Proceedings of CONF-FMCE 2025 Symposium: Semantic Communication for Media Compression and Transmission
DOI: 10.54254/2755-2721/2025.GL25781

A Study on the Photovoltaic Conversion Mechanism of High-Efficiency Lead Halide Perovskite Solar Cells

Hairui Zeng

School of Optoelectronic Engineering, Changchun University of Science and Technology, Changchun, China
2661581713@qq.com

Abstract. Organic–inorganic halide perovskite materials have emerged as a core light-harvesting medium for the new generation of solar energy devices due to their high absorption coefficients and high charge carrier mobility. Enhancing their photovoltaic conversion efficiency further depends on an in-depth understanding of their conversion mechanisms. This paper provides a detailed explanation of key kinetic processes such as light absorption and exciton dissociation, carrier transport and recombination, and interfacial charge transfer in perovskite photovoltaic materials. It reveals various potential factors affecting charge carrier recombination efficiency and emphasizes the significance of defect state passivation and recombination suppression for improving photovoltaic performance. This study serves as a valuable reference for optimizing the performance of future photovoltaic devices.

Keywords: halide perovskite materials, charge separation, energy transfer, carrier recombination, photovoltaic conversion

1. Introduction

Driven by the growing global demand for energy and increasing environmental awareness, organic-inorganic hybrid perovskite photovoltaic materials have emerged as promising optoelectronic materials due to their excellent photophysical properties. These materials exhibit tremendous development potential in the photovoltaic industry. Perovskite photovoltaic structures typically refer to a class of materials with a perovskite crystal structure, generally represented by the chemical formula ABX_3. The unit cell structure is illustrated in Figure 1(a). In this structure, the A-site cations occupy the eight corners of the cube, the B-site cation is located at the center, and halide anions are positioned at the centers of the six cube faces. A common crystallographic motif is the halide octahedral structure, in which the octahedra are interconnected through shared halide ions. The A-site cations occupy the spaces between these octahedra, while the B-site cations reside within the octahedra. These halide octahedra are arranged periodically in space, forming the entire crystal structure.

© 2025 The Authors. This is an open access article distributed under the terms of the Creative Commons Attribution License 4.0 (https://creativecommons.org/licenses/by/4.0/).

DOI: 10.54254/2755-2721/2025.GL25781

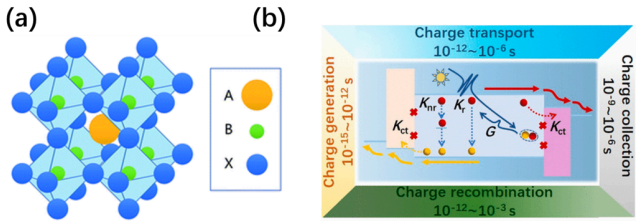

Figure 1. (a) Schematic diagram of the perovskite unit cell structure; (b) Schematic diagram of charge separation and energy transport in perovskite materials

The photoelectric conversion process in perovskite solar cells primarily includes four steps: light absorption, carrier generation, carrier transport, and carrier collection (as shown in Figure 1(b)). When sunlight irradiates the perovskite layer, the photon energy excites electrons from the valence band to the conduction band, generating photogenerated electron-hole pairs. These electrons and holes are subsequently separated under the influence of transport layers and transferred to the corresponding electrodes, ultimately producing current through an external circuit. Perovskite photovoltaic cells exhibit high photoelectric conversion efficiency and feature a relatively simple fabrication process, which facilitates their commercialization and large-scale production [1]. Moreover, the bandgap of perovskite materials can be tuned by adjusting the type and concentration of halide ions and cations, enabling the cells to adapt to different solar spectra and improve the utilization efficiency of solar energy [2].At present, further enhancing their photoelectric performance and improving device stability are critical goals for promoting the commercialization and technological advancement of perovskite solar cells. Achieving these goals relies on a deeper understanding of the photoelectric conversion mechanisms in perovskite cells. Therefore, this work aims to conduct an in-depth investigation into their photoelectric conversion behavior.

