Computational design of high performance hybrid perovskite on silicon 2-T tandem solar cells based on a tunnel junction

A. Rolland, L. Pedesseau, Y. Huang, S. Wang, D. Sapori, C. Cornet, O. Durand, and J. Even
FOTON, UMR 6082, CNRS, INSA Rennes, Université de Rennes 1, 35708 Rennes, France

M. Kepenekian, C. Katan
Institut des Sciences Chimiques de Rennes, UMR 6226, CNRS, Université de Rennes 1, 35042 Rennes, France

In this study, the optoelectronic properties of a monolithically integrated series-connected tandem solar cell are simulated. Following the large success of hybrid organic-inorganic perovskites, which have recently demonstrated large efficiencies with low production costs, we examine the possibility of using the same perovskites as absorbers in a tandem solar cell. The cell consists in a methyl ammonium mixed bromide-iodide lead perovskite, $CH_3NH_3PbI_{3(1-x)}Br_{3x}$ ($0 \leq x \leq 1$), top sub-cell and a single-crystalline silicon bottom sub-cell. A Si-based tunnel junction connects the two sub-cells. Numerical simulations are based on a one-dimensional numerical drift-diffusion model. It is shown that a top cell absorbing material with 20% of bromide and a thickness in the 300-400 nm range affords current matching with the silicon bottom cell. Good interconnection between single cells is ensured by standard n and p doping of the silicon at $5.10^{19} cm^{-3}$ in the tunnel junction. A maximum efficiency of about 27% is predicted for the tandem cell exceeding both the efficiencies of stand-alone silicon and perovskite cells taken for our simulations, which amount to 17,3% and 17,9%, respectively.

Key words: **Tandem solar cells, perovskites, tunnel junctions, numerical simulation, Photonics on silicon**

I. INTRODUCTION

In order to ensure a large part of the worldwide energy production, photovoltaics has to increase its watt produced over price ratio and match, if not exceed, the one of nuclear and fossil energies. In recent years, two strategies have emerged from this objective. The first path consists in increasing significantly the solar-cell efficiencies. In that sense, one solution is to develop group III-V multi-junction solar cells (MJSC), which can surpass the well-known Schockley-Queisser limit of an ideal single-junction solar cell [1]. However, these MJSC are currently developed on expensive GaAs and Ge substrates and required high-quality materials. Targeting terrestrial applications, less expensive alternatives have been proposed using a Si bottom sub-cell, developed on a low-cost Si substrate [2–4]. Following a different strategy, halide organic-inorganic perovskite (HOP) materials, such as lead methyl ammonium tri-iodide $CH_3NH_3PbI_3$, in so-called 'perovskite cells' have recently attracted huge attention [2]. Not only have these solar cells demonstrated remarkably high efficiencies (above 22%) and high open-circuit voltages (V_{oc}) [5], but they also offer great potential for low cost production. Taking advantage of both these strategies, this class of material is a suitable candidate as a top sub-cell absorber for tandem cells built on CIGS or Si.

As already widely developed in the III-V multibandgap systems [6], a simple tandem solar cell approach is based on a serial connection of both subcells through a tunnel junction (TJ). Although it is a key point in the optimization of device architecture, only few simulations have been reported on perovskite-based solar cells with a TJ [7,8].

In this work, we conduct numerical simulations of two-terminal tandem cells based on HOP materials as top sub-cell absorber monolithically integrated on a bottom Si sub-cell. As it has recently been shown that introducing a mixture of bromide and iodide in the halide composition of lead methyl ammonium perovskites allows for tuning the band gap [9], we chose $CH_3NH_3PbI_{3(1-x)}Br_{3x}$ as top sub-cell absorber material. We stress that the specific alloy is known however to present some stability issues under light soaking that will not be considered in the present work [10]. Moreover, the influence of the hysteresis effect related to the TiO_2 layer is neither studied. Our computational study allows designing an optimal HOP based tandem cell. The best efficiency is obtained for a bromide ratio x=0.2 and a thickness of the HOP layer between 300 and 400 nm. In these conditions the tandem cell exhibits a conversion efficiency of about 27%.

II. METHOD

Simulations are performed using the Silvaco Atlas device simulator [11], which allows to numerically solve Poisson's equation coupled with the continuity equations for both electrons and holes under steady state conditions. Quantum effects can be included, and these are mandatory to simulate a TJ. The structure consists in a 850 nm thick hole transport material (HTM) layer, a $CH_3NH_3PbI_{3(1-x)}Br_{3x}$ absorbing layer of various thickness, and a 300 nm thick TiO_2 electron

transport layer. The 2x20 nm thick $Si(n^{++})/Si(p^{++})$ TJ insures the electrical connection between the two subcells. Finally, a 280 μm thick n-type Si substrate ($N_D = 10^{16}$ cm^{-3}) includes deep trap levels, with an energy level located at 0.5 eV above the valence band edge and a density corresponding to a diffusion length of 600 μm, and a 100 nm thick n^{++} Si layer ($N_D = 10^{19}$ cm^{-3}) for the back contact.

