Name: Iram Masood

Supervisor Name: Prof. Mukesh Pratap Singh

Name of Department: Department of Applied Sciences and Humanities, Faculty of Engineering and Technology, Jamia Millia Islamia

Thesis Title: Design Optimization of Thin Film Solar Cells

Keywords: Organic Solar Cells (OSCs), Perovskite Solar Cells (PSCs), OghmaNano, Bulk Heterojunction (BHJ), Charge Transport, recombination, Electron Transport Layer (ETL), Hole Transport Layer (HTL, Power Conversion Efficiency (PCE)

FINDINGS

The increasing global demand for clean and sustainable energy has intensified research into advanced photovoltaic (PV) technologies that are capable of delivering high efficiency at reduced manufacturing costs. Among the emerging photovoltaic technologies, Organic Solar Cells (OSCs) and Perovskite Solar Cells (PSCs) have attracted considerable attention because of their lightweight nature, low-temperature fabrication, flexibility, and potential for large area production. However, despite significant progress, their widespread commercialization remains limited due to efficiency losses, charge recombination, material instability, and poor band energy alignments.

The primary objective of my doctoral research was to improve the performance of Organic Solar Cells (OSCs) and Perovskite Solar Cells (PSCs) through numerical simulation and device optimization using the OghmaNano simulation platform. Instead of relying on costly and time-consuming experimental trial-and-error approaches, the research systematically investigated the influence of material selection, device architecture, layer thickness, transport layer engineering, carrier mobility, doping concentration, and interfacial energy alignment on photovoltaic performance. The work began with the study of the physical principles governing charge generation, transport, and recombination in organic and perovskite solar cells. Mathematical models based on Poisson's equation, carrier continuity equations, drift-diffusion transport, exciton dissociation, and optical absorption were employed to accurately simulate device behaviour under solar illumination.

The first part of the research focused on Organic Solar Cells (OSCs). Initially, an inverted device architecture "FTO/TiO_2/P3HT:PCBM/PEDOT/Ag" was investigated. The thicknesses of the active layer, electron transport layer (ETL), hole transport layer (HTL), and electrodes were systematically optimized to maximize light absorption while maintaining efficient charge extraction. Structural optimization resulted in an improved power conversion efficiency (PCE) of 5.37%, establishing an optimized baseline for further studies.

Subsequently, a conventional OSC architecture ITO/PEDOT:PSS/P3HT:PCBM/ZnSe/Al was analyzed with particular emphasis on non-geminate recombination mechanisms and thermal stability. Detailed optimization of device parameters demonstrated that minimizing recombination losses significantly enhances charge collection efficiency, leading to a maximum simulated PCE of 9.60%.

To further improve device performance, a comprehensive comparative investigation of transport layer materials was conducted. A total of 45 different OSC configurations were simulated by combining nine electron transport layer (ETL) materials with five hole transport layer (HTL) materials. Materials including ZnSe, TiO_2, ZnO, C_{60}, PCBM, CuO, SnO_2, WO_3, and WS_2 were evaluated as ETLs, while CuI, NiO, MoO_3, PEDOT:PSS, and P3HT were examined as HTLs. The study demonstrated that the ZnSe/CuI transport layer combination provides the most favourable energy level alignment, efficient carrier extraction, and reduced recombination losses, resulting in a maximum simulated PCE of 10.35%. These findings provide valuable design guidelines for selecting transport materials in high-performance organic photovoltaic devices.

The second part of the research focused on Perovskite Solar Cells (PSCs) employing the standard FTO/TiO_2/$CH_3NH_3PbI_3$/Spiro-OMeTAD/Au architecture. The work investigated exciton dissociation, free carrier generation, charge transport, and recombination mechanisms responsible for efficiency losses. Optimization of recombination parameters and charge carrier extraction significantly enhanced device performance, yielding a theoretical PCE of 29.79%.

Further optimization involved systematic variation of absorber thickness, transport layer thickness, carrier mobility, and doping concentrations of both ETL and HTL. The influence of interfacial energy level offsets on charge transport and recombination was also examined. The study demonstrated that appropriate optimization of transport layer properties can effectively compensate for mobility limitations while maintaining efficient charge extraction. Under optimized conditions, the PSC achieved a maximum theoretical power conversion efficiency of 30.68%, accompanied by improvements in open-circuit voltage (V_{OC}), short-circuit current density (J_{SC}), and fill factor (FF).

Overall, this research establishes that simulation-driven optimization is an effective and economical approach for designing next-generation photovoltaic devices. The work highlights the critical importance of transport layer engineering, thickness optimization, charge mobility, recombination suppression, doping optimization, and energy level alignment in achieving high-performance solar cells.

The outcomes of this research contribute to the understanding of device physics in both organic and perovskite solar cells and provide practical design strategies for improving efficiency and stability. The findings also serve as a foundation for future studies involving tandem solar cells, environmentally stable perovskite materials, and machine learning-assisted photovoltaic device optimization, thereby supporting the development of efficient, stable, and commercially viable renewable energy technologies.