2. Literature review

Due to the structural diversity of perovskite optoelectronic devices, they have been widely applied in various fields. A classic material, $CH_3NH_3PbI_3$, serves as the light absorber, where photogenerated excited-state electrons are transferred to the electrode interface to achieve efficient photoelectric conversion [3]. By studying the processes of charge generation and separation, the general conversion mechanisms of perovskite optoelectronic devices can be summarized, providing a basis for identifying high-performance composite materials. In the photoelectric conversion process of perovskite solar cells, the charge dissociation process is the most critical step. Upon absorption of incident light, electrons in the dielectric are excited from the valence band to the conduction band, leaving behind holes in the valence band. These electron-hole pairs, still bound by Coulombic interaction at their original sites, form quasiparticles known as excitons. As shown in Figure 2, the dissociation of excitons marks the generation of free electrons and holes, which initiates the charge transport process.

DOI: 10.54254/2755-2721/2025.GL25781

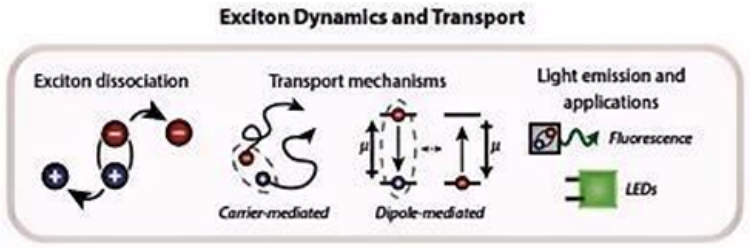

Figure 2. Schematic diagram of exciton dissociation and charge transport in perovskite materials

As illustrated in Figure 2, the transport of free charges generated by exciton dissociation to their respective electrodes is a key step in photoelectric conversion. In perovskite solar cells, the entire charge separation process consists of two stages: the transport of charges to the interface, and the transfer of electrons and holes from the interface to the electrodes. In general, the interface charge transfer (ET) process plays a more significant role in $CH_3NH_3PbI_3$-based photovoltaic cells. Through kinetic studies on charge transport dynamics (CT) in $CH_3NH_3PbI_3$ materials, these two intertwined stages can be accurately distinguished. By integrating the "diffusion-coupled charge transfer" model with ultrafast transient absorption spectroscopy, it has been found that the ET kinetic time constant typically falls within the nanosecond to microsecond range [4], indicating that the ET process occurs prior to charge trapping [5].As shown in Figure 3, exciton dissociation and charge collection lie at opposite ends of the carrier dynamics timescale, with exciton dissociation generally occurring on the picosecond timescale. Enhancing the efficiency of exciton dissociation is crucial for improving photoelectric conversion efficiency, as only efficient dissociation yielding free charges can initiate the carrier transport process [6]. For example, interfacial modification can reduce the exciton dissociation driving energy, thereby promoting more efficient charge separation.

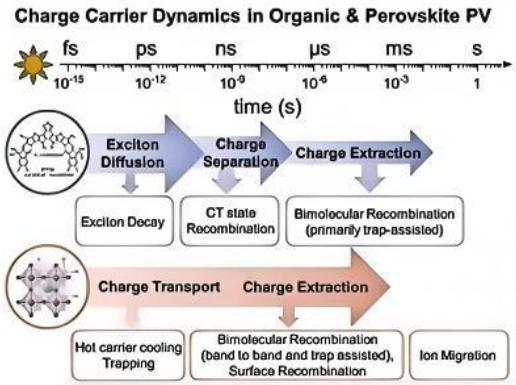

Figure 3. Schematic diagram of carrier dynamics timescales in perovskite materials

Following exciton dissociation, the prerequisite for effective interfacial charge transfer is rapid bulk transport of photogenerated charge carriers. This characteristic depends on the carrier diffusion behavior, which is typically described by the diffusion length and diffusion coefficient of the perovskite material [7]. In general, under sunlight conditions, free photogenerated carriers in perovskite materials are not significantly affected by exciton annihilation, as this is a process that occurs under intense excitation. The irradiance of sunlight is far below the threshold needed to trigger such annihilation. However, the charge recombination rate has a substantial impact on the dynamics of carrier diffusion. Therefore, increasing the diffusion length enhances the transport rate of electron–hole pairs [8]. Moreover, the diffusion rate of the carriers themselves is directly

DOI: 10.54254/2755-2721/2025.GL25781

proportional to the diffusion coefficient: the larger the coefficient, the faster the transport. As shown in Figure 4, the power density of external irradiation is closely related to the defect state density and the carrier diffusion coefficient of the material. This presents higher requirements for research into carrier recombination mechanisms [9]. Consequently, to better coordinate carrier transport and interfacial charge transfer dynamics, an in-depth understanding of the photogenerated carrier recombination mechanism is essential.

