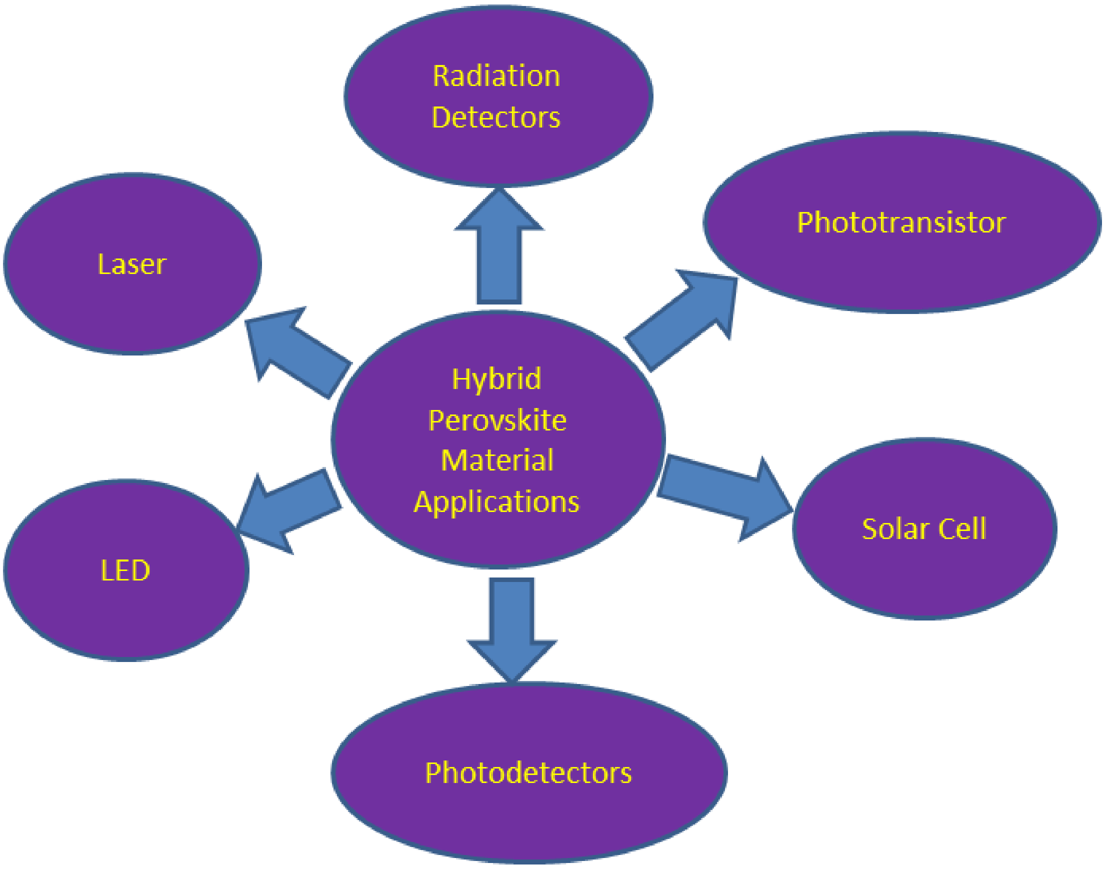
CHAPTER 6

Conclusion and Future Scope

Contents



CHAPTER 6

Conclusions and Future Scope

6.1 Introduction

Perovskite materials are widely used in many optoelectronic applications, such as solar cells, photodetectors, laser, LED, electronic sensors, radiation detectors, image sensors, etc. Hybrid perovskite materials have been projected as one the most important 4^{th} generation organic solar cell materials due to their possibility of bandgap tuning to achieve the power conversion efficiency (PCE) of more than 25%. In view of the above, the present thesis reports the fabrication, TCAD simulation and characterization of some $CH_3NH_3PbI_3$ hybrid perovskite solar cells (PSCs) with TiO_2 nanorods (TNRs)/ZnO nanorods (ZNRs) as the electron transport layer (ETL) and PTAA/ Spiro-OMeTAD hole transport layer (HTL). The major objectives of the thesis are to investigate the effects of thickness and morphological engineering of the ETL and doping engineering of the HTL on the performance optimization of the proposed PSCs in this thesis. Four types of $CH_3NH_3PbI_3$ hybrid perovskite based inverted PSC structures fabricated on the transparent fluorine doped tin oxide (FTO) substrates have been investigated in this thesis: FTO/TNRs/Perovskite/PTAA/Pd, FTO/TNRs/Perovskite/Spiro-OMeTAD/Pd, FTO/ZNRs/Perovskite/PTAA/Au and FTO/ZNRs/Perovskite/Spiro-OMeTAD/Pd. The perovskite thin film is used as an active layer (absorber layer), whereas Spiro-OMeTAD and PTAA are used as hole transport layers in solar cell structure. The fabrications and measurements have been carried out under robust open atmospheric conditions. That is why, the experimental results for FTO/TNRs/Perovskite/PTAA/Pd and FTO/ZNRs/Perovskite/Spiro-OMeTAD/Pd PSCs have been compared with the TCAD simulation data to show the deviations of the measured results under real environmental conditions from the ideal theoretical results. The present chapter summarizes the chapter-wise objectives and major findings of the thesis as described in the following:

6.2 Chapter-Wise Major Observations

Chapter-1 introduces the optoelectronic and photovoltaic properties of hybrid perovskite materials and their applications in solar cells, sensors, and LEDs. Different materials used for ETL and HTL and ETL/HTL engineering for the performance improvement of the PSCs are discussed. The optical and electrical characterization techniques such as spectrophotometry, XRD, TEM, SEM, UV-Vis spectroscopy, photoluminance spectroscopy, and impedance measurement used for the solar cells are also briefly discussed. A detailed literature survey has been carried out on the hybrid perovskite materials based solar cells. Literature surveys on various performance improvement techniques of the solar cells are also discussed. Based on the observations from the literature survey, the scopes of the thesis have been outlined at the end of this chapter.

Chapter-2 investigates the effect of ETL thickness on the electrical and optical characteristics of the FTO/TNRs/$CH_3NH_3PbI_3$/PTAA/Pd structure based perovskite solar cells (PSCs). The TNRs layer has been used for the ETL, PTAA as the HTL, and $CH_3NH_3PbI_3$ hybrid perovskite has been used for the active layer of proposed PSC. The TNRs are grown using the low-cost hydrothermal method at a temperature of 180^0 C, whereas both the $CH_3NH_3PbI_3$ active layer and HTL are deposited by the spin coating method. Both the fabrication processes and measurements are carried out in the open air condition for three proposed PSC devices with three different ETL thicknesses of 500 nm, 650 nm and 800 nm. The measured results have been compared with the TCAD simulation data to confirm the measured results with the ideal theoretical characteristics. The major observations of this chapter are listed below:

- The XRD pattern shows good crystallinity and rutile phase of the hydrothermally grown TNRs ETL.
- The effects of different ETL thicknesses on J_{SC}, V_{OC}, PCE, and EQE are compared for fabricated and simulated solar cells.
- The ETL thickness of 500 nm shows the best solar parameters for the proposed PSCs.
- The PCE of both the fabricated and simulated PSCs is decreased for ETL thickness above 500 nm.
- The optimum simulated values of V_{OC} (1.07), J_{SC} (23.71), FF (0.63) and PCE (15.69 %) against their corresponding experimentally measured values of V_{OC} (1.06), J_{SC} (22.19), FF (0.63) and PCE (15.04 %) are observed for the ETL thickness of 500 nm, perovskite thickness of 100 nm, and HTL thickness of 350 nm.
- The close proximity of the simulated electrical and optical characteristics with the experimentally measured results confirms that the TCAD tools can be effectively explored for other PSC structures.

Chapter-3 reports the effects of solvothermal etching and $TiCl_4$ treatment of the hydrothermally grown TNRs ETL of the electrical and optical characteristics of FTO/ZNRs/$CH_3NH_3PbI_3$/Spiro-OMeTAD/Pd structure based PSCs. The solvothermal etching is used to modify the surface morphology of the TNRs ETL. The performance parameters of the solvothermally etched ETL have been compared with those of PSCs with un-etched TNRs ETL. Fabrication and measurements are carried in a robust atmospheric condition with more that 60% humidity. The performance parameters of three types of PSCs have been carried out: (i) TNRs-based ETL without etching and $TiCl_4$ treatment (Device A); (ii) ETL with only $TiCl_4$ treatment but no etching of TNRs (Device B); and (iii) TNRs ETL with solvothermal etching followed by $TiCl_4$ treatment (Device C). The major observations are summarized below:

- ❖ The solvothermal etching of the TNRs ETL is shown to enhance the performance of fabricated PSC due to the increase in the effective surface-to-volume ratio of the ETL and absorption layers.
- ❖ The application of both the solvothermal etching followed by $TiCl_4$ treatment of the hydrothermally grown TNRs in "Device C" are observed to be the best among the three devices under study. This is attributed to the increased surface-to-volume ratio of the ETL by etching and increased carrier lifetime in the active layer owing to the reduced traps and voids by $TiCl_4$ treatment of the TNRs.
- ❖ The PCE, V_{OC}, J_{SC}, and FF of the fabricated champion device "C" are measured as 15.16 %, 1.04 V, 22.64 mA/cm2, and 0.64, respectively.
- ❖ The EQE of device "C" is also found to be the best among the three devices.

