Squaraine Based Organic Dyes for Dye-Sensitized Solar Cells

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ABSTRACT

In dye-sensitized solar cells (DSSCs), dye-TiO_2/electrolyte interface plays an important role in modulating the charge injection, charge recombination and dye regeneration processes. Aggregation of organic dyes on the TiO_2 surface leads to self-quenching of photo-excited states which hampers the charge injection process which in turn affects the device performace. On the other hand, it helps to broaden the absorption profile of light absorbing sensitizers due to the formation of either H or J type aggregates. Hence controlling the aggregation dyes on TiO_2 for enhancing the light harvesting efficiency and passivating the for surface reducing the charge recombination process is desired for achieving high J_{SC} and V_{OC} of the DSSC devices, respectively (**Figure 1a**). To test this hypothesis, a series of alkyl group wrapped squaraine dyes were designed and synthesized, and fabricated the DSSC devices with I^-/I_3^- electrolytes. Incident photon-to-current conversion efficiency profile showed the contribution of aggregated structures for the photocurrent generation. Furthermore, integrating the electronic effects by means of introducing electron donating and withdrawing groups, and π-conjugation within polymethine frame offers modulated HOMO energy levels of the dyes, a set of visible far-red and NIR active dyes, respectively. Visible light active squaraine dyes with more positive HOMO energy levels showed compatibility with copper electrolyte with the device V_{OC} of 1 V (**Figure 1b**). Results on the DSSC device performances of both visible and far-red active squaraine dyes will be discussed.

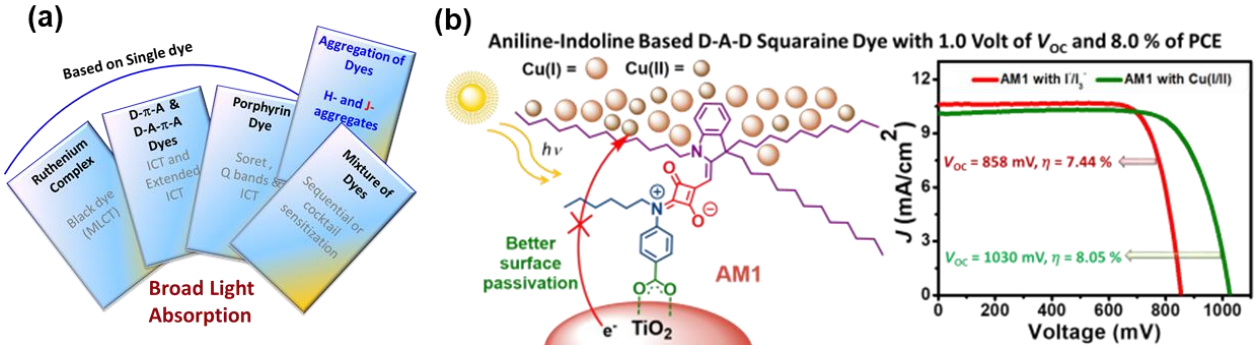

Figure 1. (a) Broadening the light harvesting efficiency of sensitizer by means of aggregation; (b) J-V profile of visible active dye **AM1** sensitized solar cell.

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Selected publications:

1. Ingole, K.B.; Deshmukh, S. S.; Verma, T. S.; Krishnamurty, S.; Krishnamoorthy, K.; Nithyanandhan, J. *ACS Appl. Energy Mater.* **2024**, *7*, 7982.
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