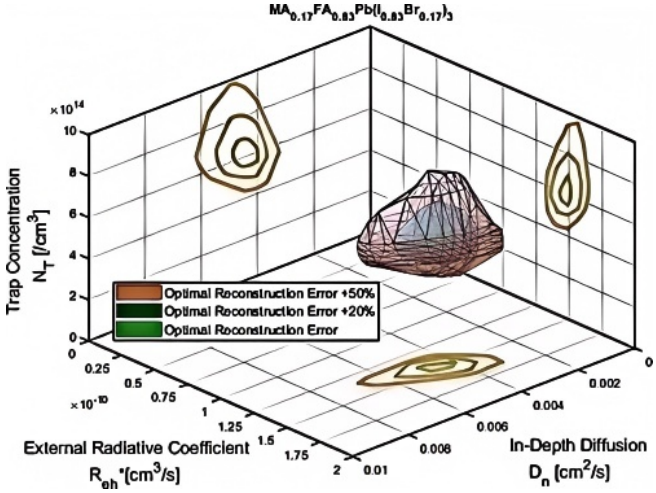

Figure 4. Functional relationship between diffusion coefficient and diffusion depth

In perovskite materials, the relatively high dielectric constant reduces the exciton binding energy, laying the foundation for efficient charge separation and the easy formation of free electrons and holes [10]. However, bimolecular recombination and trap-assisted recombination have become the two main energy loss pathways. Under gradually decreasing external illumination, free electrons and holes in perovskite materials tend to recombine spontaneously, resulting in energy loss. This leads to a sharp reduction in the number of photogenerated carriers, causing a decline in conductivity and, consequently, damaging the efficiency of photoelectric conversion [11]. Therefore, analyzing photoconductivity decay is crucial. Excited-state photons of varying speeds generate a potential difference across both ends of the photovoltaic material, and the magnitude of this variation can be detected using a micro-current detector. The potential difference is proportional to carrier lifetime and thus reflects recombination behavior [12].Additionally, time-resolved photoluminescence (TRPL) can be employed to capture the radiative lifetimes of carriers associated with recombination in the bandgap. TRPL enables the distinction between radiative and non-radiative recombination processes, and provides carrier lifetime information under different conditions by analyzing intensity data. This technique is useful for elucidating defect-assisted Shockley–Read–Hall recombination and Auger recombination processes [13].

Recent experimental studies show that the losses of photocurrent and photovoltage in lead-halide perovskite solar cells are closely related to carrier recombination at the interface, particularly recombination involving band tail states, where the possibility of trap-assisted recombination cannot be ruled out [14].Generally, bimolecular recombination can occur independently without catalytic assistance from absorbers or external additives, whereas tail state recombination relies on recombination channels formed by impurity energy levels [15].Moreover, the required concentrations of free charges and electron–hole pairs differ significantly between the two processes. Notably, tail state recombination is a non-radiative process. It is evident that

DOI: 10.54254/2755-2721/2025.GL25781

photogenerated carrier recombination in perovskite materials is a key photoelectric conversion dynamic process that is closely associated with the nature of defect states [16].

3. Conclusion

In summary, perovskite photovoltaic cells demonstrate unique advantages in energy conversion. Compared to traditional crystalline silicon solar materials, they possess higher light absorption coefficients and greater carrier mobilities, making them more favored in the photovoltaic device field. The carrier recombination process is influenced by multiple factors, including the crystal structure and defect density of the material itself, defect states at the charge separation interface, as well as external conditions such as temperature and illumination intensity. Furthermore, charge recombination occurs in various forms; both bimolecular recombination and tail state recombination release energy at interfaces, thereby reducing the operational efficiency of photovoltaic cells. Therefore, a comprehensive understanding of the carrier dynamics and associated processes in perovskite photovoltaic devices is crucial for improving their performance and efficiency. This study offers in-depth insights into the working mechanisms of perovskite solar cells and lays a solid foundation for the development of more cost-effective and highly efficient solar cell materials.

