ABSTRACT

Organic-inorganic lead halide perovskite-based solar cells (PSCs) have emerged as promising candidates for efficient energy harvesting due to their superior optoelectronic properties. While significant progress has been made in PSCs for outdoor photovoltaic applications, their performance and optimization under indoor lighting conditions—crucial for powering the rapidly growing ecosystem of IoT devices and sensors—remain relatively underexplored. This thesis focuses on the design, optimization, and development of indoor perovskite solar cells (IPSCs), integrating machine learning (ML), numerical simulations, and experimental techniques to address key challenges in material selection, device performance, and sustainable fabrication.

Initially, a ML-assisted bandgap prediction model was developed to guide the design of wide bandgap perovskite materials suitable for indoor light harvesting. Based on the model predictions, mixed-cation mixed-halide FA-Cs-based perovskites were identified as promising candidates for efficient indoor photovoltaic applications. Subsequently, an ML model was developed using recently published experimental data, with the perovskite bandgap and energy level offsets between the absorber and charge transport layers as input features, to accurately predict the photovoltaic parameters (V_{OC}, J_{SC}, FF, and PCE) of PSCs under outdoor conditions. Furthermore, another ML model incorporating additional features such as light source type and illumination intensity was developed to predict IPSC performance, closely matching experimental values. Thereafter, device performance was systematically investigated under diverse indoor light sources, including fluorescent and LED lighting (warm white and cool white), through simulation, with peak efficiency observed under cool white LED illumination. Finally, IPSCs were experimentally fabricated in ambient air using FA-Cs perovskite films, optimized through annealing temperature variations. A low-cost, stable and less-explored HTM (TOP-3) was employed, with anisole serving as both the HTM solvent and green antisolvent for eco-friendly processing. The optimized IPSC achieved a promising PCE of 25.44% under cool white LED illumination.

Keywords: Perovskite solar cells, Air ambient fabrication, Indoor Perovskites Solar Cells, Machine learning, Device Simulation, Hole transporting materials, Mixed-cation perovskites, Indoor Photovoltaics