UNRAVELLING THE ROLE OF DEFECTS IN HYBRID SEMICONDUCTOR MATERIAL: A HOLISTIC EXPLORATION OF THEIR INFLUENCE ON OPTO-ELECTRONIC DEVICE PERFORMANCE

Abstract

The thesis explores the synthesis and applications of phase-pure iron pyrite nanocrystals (FeS_2 NCs), focusing on defect states and their impact on optoelectronic properties. Two cost-effective synthesis methods, hot injection and hydrothermal, were employed, revealing variations in crystallite size, optical band gap, and Urbach energy. The influence of defects on charge carrier lifetimes and densities was investigated, particularly in photovoltaic systems using P3HT:PC_{71}BM polymer mix, with FeS_2 NCs doped via both methods. The hydrothermal method resulted in lower device efficiency compared to hot injection. Co-alloying was found to alter conductivity, transitioning from p-type to n-type, promising improved electrical properties and nonlinear absorption coefficients for optoelectronic applications.

FeS_2 NCs were further studied for their impact on enhancing photovoltaic efficiency in bulk-heterojunction solar cells and organic photovoltaic cells (OPVs), revealing optimal doping concentrations and mechanisms enhancing device performance. FeS_2 NCs were also investigated as hole transport materials (HTMs) in perovskite solar cells (PeSCs) based on $MAPbI_3$, leading to enhanced short-circuit current density and stability, suggesting a cost-efficient alternative for PeSCs under open-air conditions.

Additionally, the study explored passivating defect states in air-processed $MAPbI_3$ PeSCs using p-type semiconductors, specifically copper(I) halides (CuI and CuBr). Incorporating CuI additives reduced energy levels of defect states, facilitating improved hole transport and reduced charge carrier recombination. Optimized PeSCs using CuI showed a substantial efficiency improvement to 14.1%.

Overall, this research contributes valuable insights into defect engineering in FeS_2 NCs and the strategic use of copper(I) halide semiconductors in enhancing the efficiency and durability of optoelectronic devices, thereby advancing sustainable energy research.