ABSTRACT

Organic metal halide perovskites (OHPs) have emerged as promising contenders for photovoltaic applications, owing to their remarkable optoelectronic characteristics. In recent years, substantial enhancements in material processing and device optimization have propelled the power conversion efficiency (PCE) of perovskite solar cells (PSCs) over 26% for single-junction device. However, the prevalent practice of fabricating PSCs within glove boxes or under controlled atmospheres poses a significant barrier to commercial scalability. This thesis aims to develop protocols for the complete perovskite solar cell fabrication under air ambient conditions with controlled humidity.

The concentration of defects, including shallow, deep, and interfacial ones, plays a crucial role in recombination, carrier mobility, and overall stability in PSCs. Through simulation analysis, the impact of defect concentration on device performance is highlighted, emphasizing trapping, de-trapping, and recombination events. Employing simulations, impedance analysis, and experimental results, strategies such as doping and band offset modifications are demonstrated to mitigate ionic defects and enhance PSCs performance. Furthermore, the optimization of SnO_2 colloidal solution concentrations and successful stabilization approaches for the photoactive α-$FAPbI_3$ phase without additives in ambient conditions are showcased. Consequently, the optimized SnO_2 layer exhibits improved surface morphology and electronic conductivity. The best-performing cell achieves a PCE of 20.46%, with non-encapsulated devices retaining normalized PCE above 85% even after enduring 1200 hours under relative humidity levels below 40%. Additionally, a strategic approach is employed to tackle critical performance degradation issues associated with interfacial defects in fabricating anti-solvent-free PSCs. This involves deliberately incorporating Guanidine Sulfate (Gua-S) at the interface between SnO_2 and $FAPbI_3$. This incorporation significantly enhances the perovskite film's morphology, crystallinity, and thermal stability, improving solar cell performance. Notably, the device exhibits an increase in overall efficiency of 22.34%, retaining 87% of its initial PCE even after 2000 hours of operation. Thus, this thesis comprehensively addresses defect mitigation, stabilization of the perovskite phase in ambient air, and interfacial defect passivation in the anti-solvent-free process, enhancing the stability and efficiency of PSCs for commercial viability.

Keywords: Perovskite Solar cells, Ambient fabrication, Defect mitigation, Efficiency enhancement, Stability enhancement, Interfacial defect passivation.