Research on the Performance of Fmoc-amino Acid Passivated Peroverskite Solar Cells

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Abstract. This study investigates the effect of surface passivation of chalcogenide solar cells by introducing Fmoc-Gly-OH amino acids. The results show that the moderate amount of Fmoc-Gly-OH modification can significantly improve the photovoltaic performance and stability of chalcogenide solar cells. With the increase of Fmoc-Gly-OH concentration, the photovoltaic conversion efficiency firstly increases and then decreases, and the best effect is reached when the concentration is 1.0 mg/ml.XRD and SEM analyses show that the crystal structure of the Fmoc-Gly-OH modified chalcocite thin films is more regular, and the defect density is obviously reduced.XPS analysis shows that the Fmoc-Gly-OH modification is able to reduce the defect state density of the chalcogenide layer. The reduction of defects was further verified by steady-state fluorescence spectroscopy analysis. In addition, the electrochemical impedance spectra and dark-state I-V curve results of the devices showed that the Fmoc-Gly-OH modification was able to reduce the non-radiative complexation and charge transport resistance, and increase the fill factor and open-circuit voltage. Finally, the effectiveness of Fmoc-Gly-OH surface passivation in enhancing the performance of chalcogenide solar cells was confirmed by the analysis of J-V curves and box plots. This study provides new ideas and methods for surface engineering of chalcogenide solar cells, which has some practical application prospects.

Keywords: chalcogenide solar cells, Fmoc-Gly-OH, photovoltaic performance, stability, surface engineering

1. Introduction

Organic-inorganic hybrid halide perovskite materials have excellent properties[6], but perovskite crystals inevitably cause harmful crystal defects in the interior, grain boundaries and surface during the growth process, which ultimately leads to the reduction of the efficiency and stability of perovskite solar cells. Researchers try to reduce defects with different methods, such as solvent engineering, component change engineering, surface passivation engineering, additive engineering, etc.

Among these methods, surface passivation is considered to be the most commonly used and the most effective. The excess Pb2+ is thought to be a major source of charge traps, which neutralize their positive charge and eliminate the charge traps caused by structural defects by coordinating with lone pairs of electrons on Lewis bases. This passivation treatment usually results in a significant increase in the photoluminescent quantum yield and lifetime of the perovskite film, indicating a decrease in the non-radiative recombination center. However, the interaction between most passivating agents and Pb2+ is usually weak and the passivating effect is unstable[7], so it is crucial to find passivating agents with strong coordination capacity which will lead to recombination of non-radiative charges. Therefore, the introduction of some effective chemicals to passivate these defects will greatly help the efficiency and stability of the device. This graduation project mainly studies the efficiency and stability of the device by introducing Fmoc-Gly-OH amino acid material with two functional groups of amino (-NH2) and carboxyl (-COOH) to passivate the interface defects of perovskite.

2. Effect of Amino Acid Concentration on Photoelectric Conversion Efficiency of Cells

We adjusted the concentration of Fmoc-Gly-OH to modify the light-absorbing layer of chalcogenide, prepared trans-plate chalcogenide solar cells with different concentrations[3], and investigated the trend of photoelectric conversion efficiency with concentration. See Fig. 1, the photoelectric conversion efficiency increased and then decreased when the concentration increased from 0 mg/ml to 1.5 mg/ml, and reached the highest value of 1.0 mg/ml. when the concentration reached 1.5 mg/ml, the efficiency decreased, indicating that the excess amino acid affected the light-absorbing properties of the chalcogenide layer, which in turn reduced the photoelectric conversion efficiency. Therefore, we chose 1.0 mg/ml as the optimum concentration for subsequent studies.

