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Studies of Incorporation CsPbBr₃ Quantum Dots in Perovskite Films

Perovskite quantum dots (PQDs) represent a promising avenue for enhancing the efficiency and stability of perovskite solar cells (PSCs). The integration of PQDs into PSCs has been shown to extend absorption range, enhance photon harvesting, and improve device efficiency. Furthermore, PQDs offer the potential to stabilize PSCs structure by passivating surface defects and enhancing overall stability. The choice of ligands on the surface of PQDs significantly influences their incorporation into PSCs, impacting charge transport properties, interface formation, and device stability.

In this work, the effect of the CsPbBr₃ QDs doping on the perovskite structure and optoelectronic properties was studied. The single-phase CH₃NH₃PbI₃ (MAPbI₃) perovskite and triple cation perovskite Cs_{0.05}(MA_{0.17}FA_{0.83})_{0.95}Pb(I_{0.83}Br_{0.17})₃ (CsFAMI) layers were deposited on the ITO glass substrate by spin coating. The chlorobenzene (CB) was employed as the anti-solvent. For doping, the PQDs were mixed into the CB antisolvent. Three different concentrations of PQDs (0.05, 0.1, 0.15 mg/mL) were explored for perovskite doping. The preparation conditions were kept unchanged for a particular perovskite.

The CsPbBr₃ QDs were synthesized by hot-injection technique applying cesium oleate, PbBr₂, and two distinct ligands: oleic acid combined with oleylamine (OAOAm CsPbBr₃), and didodecyldimethylammonium bromide (DDAB CsPbBr₃). The scanning transmission electron microscopy analysis verified the uniform cubic structure and consistent shape of the CsPbBr₃ QDs, demonstrating an average size ranging from 10 to 14 nm.

The UV-Vis absorption spectra indicate absorption edges for OAOAm CsPbBr₃ QDs thin film at approximately 513 nm (band gap of 2.38 eV) and for DDAB CsPbBr₃ QDs at around 490 nm (band gap of 2.33 eV). Moreover, the band gap of the pristine perovskite layers, MAPbI₃ and CsFAMI, were determined to be 1.61 eV and 1.58 eV, respectively. The incorporation of CsPbBr₃ QDs with both types of ligands into the perovskite with the concentrations the 0.05, 0.1, and 0.15 mg/mL resulted in marginal enhancements in the absorption for the MAPbI₃ perovskite. No discernible alterations were noted for the CsFAMI perovskite.

Steady-state photoluminescence (PL) and time-resolved PL (TRPL) measurements were performed to study the effect of PQDs doping on the morphology and optoelectronic properties of the perovskite layer. The PL peak of the samples containing pristine and doped MAPbI₃ and/or CsFAMI perovskite with CsPbBr₃ QDs in different concentrations is observed for both ligands at 771 and 780.5 nm, respectively. The TRPL was measured at the wavelength where the maximum emission from the perovskite layer occurred. The TRPL data were fitted by bi-exponential decay models. Here, the fast decay PL component (t₁) is related to the charge carrier trapping by trap states, and the slower component (t₂) is assigned to the free carrier recombination.

For MAPbI₃ doped with the DDAB CsPbBr₃ PQDs, a small increase in the t₁ and t₂ components for 0.05, and 0.1 mg/mL doping concentrations was observed. A maximum increase of t₁ from 9.9 ns for the undoped MAPbI₃ layer up to 14.9 ns for the MAPbI₃ layer doped with 0.15 mg/mL was found. For OAOAm CsPbBr₃ PQDs, a similar maximal prolongation of t₁ up to 14.9 ns was observed for 0.1 mg/mL doping. For the slower component, a maximum prolongation of t₂ from 65 ns for pristine MAPbI₃ to 88.9 ns for DDAD CsPbBr₃ QDs 0.15 mg/mL doping and up to 106.2 ns for OAOAm CsPbBr₃ QDs 0.1 mg/mL doping were found.

Slightly different behavior was observed for CsFAMI perovskite doped by CsPbBr₃ QDs. For the PQDs with DDAB ligand in CsFAMI we found an almost unchanged t₁ (9.9 ns for pristine perovskite vs 10.0 for 0.1mg/mL doping). For the t₂ component, an increase from 64 ns for pristine perovskite up to 89 ns for 0.15 mg/mL doping was found. For OAOAm PQDs, maximum increase of t₁ up to 20.1 ns was found for 0.05 mg/mL doping. For t₂ maximum, an increase from 61.9 ns for pristine CsFAMI up to 100.8 ns for 0.15 mg/mL doping was found.

In summary, the CsPbBr PQDs doping could be effective for both MAPbI₃ and CsFAMI perovskites. The increased values for t_1 and t_2 for all concentrations were observed, more pronounced being for the OAOAm ligand. This could point to the possibility of suppressing the charge carriers trapping as well as free carrier recombination at the grain boundaries by the PQDs doping.

The results will be completed by SEM, AFM, and XRD studies to analyze the effect of doping on the morphology.

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