


NIR Active Squaraine Dyes for Dye-Sensitized Solar Cells: Modulating Aggregation and Electronic Properties of the Dyes

Rajesh Bisht and J Nithyanandhan

Email: rh.bisht@ncl.res.in

Dye-sensitized solar cells (DSSC) have shown great potential as an alternative to silicon based solar cells for future demand of clean and renewable energy. They are cheaper and easy to fabricate in comparison to silicon solar cells. The light absorbing sensitizer is one of main components in DSSCs along with metal-oxide based semiconductor, electrolyte and a cathode. Dye-metal oxide semiconductor interface plays a vital role in controlling the charge injection and charge recombination dynamics which eventually manifest in the device performance. While there are several sensitizers, with various architecture, have been explored and tested, there are few which absorbs in NIR region with high extinction coefficients. This talk will be focused on design, synthesis and use of squaraine based dyes in DSSC as NIR absorbing sensitizers. Several examples of high performing squaraine dyes and idea behind their design will be highlighted. Squaraine dyes in spite of being efficient absorber has not been able to perform satisfactorily as it tend to form aggregate on the surface of metal-oxide semiconductor (TiO_2). Aggregation causes the self-quenching of exciton generated upon absorption of light and reduces the current. Our recent efforts

to tackle the problem of aggregation in indolenine based squaraine dye will be discussed where we capitalized on the sp^3 carbon atom on the indolenine unit by placing an out-of-the plane branched alkyl chain on it. We have also synthesized the dyes by extending the conjugation of squaraine dye to further push the absorption towards NIR region along with the absorption in the visible region. The extension was done by attaching the -bridge like benzodithiophene (BDT) between squaraine unit and anchoring carboxylic acid group (RSQ dyes). In another approach we extended the conjugation by synthesizing a new donor by fusing fluorene moiety in indolenine unit. This donor provided two sp^3 carbon atoms and hence opportunity to insert two branched out-of-plane alkyl groups which control the aggregation of dyes on the surface (XSQ dyes). These modifications have improved the performance of the DSSC and with further tweaking better results can be expected.

References:

1. Yum, J. H.; Walter, P.; Huber, S.; Rentsch, D.; Geiger, T.; Nuesch, F.; De Angelis, F.; Grätzel, M.; Nazeeruddin, M. K. *J. Am. Chem. Soc.* **2007**, *129*, 10320.
2. Bisht, R.; M. K., M. F.; Singh, A. K.; Nithyanandhan, J. *J. Org. Chem.* **2017**, *82* (4), 1920–1930.
3. Alagumalai, A.; M. K., M. F.; Vellimalai, P.; Sil, M. C.; Nithyanandhan, J. *ACS Applied Materials & Interfaces*, **2016**, *8* (51), 35353–35367.

