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Suitability of LBSO/CuI as an Effective ETL/HTL for Perovskite Solar Cells: A Dry Lab Approach

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With rapid breakthroughs in power conversion efficiency (PCE), hybrid halide perovskites (HHPs) based solar cells have been considered as the potential candidates for the next generation solar cell technology. However, these perovskite solar cells (PSCs) are still far from the door of the photovoltaic market owing to their instability issue involved with various used materials during fabrication. In this work, we deal with the numerical simulation of PSC devices via SCAPS-1D software. For better performance, several prominent materials for absorber layer have been proposed with a combination of La-doped $BaSnO_3$ as ETL and CuI as HTL. The strong dependency of proper ETL, absorber layer and HTL on the overall device performance has been observed. Moreover, the $FAPbI_3$-based device outperformed other devices with different absorber materials, yielding an overall PCE of 22.09 %. Thus, the dry lab approach using computer simulations will be helpful for experimentalists to design and fabricate similar PSCs by reducing the cost of experimental trials.

Keywords: Hybrid halide perovskites; Power conversion efficiency; Absorber layer; Dry lab approach

1 Introduction

Hybrid halide perovskites (HHPs) have drawn unprecedented attention among photovoltaic community and emerged as a promising material for the next generation of photovoltaics. Being a magic box of various miraculous properties, HHP based solar cells have revolutionized the photovoltaic landscape with an incredible advancement in power conversion efficiency (PCE) from 3.8 %[1] to recently certified value of 26.1 %[2] just within a decade. The high efficiency along with the low-cost and facile solution-based fabrication processes paves a path for their commercialization; however, these PSCs are still confined to laboratories only, owing to their instability issue. Although the scientists have made several major efforts both on experimental and theoretical fronts, yet tackling its instability has become a challenge for the whole photovoltaic community.

In the most efficient PSCs, TiO_2 is commonly used as an electron transport layer (ETL), which must be annealed at a very high temperature (500 °C) in order to achieve the crystalline phase. In addition, it is unstable under UV illumination that impedes the device stability. In this regard, Shin *et. al*. fabricated La-doped $BaSnO_3$ (LBSO) based PSC[3], resulting in an overall PCE of 21.2 %. Moreover, the device maintained 93 % of the initial PCE even after 1000 h of one sun illumination. Similarly, the widely used organic HTL material, Spiro-OMeTAD, in PSCs has complicated synthesis processes. It also requires ultra-purity, which raises the ultimate cost of device. Moreover, organic HTLs can degrade the photovoltaic performance due to movable additives, morphological deformation, metal diffusion and so forth. In this perspective, various inorganic materials have been investigated as an alternative of organic HTLs, in order to achieve low-cost and high stability.

After thorough literature studies, we plan to consider La-doped $BaSnO_3$ as probable ETL and CuI as HTL in all the proposed PSCs consisting of different type of prominent absorber layer materials. Here, we adopt the dry lab approach using computer simulations in order to reduce the experimental trails, which in-turn reduces the ultimate cost of device fabrication.

2 Simulation Methodology

All the simulation work were accomplished using Solar Cell Capacitance Simulator version 3.3.07 (SCAPS-1D) software. It is based on three basic

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Table 1 — Input Parameters for various absorber layers, ETL (LBSO) and HTLs (PTAA, CuI)

Simulation Parameter	FTO[4,5]	ETL[6,7]	Absorber Layer[8,12,13]				HTL[9,10]	
		LBSO	MA PbI_3	FA PbI_3	Cs_xFA_{1-x} PbI_3	MAPb $(I_{1-x}Cl_x)_3$	PTAA	CuI
Thickness (nm) (t)	300	120	440	440	440	440	200	200
Band gap (eV)(E_g)	3.5	3.12	1.55	1.51	1.55	1.55	2.96	3.1
Electron affinity (eV) (χ)	4	4.4	3.9	4	3.95	3.9	2.3	2.1
Dielectric Permittivity (ϵ)	9	22	6.5	6.6	6.6	6.5	9	6.5
Conduction Band Density of State(cm^{-3}) (N_c)	2.2×10^{18}	1×10^{18}	1.6×10^{19}	1.2×10^{19}	2×10^{19}	2.2×10^{18}	2×10^{21}	2.2×10^{19}
Valence Band Density of States (cm^{-3}) (N_V)	1.8×10^{19}	2.2×10^{20}	4.66×10^{19}	2.9×10^{18}	2×10^{18}	1.8×10^{19}	2×10^{21}	5.5×10^{20}
Electron thermal velocity (cm/s) (V_e)	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7
Hole thermal velocity (cm/s)(V_h)	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7	1×10^7
Electron mobility (cm^2/Vs) (μ_e)	20	70	2	2.7	0.28	2	1	100
Hole mobility(cm^2/Vs) (μ_h)	10	70	2	1.8	2	2	40	43.9
Donor defect density (cm^{-3}) (N_D)	1×10^{19}	4.4×10^{20}	1×10^{19}	1.3×10^{16}	1.3×10^{16}	-	0	0
Acceptor defect density (cm^{-3}) (N_A)	0	0	1×10^{19}	1.3×10^{16}	1.3×10^{16}	-	1.6×10^{21}	1×10^{18}
Defect density in bulk (cm^{-3}) (N_t)	1×10^{15}	1×10^{15}	1×10^{14}	1×10^{14}	1×10^{14}	1×10^{14}	1×10^{15}	1×10^{15}

equations namely, Poisson's equation, continuity equation for holes and continuity equation for electrons. The primary simulated PSC is composed of Fluorine-doped Tin Oxide (FTO) coated Glass/LBSO/$MAPbI_3$/PTAA/Au. All the input parameters for these materials were taken from existing literature[4-9] and summarized in Table 1. At 300 K, the device was simulated under exposure of one sun AM 1.5G (100mW cm^{-2}) solar spectrum. Concurrently, the parasitic resistances, R_{series} and R_{shunt} were assumed to be 1Ω and 6800 Ω, respectively, and the work function of back contact (Au) was taken to be 5.1 eV. All the simulations were performed without considering the optical reflectance of each layer at the surface and interfaces.

