钙钛矿太阳能电池中 CsPbBr_3 纳米晶界面修饰剂的作用机制

S. Wageh ^{1,*}, Ahmed A. Al-Ghamdi ¹, 赵丽 ^{2,*}

¹ Department of Physics, Faculty of Science, King Abdulaziz University, Jeddah 21589, Saudi Arabia.

² 湖北大学材料科学与工程学院, 功能材料绿色制备与应用教育部重点实验室, 有机化工新材料湖北省协同创新中心, 武汉 430062

Insights into Mechanism of CsPbBr_3 Nanocrystal Interfacial Modifier in Perovskite Solar Cells

S. Wageh ^{1,*}, Ahmed A. Al-Ghamdi ¹, Li Zhao ^{2,*}

¹ Department of Physics, Faculty of Science, King Abdulaziz University, Jeddah 21589, Saudi Arabia.

² Hubei Collaborative Innovation Center for Advanced Organic Chemical Materials, Ministry of Education Key Laboratory for the Green Preparation and Application of Functional Materials, School of Materials Science and Engineering, Hubei University, Wuhan 430062, China.

Emails: wswelm@kau.edu.sa (S.W.); zhaoli7376@163.com (L.Z.)

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(a–b) Transient TA spectra and (c) normalized decay kinetic curves of FTO/SnO₂/PSK and FTO/SnO₂/CN/PSK.

Schematics for electron excitation and extraction at the interfaces (d) between SnO₂ and PSK or (e) between SnO₂ and CN/PSK. (f) Schematic for the changes of Fermi level at PSK/ETL interface and PSK/HTL interface.

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During the past decade, organic-inorganic hybrid perovskite solar cell (PSC) has attracted great attention in the photovoltaic field^{1,2}. As the third-generation solar cell, PSC in laboratory has already achieved certified power conversion efficiency (PCE) exceeding 25%. The superb photovoltaic performance of PSC is attributed to the unique optoelectronic properties of organic-inorganic halide perovskite light absorption layer, including low exciton binding energy, high absorption coefficients, and outstanding carrier mobility^{3,4}. Hence, the quality of perovskite film plays a decisive role in the photovoltaic performance of PSC. Defects are inevitably formed on the surface and inside of polycrystalline perovskite film during the conventional preparation methods. It's widely acknowledged that defects are the recombination centers of photogenerated electrons and holes, resulting in the loss of useful photogenerated charges^{5,6}. Therefore, decreasing the charge loss is advantageous to improving the PCE of PSC.

With the tremendous efforts of researchers in photovoltaic field, numerous research works have successfully reduced charge loss through additive engineering, heterojunction construction, and interfacial modification^{7,8}. However, the modifiers utilized in these works are typically polymers, salts, and molecules. Their components and structures are totally different from that of perovskite, leading to the poor physicochemical compatibility with perovskite film. Consequently, developing modifiers which possess similar chemical composition and crystal structure with perovskite would be a more sensible choice. Inorganic metal halide perovskite nanocrystals have crystal size in dozens of nanometers, but still maintain the outstanding photoelectric properties of bulk perovskite. Some research works have verified the significance of perovskite nanocrystal in interfacial modification. Nevertheless, the perovskite nanocrystals in these works are generally prepared through hot-injection method. In addition, none work has investigated the functions of perovskite nanocrystal in bilateral interface modification of perovskite film, and the mechanism of perovskite nanocrystal induced interface modification requires deeper exploration.

To address these aforementioned issues, **Jiaguo Yu** (Wuhan University of Technology) and **Tao Chen** (University of Science and Technology of China) *et al.* recently reported a room-temperature synthesized CsPbBr₃ nanocrystal (CN) and investigated the effects and mechanism of CN in the bilateral interface modification of CH₃NH₃PbI₃ (MAPbI₃) perovskite film (*Advanced Science* **2021**, 8, 2102648. doi: 10.1002/advs.202102648)⁹. CN is prepared by quickly injecting excess lead salt precursor into the violently stirred cesium salt precursor at room-temperature. The CN bilateral interface modification of perovskite film is composed of CN bottom modification and CN top modification. The as-synthesized CN is spin-coated on to the SnO₂ electron transport layer (ETL) to accomplish the CN bottom modification. CN top modification is realized *via* utilizing CN dispersed anhydrous toluene as the

antisolvent during the one-step preparation process of perovskite film. As for the CN bottom modification, CN at surface of SnO₂ ETL is able to serve as the seed crystal, facilitating the seed-mediated growth of perovskite film (PSK). Hence, the defects at SnO₂/PSK interface can be effectively decreased. Femtosecond transient absorption (fs-TAS) characterization is conducted to investigate the electron transfer dynamics at SnO₂/PSK interface. The photobleaching peaks at ≈ 760 nm (PB2) are ascribed to the photo-induced carrier population in perovskite film (Fig. a,b). Furthermore, the electron injection time ($\tau_{\text{injection}}$) can be obtained through bi-exponential fitting of the decay kinetic curves at 759 nm (Fig. c). The $\tau_{\text{injection}}$ is decreased from 611 to 258 ps with CN bottom modification, illustrating that CN can passivate the interfacial defects and promote the electron extraction process (Fig. d,e). Concerning CN top modification, a gradational doping of CN is formed at the upper part of perovskite film. *In situ* Kelvin probe force microscopy and *in situ* CPD detection characterizations confirm that the Femi level (E_f) of PSK surface is lowered after CN top modification both under dark condition and illumination. Accordingly, the Fermi level difference between the surface and bottom of the film has increased (Fig. f), contributing to enlarged built-in electric field. This suggests the separation of photogenerated electrons and holes is significantly improved with CN top modification. Combining the merits of CN bottom modification and top modification, CN bilateral interface modified planar PSC exhibits average PCE exceeding 20%.

To briefly conclude, this work has provided mechanism insights into the functions of CN in the interfacial modification of perovskite. Controllable preparation of CN at room-temperature is achieved, and boosted built-in electric field contribute to efficient separation of photogenerated electrons and holes inside PSC. This novel research work has also revealed the potential of perovskite nanocrystal-based modifiers in photoelectric devices including photovoltaics, LEDs, and photodetectors.

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