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Original
Trap and Band Alignment Induced Voc Losses in Wide-Bandgap Perovskite Solar Cells / Fronteddu, A., Cappelluti, F.. - ELETTRONICO. - (2026), pp. 130-131. (2026 International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD) Cork (Ire) 19-24 July 2026) [10.1109/nusod69851.2026.11687834].

Availability:
This version is available at: 11583/3015678 since: 2026-09-17T13:47:58Z

Publisher:
IEEE

Published
DOI:10.1109/nusod69851.2026.11687834

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26 November 2026

Trap and band alignment induced V_{oc} losses in wide-bandgap perovskite solar cells

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***Abstract*—Wide-bandgap perovskite solar cells suffer from large open circuit voltage losses. We use TCAD simulations of bromide-based single-halide *p-i-n* devices to isolate the coupled role of trap distribution and band alignment at the charge transport interfaces. We show that specific interfacial electrostatic conditions enhance trap-assisted recombination, causing a marked reduction in open circuit voltage.**

***Index Terms*—perovskite solar cells, wide-bandgap perovskites, trap-assisted recombination, interface band alignment, TCAD simulation**

I. Introduction

Wide-bandgap (WBG) perovskite solar cells (PSCs) are promising both as single-junction devices for applications such as building-integrated photovoltaics and the Internet of Things (IoT), and as top cells in tandem photovoltaics. However, their performance is limited by significant open-circuit voltage (V_{oc}) losses. The origin of these losses remains under debate and is commonly attributed to material defects, particularly at interfaces, and, to a lesser extent, to photo-induced phase segregation [1], [2]. In this work, we analyze V_{oc} losses induced by bulk and interface defects in Br-based single-halide perovskites, which are not affected by phase segregation. We also study the interplay between trap-assisted recombination and band alignment at the charge transport layers, which is often tuned through transport layer engineering approaches [3], and assess its influence on device performance.

II. Simulation Method and Results

The device under study is a planar *p–i–n* solar cell composed, from bottom to top, of a $30\,\mathrm{nm}$ electron transport layer (ETL, $E_g = 3.3\,\mathrm{eV}$), a $280\,\mathrm{nm}$ formamidinium lead bromide ($FAPbBr_3$, $E_g = 2.27\,\mathrm{eV}$) absorber, and a $30\,\mathrm{nm}$ hole transport layer (HTL, $E_g = 3.2\,\mathrm{eV}$). To model the effect of interface engineering, the ETL and HTL electron affinities are varied and determine the valence band offset $\Delta E_V = E_V^{PVK} - E_V^{HTL}$ at the HTL/PVK interface and the conduction band offset $\Delta E_C = E_C^{PVK} - E_C^{ETL}$ at the PVK/ETL interface. The simulations are performed with Synopsys TCAD Sentaurus [5], employing transfer matrix method for optical generation and Poisson and drift-diffusion equations for charge transport. Bulk and interface defects are described through a spatially dependent profile inspired by experimentally reported trap distributions in perovskite films of comparable thickness [4]. As shown in Fig.1c, the trap density is higher at the interfaces and decreases toward the center of the film. The adopted fitting function is:

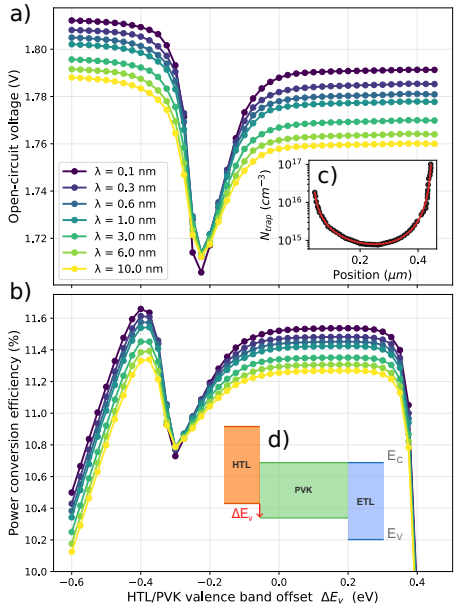


Fig. 1. (a) Open-circuit voltage and (b) Power conversion efficiency as a function of the HTL/PVK interface valence band offset, for different values of the effective length λ of the defects spatial distribution, with constant total areal trap density of $10^{11}\mathrm{cm}^{-2}$. (c) Example of fitting of experimental spatial distribution of traps from [4] using (1). (d) Schematic of the solar cell band alignment.

$$N_{\mathrm{trap}}(x) = D_T\left(1+\frac{x}{\lambda_T}\right)^{-p_T} + D_B\left(1+\frac{L-x}{\lambda_B}\right)^{-p_B}, \quad (1)$$

where $D_{T,B}$ (T: top, B: bottom) are the interface peak densities, $p_{T,B}$ control the decay, $\lambda_{T,B}$ are the effective lengths at which the density is half of the peak value at the respective interface, and L is the perovskite film thickness. Traps are modeled as deep states at mid-gap, with electron and hole cross-sections of $10^{-15}\mathrm{cm}^2$.