Table 1 summarizes the physical key parameters from the literature used in this study for the HTM, HOP, TiO$_2$ and Si materials [7]. Deep traps are also considered with an energy level located 0.5 eV below the conduction band edge and a density $N_T = 10^{15}$ cm^{-3} [29,30], which corresponds to a carrier diffusion length of about 700 nm in good agreement with available experimental data [7, 12].

In a tandem cell, in addition to the thickness of the absorber, the bandgap is among the essential parameters that need to be optimized. Here, the choice for CH$_3$NH$_3$PbI$_{3(1-x)}$Br$_{3x}$ mixed halide allows to monitor a wide range of bandgaps from 1.55 eV (x=0) to 2.3 eV (x=1). Bandgap energies and electron affinities of mixed compositions were computed from linear interpolation of the values reported for the pure tri-iodide and tri-bromide compounds (Table 1).

TABLE I
INPUT PARAMETERS FOR DEVICE SIMULATION

Parameter	CH$_3$NH$_3$PbI$_{3(1-x)}$Br$_{3x}$	HTM	TiO$_2$	Si
E_g (eV)	1.55+0.75x	3.0	3.2	1.12
χ (eV)	3.9-0.55x	2.45	3.9	4.17
ε_r	6.5	3.0	9	11.8
μ_n/μ_p (cm^{2}V^{-1}s^{-1})	2/2	2 10^{-4}/2 10^{-4}	20/10	1500/480
τ_n/τ_p (s)	10^{-6}/10^{-6}	10^{-7}/10^{-7}	10^{-7}/10^{-7}	10^{-4}/10^{-4}

III. RESULTS

Figure 1 shows the band diagram of the tandem cell at room temperature and at thermal equilibrium for various halide compositions. Whatever the halide composition, when an electron-hole pair is created in the perovskite layer, the electrons will easily flow to the TiO$_2$ layer without encountering any potential barrier. The behavior of the holes is similar from the perovskite layer to HTM layer. Figure 2 shows an example of simulated current-voltage characteristics (J-V) of the top HOP sub-cell (with x = 0.2), the bottom silicon sub-cell and the HOP-based tandem cell under AM1.5 illumination. Our simulation shows that *(i)* 5.10^{19} cm^{-3} *p* and *n* doping levels of Si are high enough to guarantee appropriate tunneling properties in this device and *(ii)* the optimum configuration is obtained for a perovskite thickness between 300 and 400 nm and a bromide concentration of 20%, which

corresponds to photovoltaic efficiency of the tandem cell of about 27%.
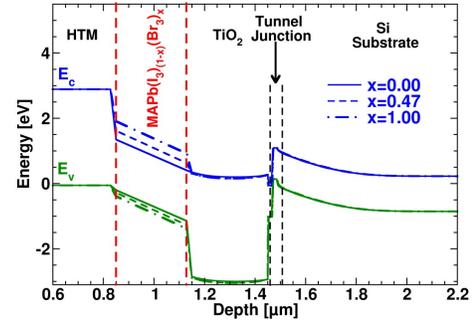
Fig. 1. Energy Band diagrams of the tandem cell. The valence and conduction band edges (resp. E_V and E_C) are depicted in green and blue, respectively. Effect of halide composition in the HOP absorber CH$_3$NH$_3$PbI$_{3(1-x)}$Br$_{3x}$ is illustrated for x=0.0 (solid line), 0.47 (dashed line) and 1.0 (dashed dotted line). The thickness is kept constant at 300nm.
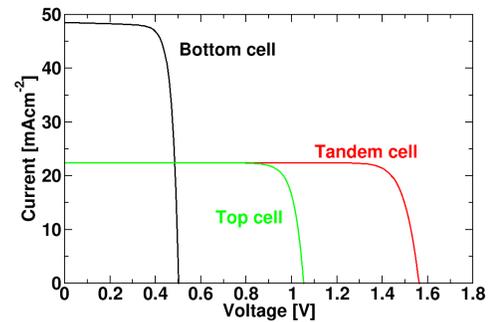
Fig. 2. J-V characteristics of the bottom cell, top cell and tandem cell under AM1.5 illumination. The HOP absorber material is CH$_3$NH$_3$PbI$_{3(1-x)}$Br$_{3x}$ with x=0.2 and a thickness of 300 nm.

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