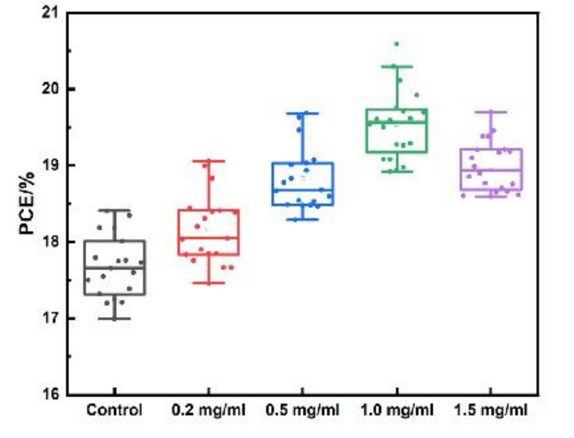

Figure 1 Variation of photoelectric conversion efficiency with concentration of Fmoc-Gly-OH.

3. Microscopic Morphology Analysis of Hole Transport Layer Thin Films

In order to verify the passivation effect of Fmoc-Gly-OH on chalcogenide films, we analyzed unmodified and modified chalcogenide films by scanning electron microscopy[4]. Figure 3 shows that the unmodified films have defects such as excessive P crystal particles on the surface, resulting in relatively weak light absorption intensity. In contrast, the Fmoc-Gly-OH-modified films exhibited a more compact and flat crystal grain stacking. Specifically, the addition of 1.0 mg/ml modifier promoted grain growth, resulting in larger and denser stacking of grains in the chalcogenide layer. However, when the modifier concentration reached 1.5 mg/ml, grain growth was inhibited and aggregation was produced on the film, which further verified the change in light absorption intensity[10].

In order to verify the uniform doping of Sr, we analyzed the Sr:NiOx films by facet scanning, as shown in Fig.2(a), the three elements of Sr, O, and Ni were uniformly distributed on the surface of the films, confirming the uniform doping of Sr. In Fig.2(b), we compare the SEM images of the hole transport layer films with different structures and find that the grain agglomeration is more obvious in the Sr-doped film, which is due to the expansion of the NiOx lattice by the larger Sr atoms. However, the grain agglomeration of Sr:NiOx/Sr:NiOx films is lighter than that of Sr:NiOx/Sr:NiOx films because the lattice expansion is slowed down by the surface of NiOx films. In addition, the surface of NiOx/Sr:NiOx films is smoother, more continuous and denser, which reduces the non-radiative complexation at the interface and provides a good basis for the deposition of high quality chalcogenide films. Figure 2(c) demonstrates the cross-sectional SEM image of the prepared trans chalcogenide solar cell, which highlights the importance of having a uniform and dense charge transport layer for the solar cell performance, especially the preparation of the hole transport layer is the first step in building a trans flat plate chalcogenide solar cell.

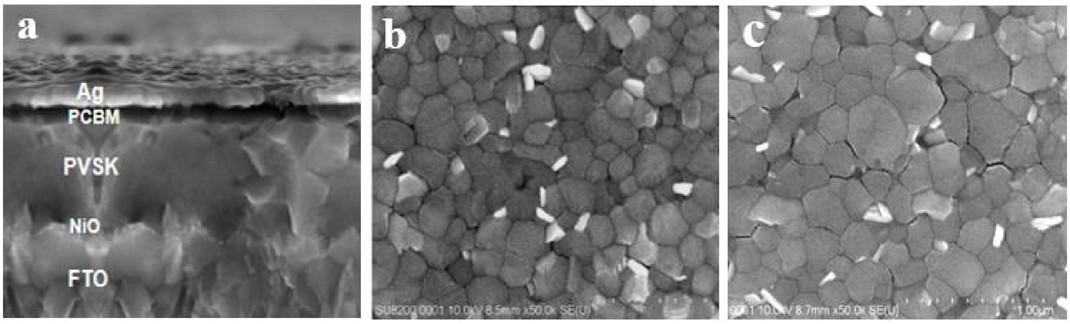

Figure 2 Cross-sectional SEM image of the device with Fmoc-Gly-OH modified MAPbI3 film (a) and SEM images of (b) pristine perovskite and (c) 1.0 mg mL–1 Fmoc-Gly-OH added perovskite thin films at the same scale.

