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Hybrid Perovskite/GaP nanowires solar cells with enhanced photovoltaic performance

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Abstract. In this work we report an improved photovoltaic performance of hybrid halide perovskite solar cell with integrated into a active layer GaP nanowires. The incorporation of GaP nanowires improves charge extraction from a perovskite layer. As a consequence, we boost the $MAPbI_3$ perovskite solar cell efficiency up to 18.8% by open-circuit voltage and short-circuit current density enhancement. The provided multi-physical theoretical simulations of the solar cells with the incorporated GaP nanowires describe the mechanism of charge extraction and optical absorption improvement.

Keywords: perovskite solar cells, GaP nanowires, electric field management, photon management

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Материалы конференции
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Металло-органические галогенидные перовскитные солнечные элементы с интегрированными нитевидными нанокристалллами фосфида галлия с улучшенными фотовольтаическими характеристиками

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Аннотация. В этой работе сообщается об улучшенных фотофольтаических характеристиках металло-органического галогенидного перовскитового солнечного элемента с интегрированными в активный слой нитевидными нанокристаллами GaP. Включение нитевидными нанокристаллов GaP улучшает извлечение заряда из слоя перовскита. Как следствие, был повышен коэффициент полезного действия перовскитного ($MAPbI_3$) солнечного элемента до 18,8% за счет повышения напряжения открытой цепи и тока короткого замыкая элемента. Предоставленное мультифизическое теоретическое моделирование солнечных элементов с включенными нитевидными нанокристаллами GaP описывает механизм извлечения заряда и улучшения оптического поглощения.

Ключевые слова: перовскитные солнечные элементы, GaP нитевидные нанокристалллы, управление электрическим полем, управление фотонами

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Introduction

Since the very first report on lead halide organo-inorganic perovskite solar cells (PeSCs) was published in 2009 [1] this research area saw an expeditious development due to the perovskites' unique electronic and optical properties, such as tunable direct bandgap, high absorption coefficient, low nonradiative recombination rate, high defects tolerance, and high charge carriers' mobility [2]. The record perovskite solar cell PCE constitutes 25.8% to date. PCE [3], Integration of low dimension structures [4] into the perovskite active material aid the PeSCs performance enhancement beyond physical limitations (i.e. optical losses in substrates and charge transport materials, the lower light absorption of perovskite in the red spectral range and charge recombination at interfaces between the perovskite and transport layers as well as between perovskite grains). GaP nanowires are promising nanostructure to incorporate in PeSCs due to high refractive index (n >3) allowing for strong light confinement, high transparency in the visible wavelengths range [5], optimal thermal conductivity for optoelectronic applications in addition to the band gap tunability via doping [6]. Here, we incorporate GaP (i-type) and GaP:Be (p-type doping) NWs to be placed between a mesoporous TiO_2 hole-transport layer (HTL) and $MAPbI_3$ perovskite photoactive layer of n-i-p PSC to enhance light-harvesting and improve electrical charge extraction inside of the perovskite layer. We report PCE 5.45% increment value for PSC with integrated i-GaP NWs and 8.48% PCE increment for GaP:Be NWs with the best device possessing PCE 18.8%.

Materials and Methods

The numerical modeling of SC optical properties was performed with COMSOL Multiphysics software. Self-catalyzed GaP NWs grown on Si(111) substrates by solid-source MBE using Ga as a catalyst were used in this study. The PeSCs were fabricated in n-i-p architecture with Glass/FTO/c-TiO_2/m-TiO_2/GaP NWs/$MAPbI_3$/SPIRO-MeOTAD/Gold structure. Our PeSCs underwent optical (i.e. photoluminescence (PL) intensity spectra, time-resolved photoluminescence (TPL) decay spectra) and functional (i.e. J-V curves characteristics, external quantum efficiency (EQE) and photocurrent) characterization.

The J-V characteristics of the measured cells have been measured under a solar simulator (ABET Sun 2000, class AAA) at light spectra of AM 1.5 G and 100 mW/cm^2 illumination power calibrated with a certified reference Si cell (RERA Solutions RR-1002). The incident power was checked with a Skye SKS 1110 sensor. The measured area of cells was 0.1 cm^2.

The external quantum efficiency and photocurrent at $V = 0$ have been performed via a commercial machine Arkeo – Cicci Research with an integrated xenon lamp and a monochromator (Newport 74 000) and was able to acquire spectrum from 300 to 1100 nm with a measurement step of 20 nm. The calibration has been performed by a commercially certified reference Si cell. All measured cells were covered by a metal mask with a certain square size of 0.1 cm^2.

Results and Discussion

According to our simulation results introduction of GaP NWs leads to the bending of bands near the NW edge, see Fig. 1, resulting in the emergence of a conductive channel inside of the perovskite layer around the surface of the nanowire for holes, in case of the p-doped GaP NWs, and holes and electrons in case of i-doped GaP NWs, respectively.

