

Synthesis and Photophysical Characterizations of Novel NIR Dyes bearing Double Anchoring Groups for Enhanced PCE and Stability

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Keywords: Squaraine dyes, Anchoring group, Photovoltaic performance, Anchoring stability, Dye sensitized solar cell

Dye sensitized solar cell (DSSCs) have attracted significant attentions as one of the potential candidates amongst third-generation solar cells due to their relatively ease of fabrication and low fabrication cost, good Photo-conversion efficiency especially under low light conditions. State-of-art dye-sensitized solar cells (DSSCs) having photo conversion efficiencies (PCE) beyond 12 % in spite of photon harvesting window mainly in the visible wavelength region. Development of near infrared (NIR) dyes is, therefore, inevitable for the further improvement in the efficiency. Dye molecules are adsorbed onto the mesoporous TiO₂ surface chemically through an anchoring group. Anchoring group of the sensitizer is not only responsible for the improvement of the PCE but also impacts the stability of the solar cell. Previously published results have indicated that phosphonic acid anchoring group exhibits very high stability as compare to the most commonly used carboxylic acid. Owing to this, a series of unsymmetrical squaraine dyes (SQ) having same π -conjugated mother core but different dual anchoring groups were designed and subjected to QC calculations using Gaussian program. Two of the potential sensitizers viz. **SQ-161** and **SQ-162** having chemical structure as shown in the Fig. 1 were successfully synthesized, characterized and subjected to their Photophysical, and photovoltaic characterizations.

Both the sensitizers have a common main π -conjugated mother core and phosphonic acid anchoring group but differ in the 2nd anchoring group such as cyanoacrylic acid in SQ-161 and acrylic acid in the SQ-162. Both of the sensitizers are energetically suitable for DSSC as verified by theoretical QC calculation as well as by the experimentally constructed energy band diagram. Electronic absorption spectra of SQ-162 in the solid-state as well as in the ethanol solution has been shown in the Fig. 1 indicating structural rigidity due to lack of significant spectral difference and especially the extent of the lower vibronic shoulder appearing around 610 nm. Apart from their synthesis and characterization, these dyes were also subjected to their photophysical characterizations along with the investigation of their anchoring behavior and stability of dyes (binding strength) on to the mesoporous TiO₂ by rate of dye adsorption and dye desorption studies, respectively, which will be discussed in detail during my presentation.

Acknowledgement: SSP would like to thank Japan Society for Promotion of Science for the financial support by Grant-in-Aid for scientific research (C) [Grant No.-18K05300].

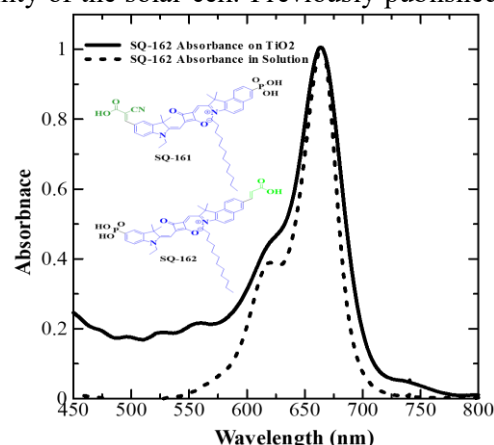


Figure 1. Chemical structure unsymmetrical squaraine dyes SQ-161 and SQ-162 bearing double anchoring groups and Electronic absorption spectra of SQ-162 in the solid-state (solid lines) and in solution (dotted line).