4. Absorbance and Steady-state Photoluminescence Analysis

We tested the absorbance of FTO/calcite layers doped with different concentrations of Fmoc-Gly-OH by UV spectrophotometry, and the results are shown in Figs. As can be seen from Figs.3, the light absorption of the chalcogenide films improved with the addition of Fmoc-Gly-OH in the visible range of wavelengths 380-800 nm. However, when the amount of additive was greater than 1.0 mg/mL, the formation of chalcogenide was inhibited to some extent due to the interaction of excess Fmoc with more Pb2+ in the chalcogenide layer, and aggregation was generated at the top of the film layer, which blocked the absorption of light by chalcogenide. This is also corroborated with the final photoelectric conversion efficiency.

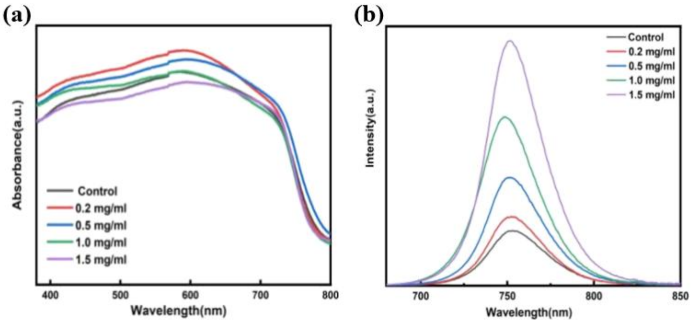

Figure 3 (a) UV-Vis spectrum, (b) steady-state photoluminescence (PL) spectra of perovskite films with different concentrations of Fmoc-Gly-OH added.

We investigated the effect of Fmoc-Gly-OH on the chalcogenide layer by fluorescence spectroscopy analysis. The results showed that the PL intensity increased with the increase of Fmoc-Gly-OH concentration, indicating that the modified chalcogenide film had a lower defect density and reduced non-radiative complexation. This confirms that Fmoc-Gly-OH amino acids passivate the chalcogenide defects and reduce the non-radiative complexation sites, thus decreasing the probability of carrier complexation.

5. Analysis of Photoelectric Performance of Solar Cells

The curve that most intuitively reflects the improvement of solar cell performance by Fmoc-Gly-OH passivation is the current-voltage curve, and the current-voltage curve of the cell with the best performance is shown in Fig. 4, and its various optical property parameters are also summarized in Table 3-2. From this table, it can be seen that the addition of Fmoc-Gly-OH significantly improved the photovoltaic performance of the chalcogenide solar cell, in which the optimal concentration was 1.0 mg/ml, and its photovoltaic conversion efficiency was 20.61%, the open-circuit voltage was 1.00 V, the short-circuit current was 23.02 $\mathrm{mA \cdot cm^{-2}}$ and the filling factor was 0.79, which was a significant improvement relative to the initial solar The comprehensive performance of the solar cell has an obvious improvement.

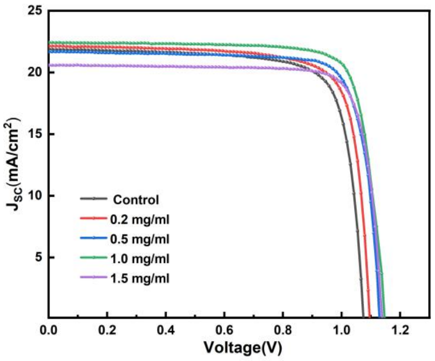

Figure 4 The J-V curves of best PSCs without and with Fmoc-Gly-OH of reverse scan.

6. Conclusion

Surface passivation of Fmoc-Gly-OH produces highly efficient and stable PSCs.SEM images show that Fmoc-Gly-OH-modified films have tighter grains, smoother crystal surfaces, and greatly reduced trap density. PL, TRPL tests show the reduction of non-radiative composites and the decrease of defect density.Uv-Vis, EIS, and other data demonstrate the quality enhancement of chalcogenide thin films and corresponding devices modified by Fmoc-Gly-OH.Passivation passivates defects at the grain boundaries of chalcogenide thin films while inhibiting unfavorable ionic migration, effectively enhancing the open-circuit voltage. This method is simple to operate and has some guiding significance for chalcogenide surface interface modification engineering.

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