INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Programme of Study : Ph.D.

Thesis Title:
Development of New Materials and Methods for Dye Sensitized and Perovskite Solar Cells

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Thesis Submitted to the Department/ Center : Chemistry

Date of completion of Thesis Viva-Voce Exam : 30.06.2020

Key words for description of Thesis Work : Renewable Energy, Dye sensitized solar cells, perovskite solar cells,

SHORT ABSTRACT

A number of sources have been discovered and techniques developed in pursuit of renewable energy to overcome the energy crisis and reduce carbon foot print. Solar energy is considered as the most sustainable renewable energy source owing to the large amount of energy supply from the sun to the earth. Among photovoltaic technologies, dye-sensitized solar cells and perovskite solar cells are very attractive due to their lower production cost and easy fabrication. Dye-sensitizer is a key component in dye-sensitized solar cells and it has a similar role as the chlorophyll in plants. It harvests the sunlight and transfer the energy via electron transfer to an appropriate material (TiO2 in this case) for the production of electricity. With the aim to further enhance the conversion of sunlight to electricity, perovskite solar cells have been developed from dye-sensitized solar cells by replacing the sensitizer with perovskite materials having comparatively better charge transport properties. These solar cell devices fabricated with cheap and abundant materials seems a significant contributor to commercial photovoltaic technology in the near future.

This thesis is broadly organized into two parts. The first part focuses on the development of new sensitizers using several strategies to further advance the performance of dye-sensitized solar cells. The second part covers regulation of crystallization and trap states in perovskite through additive engineering to achieve high efficiency, stability and reproducibility of perovskite solar cells. Firstly, with the aim to achieve high efficiency in the dye-sensitized solar cells and understand the structure property relationship, a series of organic dyes having a carbazole donor, cyanoacrylic acid as an acceptor, and phenylene ring as a spacer with the difference in the positions and number of fluorine substitution were synthesized. The study revealed that fluorine substitution leads to a red shift in the absorption spectra of the dyes and reduces the band gap. As a result, the dye MA1F-o with o-fluoro substitution outperformed other dyes with a power conversion efficiency of 4.02%. Subsequently, to study and control the aggregation effect of sensitizers, mono- and di-anchor dyes having carbazole donor were synthesized. The results demonstrated that the presence of two acceptor groups provide efficient electron extraction from carbazole donor, reduces dye aggregation, and improves charge transfer. Therefore, an attractive power conversion efficiency of 5.35% was observed for di-anchor dye with iodide based redox electrolyte. A comparatively lesser efficiency was achieved in solid state dye sensitized solar cell.

Later, with the objective to regulate the crystallization process that could provide smooth perovskite films with large grains, Lewis acid-base adduct formation approach in concurrence with hot casting technique was employed. Uniform films of $MAPbCl_xI_{3-x}$ having large grain size were formed reproducibly on addition of 1.5 equivalents of dimethyl sulfoxide to the precursor solution. Perovskite solar cells fabricated using this solution resulted in power conversion efficiency of 14.11% with enhanced stability. Following this work, oxalic acid was used as additive in perovskite solution to regulate the crystallization, minimize ion migration and charge recombination in perovskite solar cells. As a result, 17.12% power conversion efficiency was obtained. Finally, benzene carboxylic acid derivatives (benzoic, isophthalic, and trimesic acids) were utilized to simultaneously control crystallization kinetics and passivate trap states in perovskite film resulting in maximum power conversion efficiency of 18.08%.

The efforts made in this thesis highlights the usefulness of molecular engineering of sensitizers as well as additive engineering of perovskites and provides the basis for facilitating the commercialization of dye sensitized and perovskite solar cells in the near future.