Chapter-4 investigates the electrical and optical performance characteristics of FTO/ZnO Seed Layer/ZNRs/$CH_3NH_3PbI_3$/PTAA/Au structure based PSCs where PTAA is used for HTL in the device. Four devices containing four different morphologies of ZNRs-ETLs grown by the hydrothermal method on four different types of seed layers (of drop-casted ZnO, spin-coated colloidal ZnO nanoparticles (NPs), spin-coated colloidal ZnO quantum dots (QDs), and hydrothermally grown ZnO NRs) were studied in this chapter. The major findings of the chapter are summarized below:

- The surface and structural morphologies of different types of ZNRs ETLs grown from different seed layers are analyzed by XRD and SEM measurements. The XRD confirms the uniform crystallinity of ZNRs while SEM confirms the growths of good quality ZNRs
- The PSC with the ZNRs-ETL grown from ZnO QDs based seed layer gives better electrical and optical performances over ZNRs-ETL based devices. The device shows improved shunt and series resistance over the other three devices.
- The values of J_{SC}, V_{OC}, FF and PCE of the ZnO QDs seed layer based PSC are 19.14 mA/cm^2, 1.01, 0.64, and 10.69% respectively.

Chapter-5 investigates the effects of doped and undoped spiro-OMeTAD based HTL on the performance of FTO/ZNRs/$CH_3NH_3PbI_3$/Spiro-OMeTAD/Pd solar cell. The hydrothermally grown ZNRs layer is used as the ETL of the device. The device parameters are compared for undoped and doped spiro-OMeTAD HTL based PSCs. The devices are fabricated and characterized in open air environment. The measured results have been compared with the numerical simulation data using Setfos^{TM} TCAD simulation tool for validating the measured data. The major observations of this chapter can be summarized as follows:

- The small molecules TBP and LiTFSI are used as additives in Spiro-OMeTAD to enhance the conductivity of the HTL layer. The doped Spiro-OMeTAD HTL based PSCs give better performance over the undoped Spiro-OMeTAD HTL based PSCs.

- For undoped HTL, the fabricated PSC gives an optimized *PCE* value of 9.51% with V_{OC} of 0.98 V, J_{SC} of 15.84 mA/cm^2, and fill factor (*FF*) of 61% under ambient-air environment. However, improved performance with *PCE* of 10.18%, V_{OC} of 1.01 V, J_{SC} of 18.57 mA/cm^2, and *FF* of 64% are obtained for the doped Spiro-OMeTAD HTL based PSC.
- The results are compared with the commercially available SetFos™ TCAD tool for showing the reliability of the measured data. Reasonably good matching is observed between the experimental results and TCAD simulation data.
- In simulated PSC, the PCE, V_{OC}, J_{SC}, and FF for undoped and doped HTL devices are observed as 10.13%, 1.001 V, 15.83 mA/cm^3, and 0.60: and 11.53%, 1.001 V, 17.27 mA/cm^3, and 0.66, respectively.

6.3 Future Scope of Work

- The PSCs based on the organic ETL and HTL can be fabricated on flexible substrates such as polyamide, PET, PEN, etc., for the flexible device.
- 2D/3D perovskite can be introduced as an active layer to make more stable PSCs.
- The introduction of perovskite quantum dots with a suitable bandgap can enhance photo absorbance in perovskite material.
- Doping of lanthanide materials can also be used to improve the device efficiency by up conversion and down conversion phenomenon.
- The blending of nanoparticles in ETL as a metamaterial can be used as an anti-reflection layer and enhanced optical properties by the plasmonic effect.

- Composites of graphene with metal oxides (ZnO, TiO_2, SnO_2, etc.) can be used as ETL in PSCs for fast charge transportation in the photovoltaic device.
- Multifunction tandem architecture could be explored to overcome the Shockley-Quiesser limit by utilizing larger spectrum absorbance.