INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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SHORT ABSTRACT

The whole thesis has been organized into six chapters. The first chapter is about the brief introduction of Organic Photovoltaic devices and some recent developments in the Dye sensitized solar cells (DSSC), basic working principle of dye sensitized solar cell (DSSC), a detail explanation of components including in device. This chapter is concluded with the current state-of–the-art scenario and challenges related to design and synthesis of various wide band gap D-π-A, D-A- π-A dyes with a brief literature survey, including performance parameters and stability. The second chapter includes the design and synthesis of four new series of organic dyes based on meta-fluorine substituted phenyl moiety, used as a π-linker in various dyes, used for dye sensitized solar cell (DSSC) application. Without addition of any co-absorbent on TiO_2 layer we achieved highest efficiency (PCE) of 4.4% by using a simple m-Cz-dye due to the deep HOMO level, high molar absorption coefficient (13,126 $M^{-1}Cm^{-1}$), planarity of backbone and long excitation life time value (ns) = 1.25. The third chapter demonstrates the effect of various TiO_2 thicknesses with new series of dyes having ortho-fluorine substituted phenyl spacers contain different donors like carbazole, triphenylamine and phenothiazine moieties. The Optical, electrochemical, molecular orbital calculation and photovoltaic properties for different TiO2 thicknesses (9-12μm) of the new dyes were investigated. Thicknesses of TiO_2 film have effects on open circuit voltage (V_{oc}), short circuit current (J_{sc}) and efficiency. We observed that the Jsc and V_{oc} of o-Cz dye with a TiO_2 film thickness of 12 μm (8.91 mA/cm^2 and 0.63 V) are larger than film thickness of 9 μm (8.40 mA/cm^2 and 0.57 V). It could be due to the increase in thickness of TiO_2 film. At optimum thickness of TiO_2 film (12 μm), o-Cz dye exhibits power conversion efficiency (η) of 3.63(± 0.4)%. This was improved efficiency of o-Cz dye from 3.3% to 4.0% without using any coabsorbents, while changing the thickness of TiO_2 film. The fourth chapter explains about the synthesis of new AIEE based materials and its application in DSSC. Two chromophores TPA-PHA, TPA-PFA exhibits AIEE property due to the formation of excimer in aggregation state. The results reveal that, the TPA-PFA had less quantum yield (Φsolid=82.13) than TPA-PHA (Φsolid=88.32) in aggregated state, the reason behind that m-fluorine substitution on phenyl contains chromophore makes “inductive effect”, the substitution of fluorine atom has causes of more formation of ICT from Donor to Acceptor. From FESEM analysis we conclude that,

both AIEE chromophores are exhibits two different kinds of nano aggregates in solid state. These AIEE chromophores were utilized and developed as new dyes i.e., Dye-1, Dye-2 for DSSC application. The dye-1, dye-2 exhibit a power conversion efficiency (PCE) of 2.1% (J_{sc}= 5.05 mA/cm^2, V_{oc}= 0.67 V and FF= 0.61) and 1.9% (J_{sc}= 4.68 mA/cm^2, V_{oc}= 0.70 V and FF= 0.59), respectively. The fifth chapter describing about the synthesis of new thiophene 3,4-disubstituted dyes and effect of the electrolyte system on DSSC performance. New π-spacer contains thiophene 3,4- di substituted organic dyes with double acceptor at 2,5-position frame work. Influence of triphenylaime and carbazole units substitution at 3,4-position of thiophene based dyes optical, electrochemical, theoretical and photovoltaic properties with various electrolytes (Iodide and Co^{+2}/Co^{+3}) are studied. Without using any additives, 2Cz-Th dye and NPh3-Th dye in presence of cobalt (II/III) redox shuttle resulted in an overall power conversion efficiency (PCE) 3.3% and 3.1%, respectively. Final chapter describes facile alkylation method of CPDT and brominated CPDT. Our initial attempts 50% aq NaOH, TBAI, 1-bromo octane, CPDT were used for dialkylation in atmospheric conditions, but result, formation of a mixture of unwanted products in major amounts. The same reaction again started with careful degassing of the reaction mixture comprising three freeze–thaw cycles During the course of 5 minutes we observed that the colour of the reaction mixture changed into greenish black at 75 °C, however, no starting material was observed in the reaction mixture after 3h. This modification in the reaction conditions resulted in the development of highly successful dialkylation reaction of CPDT without the use of any organic solvents, metal catalyst, inert gases, strong acids, and high pressure/temperature, yet 82–96% isolated yield of the desired product 4,4'- dialkyl CPDT could be achieved with a variety of alkyl halides including chloro alkanes. This facile method has several advantages such as the exclusive use of water instead of high boiling toxic solvents, simple separation of the defect free dialkylated CPDT product and the use of mild reaction conditions.