References

[1] Duan, L., Uddin, A., Progress in Stability of Organic Solar Cells, Adv Sci (Weinh), 7, (2020), 1903259.
[2] Gramlich, M., Lampe, C., Drewniok, J., Urban, A. S., How Exciton-Phonon Coupling Impacts Photoluminescence in Halide Perovskite Nanoplatelets, J. Phys. Chem. Lett., 12, (2021), 11371-11377.
[3] Xiang Zhang, et al. Metal Halide Perovskite as Down-Conversion Materials for Advanced Display. Adv. Mater. 2025, DOI: 10.1002/adma.202410194.
[4] Xu, Lili, Liu, Gaoyu, Xiang, Hengyang, Wang, Run, Shan, Qingsong, Yuan, Shichen, Cai, Bo, Li, Zhi, Li, Weijin, Zhang, Shengli, Zeng, Haibo, Charge-Carrier Dynamics and Regulation Strategies in Perovskite Light-Emitting Diodes: From Materials to Devices, Applied Physics Reviews, 9, (2022).
[5] Xie, Yongchao, Zhang, Jia, Yu, Haomiao, Li, Jinpeng, Wang, Kai, Zhu, Xixiang, Broad Two-Photon up-Conversion Photoluminescence Realized by Locally Polarized Heterostructures in 2D Perovskite, J. Phys. Chem. C, 127, (2023), 21220-21226.
[6] Baranowski, Michal, Plochocka, Paulina, Excitons in Metal-Halide Perovskites, Adv. Energy Mater., 10, (2020).
[7] Zhu, T., Snaider, J. M., Yuan, L., Huang, L., Ultrafast Dynamic Microscopy of Carrier and Exciton Transport, Annu. Rev. Phys. Chem., 70, (2019), 219-244.
[8] Savenije, T. J., Ponseca, C. S., Jr., Kunneman, L., Abdellah, M., Zheng, K., Tian, Y., Zhu, Q., Canton, S. E., Scheblykin, I. G., Pullerits, T., Yartsev, A., Sundstrom, V., Thermally Activated Exciton Dissociation and Recombination Control the Carrier Dynamics in Organometal Halide Perovskite, J. Phys. Chem. Lett., 5, (2014), 2189-2194.
[9] Liu, N., Liu, P. F., Zhou, H. P., Bai, Y., Chen, Q., Understanding the Defect Properties of Quasi-2D Halide Perovskites for Photovoltaic Applications, J. Phys. Chem. Lett., 11, (2020), 3521-3528.
[10] Ryu, H., Park, D. Y., McCall, K. M., Byun, H. R., Lee, Y., Kim, T. J., Jeong, M. S., Kim, J., Kanatzidis, M. G., Jang, J. I., Static Rashba Effect by Surface Reconstruction and Photon Recycling in the Dynamic Indirect Gap of APbBr3 (a = Cs, CH3NH3) Single Crystals, J. Am. Chem. Soc., 10.1021/jacs.0c09132, (2020).
[11] Rundong Fan, et al. Tungstate-mediated In-situ Passivation of Grain Boundary Grooves in Perovskite Solar Cells. Angew. Chem. Int. Ed. 2023, DOI: 10.1002/anie.202303176.
[12] Mengjiong Chen, et al. Gas-medium annealing for perovskite solar cells with state-of-the-art energy loss. EES 2025, DOI: 10.1039/D5EE00851D.
[13] Yulin Liu, et al. Structurally Dimensional Engineering in Perovskite Photovoltaics. Adv. Energy Mater. 2023, DOI: 10.1002/aenm.202300188.
[14] J. Even, et al., "Perovskite photovoltaics: Life cycle and critical materials assessment, " Joule, vol. 1, no. 1, pp. 167-181, 2017.
[15] M. M. Lee, et al., "Efficient hybrid solar cells based on mesoscopic electrodes with quantum-sized CdSe nanoparticles, " Science, vol. 318, no. 5856, pp. 634-637, 2007.

DOI: 10.54254/2755-2721/2025.GL25781

[16] X. Gao, et al., "Ammonia gas-assisted solution process for perovskite solar cells with improved stability and efficiency, " Adv. Mater., vol. 28, no. 24, pp. 4991-4998, 2016.