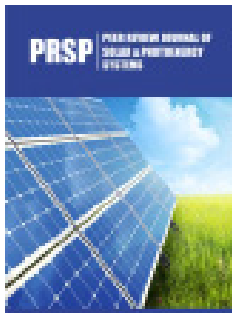


Surface Passivation: A Path Forward For Performance Improvement of Perovskite Solar Cells

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Opinion

Recently the power conversion efficiency (PCE) of perovskite solar cells (PSCs) has approached 25.2%. The theoretical Shockley-Queisser limit of power conversion efficiency of such materials with a bandgap of 1.6 eV is 30%. The remaining gap between theoretical limit and experimentally achieved PCE is possibly due to various types of defects distributed at the grain boundaries, surfaces and interfaces in the perovskite material hamper the efficiency improvements in the perovskite solar cells. In order to address surface defects different passivation schemes have been proposed recently. Here in this document, an overview of recent advancements in the knowledge of passivation schemes for PSCs has been summarized.

Introduction

Recent research has revealed that the metal halide perovskites have several noteworthy optoelectronic properties, such as large absorption coefficient, long charge carrier diffusion length and tunable band-gap [1]. In recent years, the power conversion efficiency (PCE) of perovskite solar cells (PSCs) have been improved from 3.8% to 25.2% [2]. The defect distribution in the PSCs at the grain boundaries, surfaces, and interfaces hinders photo-generated charge carrier transport through the radiative recombination and adversely affect the improvement of the PCE [3]. In order to address surface defects various passivation schemes have been described as an efficient approach for encouraging the efficiency of PSCs [4].

In a recent paper, guanidinium cation (Gua) has been discovered as an effective dopant to modify the crystal structure of MAPbI_3 [5-8] and mixed-cation $(\text{Cs})_x(\text{FA})_{1-x}\text{PbI}_3$ [9] perovskites, resulting in an improved photo-generated charge carrier lifetime and PCE. In another recent paper, compositional engineering of mixed-cation and mixed-halide perovskite compositions with guanidinium iodide (GuaI) enhanced the performance of PSC due to high values of open circuit voltage (V_{oc}) and reduced the interfacial charge recombination [10-15]. Remarkably, these studies examine the effect of guanidinium cation on the electrical output of PSC by mixing all perovskite precursors together [16]. Further, Luo et al. [17] described the use of guanidinium bromide, which forms a wide band gap over layer at the interface between the perovskite/HTL and consequently improves the value of V_{oc} [17]. Perhydropoly (silazane) (PHPS) is another material reported recently for passivation of PSC on the hole transport layer (HTL) side, whereas guanidinium iodide (GuaI) acts on the electron transport layer (ETL) side [1].

Theoretical Background

The V_{oc} is the potential difference measured experimentally between the external terminals of the PSC, but it is closely related to the internal quasi-Fermi level separation (QFLS) between the charge density in the conduction band and the valence band of the absorbing material (perovskite material). The quasi-Fermi levels, E_{Fe} and E_{Fh} represent the density of the free photo-generated electron and holes in the conduction band and valence band respectively under the limits of quasi-equilibrium. The net current density across the external terminals of the PSC is given by:

$$J = J_{ph} - J_R \quad (1)$$

Where, J_{ph} is the photo-generated current density and J_R represents the bimolecular recombination current density within the PSC during its operation. The value of J_R is given by [18]:

$$J_R = J_0 \exp(QFLS / (n \kappa_B T)) \quad (2)$$

Where, J_0 is the total dark recombination current due to radiative and nonradiative processes,

$$QFLS = E_{F_{ie}} - E_{F_{ih}}$$

T represents temperature in Kelvin, n represents diode ideality factor, and κ_B represents the Boltzmann constant. When the quasi-Fermi levels aligns with respective electrode work function then there is no bending of conduction band (CB) and valence band (VB) energy levels and then $QFLS = qV_{oc}$. The bending of the CB and VB levels decreases the effective value of QFLS. By adopting passivation schemes on the absorbing layer (perovskite layer) the extent of the band bending decreases and therefore the QFLS increases as shown in Figure 1, where PHPS acts on the HTL side [4] and Gual acts for passivation of PSC on the ETL side [16]. The gap between dashed lines representing the quasi-Fermi level's separation increases with passivation (using PHPS and Gual) as shown in Figure 1 in reference to cited papers.

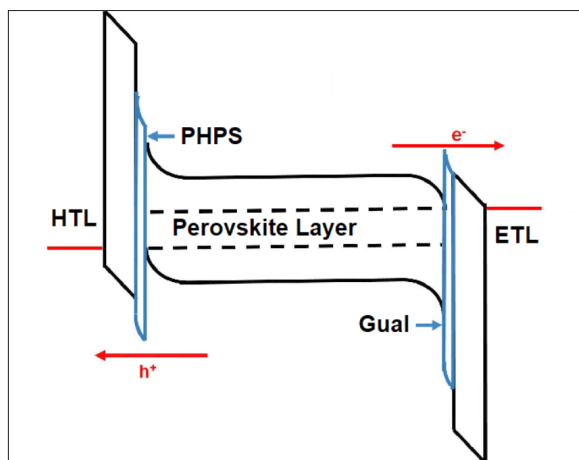


Figure 1: Band diagram revealing arrangement of passivation layers (PHPS and Gual) in the band structure of perovskite solar cell.

Conclusion

An opinion to outline the effect of surface passivation in the perovskite solar cells has been presented in this document. The recent research results have been summarized. For a better understanding, the band diagram based theoretical description has

been presented to reveal the effect of surface passivation on the electron transport process after photo-generation. It is clear that the recombination can be reduced by a suitable surface passivation strategy, which can help in improving the power conversion efficiency of perovskite solar cells.

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