ABSTRACT

Photovoltaic technologies have the potential to become one of the world's major renewable energy sources in the future, provided they can meet rising global energy demands at much lower generating costs than traditional non-renewable energy sources. Initially, solar cell devices were based on silicon material, but these solar cells are prohibitively expensive because of the high material cost and its processing. Bulk heterojunction (BHJ) based organic solar cells (OSCs), which can be produced at a lower cost with earth-abundant materials and have long-term stability, have emerged as a potential candidate to replace high-priced silicon solar cells. The low power conversion efficiency of thin-film OSCs has become a major constraint in employing OSCs, which is mainly caused by insufficient light absorption of thin active layers. In order to increase the light absorption in the BHJ based thin-film active layer, several light trapping techniques have been introduced. The application of nanophotonics to thin-film OSCs is a great scientific approach which allows the possibility of shrinking the active layer (AL) thickness while maintaining the high levels of absorption in thin AL. This creates a great scope for new device structures i.e, plasmonic OSCs, which enable the manipulation and modeling of light in nanoscale dimensions.

The work presented in this thesis is primarily focused to design and modeling of OSCs comprising of an AL of a low bandgap polymer containing plasmonic nanostructures in different regions of the solar cells such that the presence of the plasmonic nanostructures leads to an enhancement in the absorption in the AL, the short circuit current density, as well as the efficiency of the solar cells. Firstly, a BHJ based OSCs comprising of low bandgap photoactive layers with a 2-dimensional array of either Ag nano-spheres, nano-hemispheres, or nano-parabolas embedded at the bottom of the cell has been proposed. Numerical modeling using Finite Difference Time Domain (FDTD) was employed to study and compare the photovoltaic

properties of OSCs containing the different plasmonic nanostructures, in terms of optical absorption, short circuit current density (J_{SC}) and power conversion efficiency (PCE). Various geometrical parameters of the plasmonic nanostructures were optimized to obtain a substantial enhancement of light absorption in the AL. It was observed that the highest values of J_{SC} and PCE were obtained for optimized structure OSC having 2D arrays of Ag nano-parabolas at the back of the solar cell. An increase in J_{SC} and PCE of 26.41% and 26.37%, respectively, compared to a planar OSC was obtained for the OSC having a 2D array of parabolas at the bottom of the cell. The enhancement in photon absorption can be attributed due to the enhancement of light scattering from metallic nanostructures near their localized plasmon resonance. BHJ-based OSCs comprising of low bandgap photoactive layers and a combination of plasmonic nanostructures embedded in the cathode buffer layer and on top of the back Ag layer of OSCs have also been proposed in this thesis. These OSCs have a substantially enhanced absorption, short circuit current density (J_{SC}), and PCE as compared to a planar solar cell. FDTD simulations were performed to study and compare the photovoltaic characteristics of these OSCs having plasmonic nanostructures in different regions of the solar cells. Various geometrical parameters of plasmonic nanoparticles were optimized to obtain a substantial light absorption enhancement in different spectral regimes, corresponding to the absorption bands of the AL materials. Furthermore, this thesis also presents a comparative analysis of OSCs comprising of an AL of low and high bandgap polymers containing a combination of plasmonic nanostructures at the bottom of the cell and on the top of ITO.