We first reproduced the experimental results of Shin[3] *et. al*. which proves the authenticity of our simulated work. The output photovoltaic parameters are listed in Table 2.

Table 2 — Output photovoltaic parameters of experimental and simulated primary PSC.

Parameters	V_{oc} (V)	J_{sc} (mA.cm^{-2})	FF (%)	PCE (%)
Experimental	1.12	23.4	81.3	21.3
This work	1.12	23.0	81.0	20.8

Table 3—Performance of LBSO/CuI as ETL/HTL with different absorber layer materials.

Structure	V_{oc} (V)	J_{sc} (mA.cm^{-2})	FF (%)	PCE (%)
$MAPbI_3$	1.12	22.95	78.92	20.35
$FAPbI_3$	1.17	24.38	77.75	22.09
$Cs_xFA_{1-x}PbI_3$	1.20	22.94	77.75	21.41
$MAPb(I_{1-x}Cl_x)_3$	1.20	22.95	79.30	21.84

3 Results and Discussions

In order to obtain a suitable alternative of organic HTLs, we considered CuI as HTL for the present work. The input parameters for CuI are taken from existing literature[10]. Various literature studies incorporating CuI as HTL showcased its better impacts on overall photovoltaic performance[11]. It is also chosen because of its ease of preparation and good electrical properties. Further, it preserves HTL/perovskite interface from degradation which in turn improve the stability of the device. Here, we simulated the PSC with a device architecture: FTO/LBSO/$MAPbI_3$/CuI/Au. Moreover, the simulated device demonstrated a PCE of 20.35 % with a Short circuit current density (J_{sc}) of 22.95 mA/cm^2, open-circuit voltage (V_{oc}) of 1.12 V and Fill factor (FF) of 78.92 %.

3.1 Suitability of LBSO/CuI as ETL/HTL with various absorber layers

To investigate the influence of LBSO/CuI as ETL/HTL on overall PV performance with various absorber materials, we proposed different prominent inorganic/organic absorber materials and also their combinations. The selected materials for the same were $FAPbI_3$ (formamidinium lead iodide), $Cs_xFA_{1-x}PbI_3$, $MAPb(I_{1-x}Cl_x)_3$ along with $MAPbI_3$ (methylammonium lead iodide). The input parameters of these proposed materials were taken from previous literature studies[8,12,13] as listed in Table 1. Concurrently, a thickness of 440 nm was chosen for each absorber materials. Table 3 exhibits the output photovoltaic metrics for the PSCs with different absorber materials. In accordance with the obtained dataset, the combination of LBSO/CuI with $FAPbI_3$

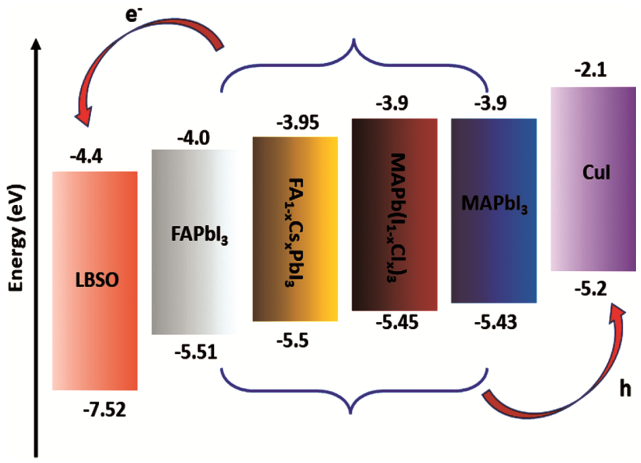

Fig. 1—Band alignments of LBSO, CuI and various proposed absorber layer materials.

perovskite highlights the better performance (PCE and J_{sc} value) among all the proposed absorber materials. It is noteworthy that all proposed materials with LBSO/CuI as ETL/HTL display good performance. This better performance may be ascribed by the suitable band alignment between the conduction band of LBSO and the lowest unoccupied molecular orbital (LUMO) of different organic/ inorganic perovskite materials as well as between the highest occupied molecular orbital (HOMO) of different organic/inorganic perovskite materials and the valence band of CuI, as depicted in Fig. 1. This alignment enables the efficient electron transport to the ETL from absorber layer and also holes transport from absorber layer to CuI. In a nutshell, we can infer that LBSO and CuI are the suitable ETL and HTL, respectively, for all the proposed organic/inorganic perovskite absorber layers considered.

4 Conclusion

The present study deals with the numerical simulation of PSCs via SCAPS-1D software. Here, we considered LBSO and CuI as ETL and HTL, respectively. Our simulated work authenticates the suitability of LBSO and CuI as ETL and HTL, respectively, not only for $MAPbI_3$ absorber layer but also for various absorber materials such as $FAPbI_3$, $Cs_xFA_{1-x}PbI_3$ and $MAPb(I_{1-x}Cl_x)_3$. These simulated results will help the material's scientists to design similar PSCs by reducing the experimental trials for optimization.

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