

Correlation between Capping Ligands and Photovoltaic Properties in PbS

Quantum Dot Solar Cells

°Jin Chang,^{1,4} Yuki Kuga,¹ Taro Toyoda,^{1,4} Yuhei Ogomi,^{2,4} Shuzi Hayase,^{2,4} Kenji Katayama,³ and Qing Shen^{1,4}

Univ. Electro-Commun.¹, Kyushu Inst. Tech.², Chuo Univ.³, CREST JST⁴

Email: shen@pc.uec.ac.jp

Introduction

Colloidal quantum dots (QDs) are generally capped with long-chain, electrically insulating ligands which are introduced during the synthetic procedures. Replacement of these molecules with shorter chain ligands has been shown necessary to decrease the inter-dot spacing and improve the electron transfer in QD thin films. This work investigate the impact of the ligand chain length and scaffold on the photovoltaic properties and carrier dynamics in PbS quantum dot solar cells (QDSCs) by ultrafast transient absorption (TA) spectroscopy, temperature-dependent photoluminescence (PL) and transient photovoltage decay measurements.

Experimental Method

Native oleic acid ligands on PbS QD surfaces were replaced by mercaptoalkanoic acids with various chain length using the solid state ligand exchange method as shown in Fig. 1. The structure and fabrication method of PbS quantum dot solar cell (QDSCs) are similar with that of previous reports.¹ As prepared PbS solid films were characterized by the fourier transform infrared spectroscopy (FT-IR), transmission electron microscopy (TEM), steady state optical spectroscopy and transient absorption spectroscopy. The photovoltaic properties of QDSCs were characterized by the photocurrent density-voltage (J - V) curves, incident photon to electron conversion efficiency (IPCE) and transient photovoltage decay measurements.

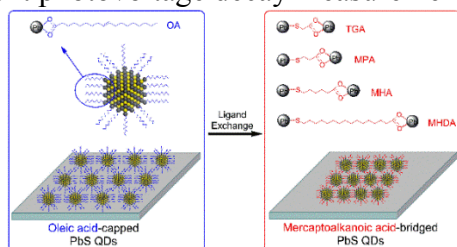


Fig. 1 Schematic illustration of the ligand exchange of PbS QD thin films.

Results and Discussion

According to FT-IR spectra (Fig. 2), native OA ligands were completely replaced by mercaptoalkanoic acids after ligand exchange. The inter-dot spacing in PbS QD films was narrowed as the ligand chain length decreased. The photoluminescence (PL) spectra in Fig. 3(left) shows that the emission peak was red-shifted as the inter-dot spacing decreased, indicating the enhanced coupling between QDs. It was found that 3-mercaptopropanoic acid (MPA) gave the highest photocurrent of 15.3 mA/cm² and power conversion efficiency of 2.64%. Although the shortest ligand thioglycolic acid (TGA) leads to the smallest inter-dot spacing, it does not give the highest photocurrent, which could be due to its acidity and ligand-induced defects on QD surfaces. Our findings in this work are useful for the deeper understanding on the effect of surface ligands on QDs and would shed light on the further improvement of QDSCs.

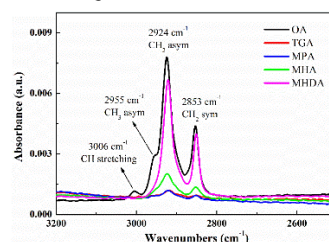


Fig. 2 Reflective FT-IT spectra (3200-2500 cm⁻¹) of PbS QD films capped with various surface ligands.

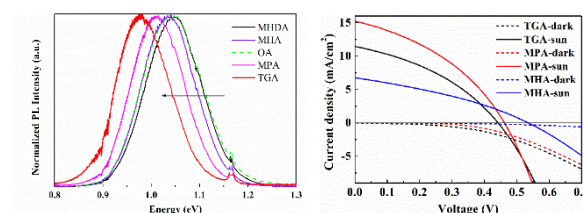


Fig. 3 Left: PL of PbS QD films at 77 K with various surface ligands. Right: J - V curves of PbS QDSCs with different ligands.

[1] J. Chang, Y. Kuga, I. Mora Sero, T. Toyoda, Y. Ogomi, S. Hayase, J. Bisquert and Q. Shen, *Nanoscale*, 2015, 7, 5446-5456.