ABSTRACT

The work presented in the Thesis was oriented towards both material and device (dye sensitized and perovskite solar cell) investigation and optimization. The initial research was dedicated on further improvement of the dye sensitized solar cells and subsequently, transferring the technological know-how, to the study and optimization of the perovskite solar cells.

Optimization and efficiency increment of PV devices was achieved by employing a surface post-treatment to modify the TiO_2 photoanodes, and further on, by employing composite SWCNT/TiO_2 photoanodes. It was established that the TiO_2 nanoparticle post-treatment operates in a manner of passivating the surface of the photoanode altering the recombination mechanism of the photogenerated carriers by reducing the surface trap states and enabling improvement of the photovoltaic parameters of the dye cells.

The results of a systematic study of the influence of the SWCNT loading in the composite photoanode, on different solar cell architectures, such as, liquid and solid state dye cells and perovskite solar cells, show that an efficiency increase due to the facilitated electron transport through the composite photoanodes can be achieved only within small concentrations of SWCNT loadings; at high concentration negative effects due to metallic nanotubes and aggregation are dominant. An increase of efficiency was evidenced for all three solar cell types with respect to plain TiO_2 photoanode reference cells.

Further on during the course of the PhD, the research was focused on the perovskite solar cell investigation and perovskite material properties. The morphological properties confronted by the photophysics of the perovskites, under illumination in cell configuration (charge generation and extraction), were studied by laser scanning techniques. Furthermore, investigation of planar perovskite solar cells and optimization with respect to low temperature processed solar cells was performed. It was established that O_2 had a curing effect on photovoltaic properties of the solar cells and the low temperature processed solar cell efficiencies were matching the high temperature processed opponent. Additionally, initial degradation studies did not show faster degradation channels due to presumably higher intrinsic humidity.

Improving the knowledge and understanding of the most utilized perovskite material in solar cell applications, methylammonium lead iodide ($CH_3NH_3PbI_3$), the physics of the interaction between the CH_3NH_3 cation and the PbI inorganic cage was studied by investigating the IR and Raman vibrational response in the frequency range from 30-3300 cm^{-1}, throughout a temperature interval spanning form 80-360K. Taking into account the vibrational relaxation, the reorientation activation energies and phonon-phonon interactions were studied. The results obtained give indication on cation dynamics, H-bond strength and methylammonium ordering in the orthorhombic phase; while Far-IR photoinduced absorption measurements show polaronic states formation. These results can help in understanding the fundamental connection between the charge transport and crystal structure of the perovskite materials, which can allow material tailoring and manipulation on an atomic level by exchanging the cation, metal or halide ion, to acquire specific material properties and utilize for specific applications.