To investigate the interplay between trap distribution and band alignment, we consider a case study in which the HTL/PVK band offset is varied while keeping the PVK/ETL interface perfectly aligned ($\Delta E_C = 0$), so as to isolate the contribution of a single interface. If not otherwise stated, a

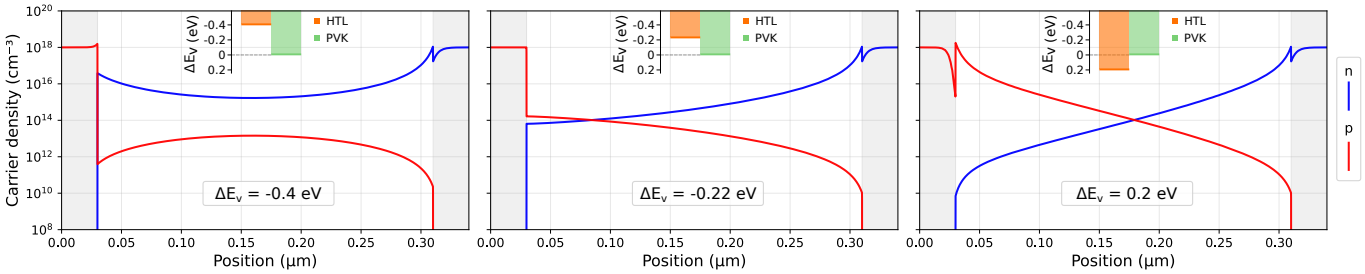


Fig. 2. Electron (blue) and hole (red) densities for different HTL/PVK interface band offsets, considering the PVK/ETL interface perfectly aligned ($\Delta E_{\mathrm{C}} = 0$). All figures are obtained at 1.71 V, *i.e.* at the open circuit voltage of the case with $\Delta E_{\mathrm{V}} = -0.22\,\mathrm{eV}$, and $\lambda = 1\,\mathrm{nm}$.

symmetric trap profile is used, with total areal density of $10^{11}\mathrm{cm}^{-2}$, $p_{T,B} = 1$ and interface peak density determined by the value of the effective length (e.g. for $\lambda = 1\,\mathrm{nm}$ we have $D \simeq 10^{17}\mathrm{cm}^{-3}$).

Fig. 1a shows a non-monotonic dependence of V_{oc} on ΔE_{V}, with a marked minimum (V_{oc} =1.71 V) for $\Delta E_V = -0.22\,\mathrm{eV}$ (condition where the HTL valence band is above the PVK one), and two plateau regions at negative and positive offsets. As shown in Fig. 1b, the power conversion efficiency (PCE) is maximized within the left-side V_{oc} plateau, at about $\Delta E_V = -0.4\,\mathrm{eV}$, and degrades toward the edges of the explored offset range. Since the short-circuit current is essentially unaffected, this trend mainly reflects the trend of the fill factor. It is worth noticing that the $\Delta E_{\mathrm{C}} = 0$ case is studied here as representative cut of the broader two-dimensional band-offset space. In fact, band-offset maps (not reported here, [6]) show that the same non-monotonic V_{oc} behavior is generally preserved, although the absolute V_{oc} and PCE maxima can occur on either side of the minimum region depending on the value of ΔE_{C}.

The physical origin of these regimes is clarified by the carrier profiles in Fig. 2 and the recombination profiles in 3, calculated for the three case studies at 1.71 V, *i.e.* the V_{oc} of the worst case ($\Delta E_V = -0.22\,\mathrm{eV}$). For $\Delta E_V = -0.4\,\mathrm{eV}$ the energy barrier at the HTL/PVK interface significantly limits hole injection (Fig. 2). The resulting carrier separation reduces trap-assisted recombination especially at the interfaces, where the trap-density is higher, and leads to the high V_{oc} plateau.

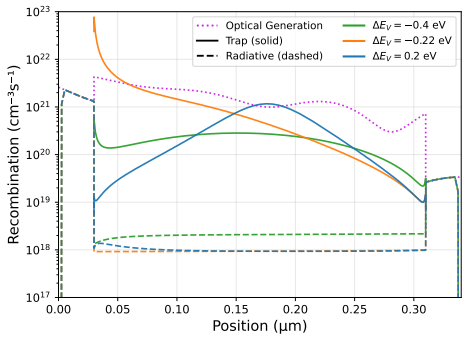


Fig. 3. Optical generation and recombination profiles for the three alignment cases described in figure 2.

At $\Delta E_V = -0.22\,\mathrm{eV}$, instead, the device electrostatics induce interfacial conditions under which electron and hole densities are comparable near the HTL interface. This causes large trap-mediated recombination, as seen in Fig. 3, and gives rise to the V_{oc} minimum. The depth of this minimum is further modulated by the PVK/ETL band offset: when this interface is brought into an equivalent unfavorable alignment condition, electron and hole densities become closer across the entire absorber and V_{oc} is further reduced. Finally, for a positive band offset, such as $\Delta E_V = 0.2\,\mathrm{eV}$ analyzed in Fig. 2, electrostatics band realignment leads to a more symmetric (*p-i-n* like) carrier density profile, with comparable electron and hole densities in the middle of the absorber. As a result, recombination is no longer dominated by the HTL/PVK interface, but by bulk traps (Fig. 3). This explains the stronger sensitivity of the right-side V_{oc} plateau to the parameter λ shown in Fig. 1, since increasing λ redistributes traps from interfaces toward the bulk. In contrast, the minimum is weakly affected, since the carrier balance in this configuration extends over the entire film thickness. Moreover, it is worth mentioning that increasing the total trap density shifts the entire V_{oc} curve down (Fig.1a), and causes the PCE peak in the left-side band offset range (Fig.1b), that is observed at the baseline trap density value, to disappear, while the plateau in the positive offset remains stable.

In conclusion, the study shows the non trivial, coupled role of trap distribution and interface band alignment in the voltage deficit of wide-bandgap perovskite solar cells, highlighting the need for further experimental and theoretical studies on these aspects.

Acknowledgment

This study was carried out within the CLAIRE project – funded by European Union – Next Generation EU within the PRIN 2022 program (D.D. 104 - 02/02/2022 Ministero dell'Università e della Ricerca).

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