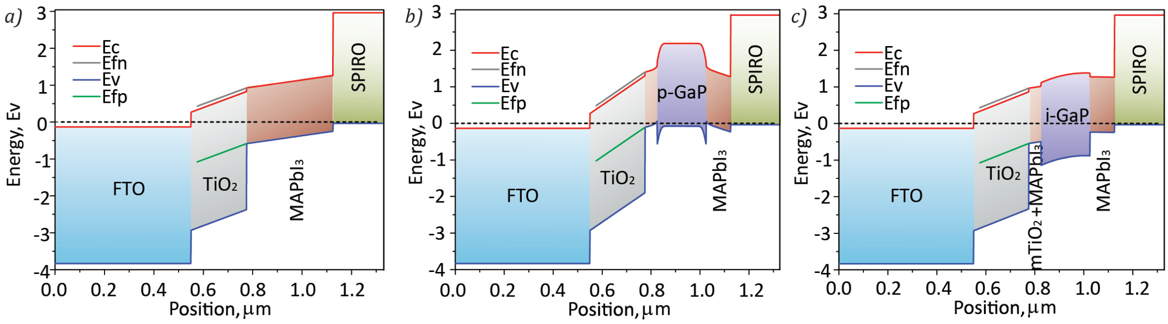

Fig. 1. Simulated energy level band diagrams for mesoporous perovskite solar Cells: reference cell (*a*); cell with p-GaP NWs (with Be doping concentration of 10^{18}cm^{-3}) (*b*); cell with i-GaP NWs (with Be doping concentration of 10^{17} cm^{-3} the band diagram is equivalent)

Both effects improve PeSCs EQE, and, consequently enhanced when compared to the reference cell photocurrent at the wavelength range from 550 nm to 780 nm, see Fig. 2, *b*.

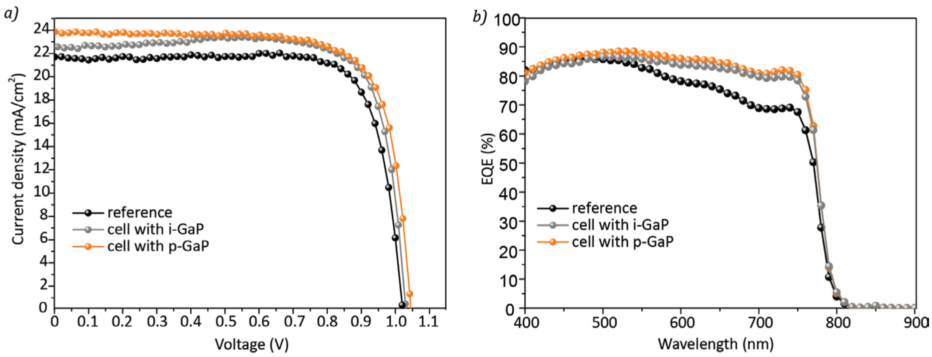

Fig. 2. Experimental data for PSCs with and without GaP NWs: (*a*) J—V curves for the best devices: reference (dot-line black curve), with p-GaP NWs (dot-line orange curve) and with i-GaP NWs (gray data); (*b*) EQE for the best PSCs related to the J—V curves shown in (*a*)

After GaP NWs introduction perovskite film PL signal is improved by 12% and by 15% for the case of i-GaP and p-GaP NWs, respectively, see Fig. 3.

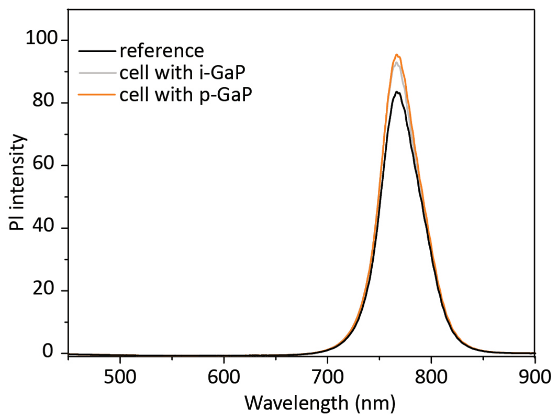

Fig. 3. Photoluminescence intensity signal for $MAPbI_3$ thin films with integrated GaP NWs compared to the reference sample

PeSC reference best performance: PCE = 17.5%, VOC 1.00 V, JSC = 21.9 mA/cm^2 and FF of 80.2%, see J-V curves in Fig. 2, *a*. The cell with the highest PCE (18.8%) contained p-GaP NWs and demonstrated a VOC of 1.04 V, JSC of 23.6 mA/cm^2 and FF of 76.3%. The best cell with i-GaP NWs was achieved a PCE of 18.5% with VOC of 1.03 V, JSC of 22.4 mA/cm^2 and FF of 80.4%.

Conclusion

We proposed a novel approach to PeSCs performance advancement via GaP NWs incorporation. The GaP NWs introduction improves electrical charge extraction and enchances light-harvesting inside of the perovskite layer We report PCE 5.45% increment value for PSC with integrated i-GaP NWs and 8.48% PCE increment for GaP:Be NWs with the best device possessing PCE 18.8%.

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