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Topic of Research: Study of Perovskite Photovoltaic Materials for Energy Harvesting

Findings

Hybrid organic-inorganic metal halide perovskite (MHPs) materials have proven to be efficient photoabsorber materials during past decade. This unprecedented progress in the field of photovoltaic has revolutionized the field of renewable energy. These materials can be prepared at low temperature using solution processed methods as compared to the capital intensive conventional Si based photovoltaic (PV) technology. Metal halide based perovskite (MHPs) exhibits number of desired optoelectronic properties such as high absorption coefficient, high mobility, large diffusion length, high defect tolerance and low exciton binding energy that make them suitable photoabsorber material for their application in solar cells. However, MHP photoabsorber materials suffers with various factors such as interface defects, ion migration and toxicity that leads to reduction in PCE and stability degradation of solar cells. For further device optimization and enhancement in device performance, these factors needs to be address in order enhance the PCE and stability of perovskite solar cells.

The research work present in the thesis mainly focused on the methodology and concepts to address aforementioned factors that suffers the performance of MHP solar cells. Synthesized methods were optimized to grown MHP materials with less bulk trap states. The detailed overview and analysis of pure and doped MHP materials has presented in this work to provide better understanding of octahedral PbX_6 dynamics, mixed ionic-electronic nature, interface trap defects, non-radiative loss and their effects on the optical, electrical and transport properties of the materials

Polycrystalline as well as single crystal samples of $MAPbX_3$ (MA = CH_3NH_3, X= I, Br, Cl) and of Cd^{2+} doped $MAPbBr_3$ were synthesized using a low temperature assisted solution growth technique. The samples were analyzed using XRD, SEM/TEM, UV-Vis., steady and transient photoluminescence, dielectric response, and space charge limited current dark I-V. The materials were also studied using computational simulations. An ionic-electronic model was used to understand the effects of ion migration. The role of trap state density on the performance of solar cell at different temperatures was studied using a drift-diffusion model.

The $MAPb_{1-x}Cd_xBr_3$ samples showed non-monotonic effects of doping on structure, optical bandgap and carrier lifetimes. Single carrier devices of different morphologies for $MAPbX_3$ (X= I, Br, Cl) were studied to understand the effects of ion migration, and interface defects on carrier transport properties. The single crystal devices exhibited enhanced transport properties such as mobility (μ) upto ~195 cm^2/V-s, diffusion length (L_D) ~ 5 µm with low trap state density (N_{trap}) ~ 10^8 cm^{-3}. Temperature dependent studies (100 K – 375 K) of the effects of defect capture cross-section ($\alpha\_$) and N_{trap} on the transport properties showed enhanced mobility upon carrier detrapping at high temperatures.