ABSTRACT

This PhD thesis makes a significant contribution to the fields of natural sciences and engineering and technical sciences in the disciplines of physical sciences and materials engineering by investigating the potential of perovskites and metal-organic complexes in optoelectronic and photovoltaic applications.

The research focused on the development and characterization of materials in the form of nanostructures and thin layers, intending to enhance efficiency and stability and accelerate the sustainable development of next-generation solar cells and light-emitting devices.

The presented work covers the study of linear and nonlinear optical properties as well as morphological features of functional materials, using experimental techniques supported by calculations and theoretical simulations.

The thin films were fabricated by physical vapor deposition (PVD) technique and analyzed using advanced characterization techniques, including Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM), Photoluminescence (PL), Fourier Transform Infrared Spectroscopy (FTIR), UV-Vis Spectroscopy, and X-ray Fluorescence (XRF). Perovskite materials, particularly $RbSn_{0.5}Ge_{0.5}I_3$ and $MAPbI_3$, exhibited exceptional light absorption properties and significant photovoltaic potential upon integration into solar cells.

In addition, thin films of Znq_2, a metal-organic complex doped with organic molecules (red-dye-DCM), were studied for their structural, linear and non-linear optical properties, demonstrating energy transfer by Förster resonance, which is crucial for optoelectronic applications.

Furthermore, Density Functional Theory (DFT) calculations have provided a detailed analysis of the electronic structure of these materials, contributing to a better understanding of the mechanisms involved and leading to improved stability and performance in practical applications.

Through experimental as well as computational research, this work discovered promising materials for making solar cells having sub-micrometer thickness with efficiency comparable to silicon solar cells but with environmental compatibility. Those findings in this thesis are an important achievement towards building future-generation photovoltaic as well as optoelectronic photovoltaic devices, allowing innovative as well as sustainable industrial applications.