}$	2.5
Shallow uniform donor density ND (cm-3)	0	0	0	0	0	0	0	0	$1E^{+19}$
Shallow acceptor density NA (cm-3)	$9 X 10^{21}$	$3 X 10^{18}$	$1.38X^{18}$	$1X10^{15}$	$1X10^{18}$	$2X10^{18}$	$3.17E^{13}$	$1E^{+17}$	$1E^{+19}$
Total defect density Nt (cm-3)	$1 X 10^{14}$	$1X 10^{14}$	$1 X 10^{14}$	$1 X 10^{14}$	$1 X 10^{14}$	$1 X 10^{14}$	$1 X 10^{14}$	$1 X 10^{14}$	$1 X 10^{14}$

TABLE 1 INPUT PARAMETERS OF ETLs

PARAMETERS	FTO	TiO2	Zno	STO	IGZO	PCBM	Znse	CdS	WO3
Thickness (nm)	500	30	30	30	30	30	30	30	30
BandGap , Eg(eV)	3.2	3.2	3.3	3.2	3.05	2	2.81	2.4	2.92
Electrno affinity X (eV)	4.4	3.9	4.1	4.0	4.16	3.9	4.09	4.18	4.590
Realtive Dielectric Permittivity	9	9	9	8.7	10	4	8.6	10	5.76
CB , Effective density of states Nc (cm-3)	$2.2X10^{18}$	$1X10^{21}$	$4X10^{18}$	$1.7X10^{19}$	$5X10^{18}$	$1X10^{21}$	$2.2X10^{18}$	$2.2X10^{18}$	$1.96X10^{19}$
VB , effective density of states Nv (cm-3)	$1.8X10^{19}$	$2X10^{20}$	$1X10^{19}$	$2X10^{20}$	$5X10^{18}$	$1.8X10^{19}$	$1.8X10^{18}$	$1.9X10^{19}$	$1.96E^{19}$
Electron mobility (cm2v-1s-1)	90	20	100	$5.3X10^{3}$	15	$1E^{-2}$	$4x10^{2}$	100	$1E^{+1}$
Hole mobility (cm2v-1s-1)	90	10	25	$6.6X10^{2}$	0.1	$1E^{-2}$	$1.1x10^{2}$	25	$1E^{+1}$
Shallow uniform donor density ND (cm-3)	$7X10^{2}$	$1X10^{19}$	$1X10^{18}$	$2X10^{16}$	$1X10^{18}$	$1E^{+20}$	$1x10^{18}$	$1X10^{18}$	$3.68E^{+19}$
Shallow acceptor density NA (cm-3)	0	0	0	0	0	0	0	0	0
Total defect density Nt (cm-3)	$1X10^{14}$	$1X10^{14}$	$1X10^{14}$	$1X10^{14}$	$1X10^{14}$	$1X10^{14}$	$1X10^{14}$	$1X10^{14}$	$1X10^{14}$

Structure of PSCs	Voc (V)	Jsc (mA/cm2)	FF (%)	PCE(%)
Au/ CUALO2 / Cs2TiBr6 / IGZO/FTO	1.1231	23.543828	73.88	19.53
Au/ CUALO2 / Cs2TiBr6 / ZNO/FTO	1.1231	23.543129	73.86	19.53
Au/ CUALO2 / Cs2TiBr6 / TIO2/FTO	1.1267	23.546622	72.46	19.22
Au/ CU2O / Cs2TiBr6 / ZNSE/FTO	0.6726	23.54986	69.26	10.97
Au/CU2O/ Cs2TiBr6 / PCBM/FTO	0.6732	23.551993	68.38	10.84
Au/ CU2O / Cs2TiBr6 / TIO2/FTO	0.6727	23.549836	67.41	10.68
Au/ CU2O / Cs2TiBr6 / ZNO/FTO	0.6614	24.16615	64.38	10.29
Au/ MOO3 / Cs2TiBr6 / CDS/FTO	0.6582	23.551529	60.16	9.33
Au/ MOO3 / Cs2TiBr6 / ZNO/FTO	0.6579	23.546039	60.16	9.32
Au/ MOO3 / Cs2TiBr6 / TIO2/FTO	0.6582	23.549529	58.43	9.06