Synthesis and photophysical characterization of far-red sensitive squaraine dyes bearing different functional groups for anchoring on mesoporous TiO_2

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Introduction: Sensitizing dye molecules play a pivotal role in the functioning and controlling the photon harvesting behavior in dye-sensitized solar cells (DSSCs). Need of efficient photon harvesting beyond the visible wavelength region is inevitable in order to enhance the photoconversion efficiency (PCE) of DSSCs, which are currently in the range of 12-14 %. Squaraine family of dyes bear Donor-Acceptor-Donor zwitterionic structure are one of the potential candidates amongst organic sensitizers owing to their intense and sharp light absorption, which can easily tailored from visible to IR wavelength region depending on the judicious selection of suitable donor moieties. Potential sensitizers for DSSCs must possess a suitable functional group, which is necessary for their attachment at the surface of wide band gap semiconductor for the photosensitization. This work focuses on the synthesis and photophysical characterizations of far-red sensitive unsymmetrical squaraine dyes bearing different anchoring groups. Man aim of the work is to investigate influence of nature of anchoring groups on the photosensitization of mesoporous TiO_2, which is one of the most commonly used wide band gap semiconductor.

Experimental: Three different model squaraine dyes having same π-conjugated mother core but different functional groups with structure shown in the Fig. 1 have been successfully synthesized. These dyes were then subjected to structural and photophysical characterizations using electronic absorption and fluorescence emission spectroscopies, their adsorption behavior on TiO_2 and estimation of the energies HOMO and LUMO energies.

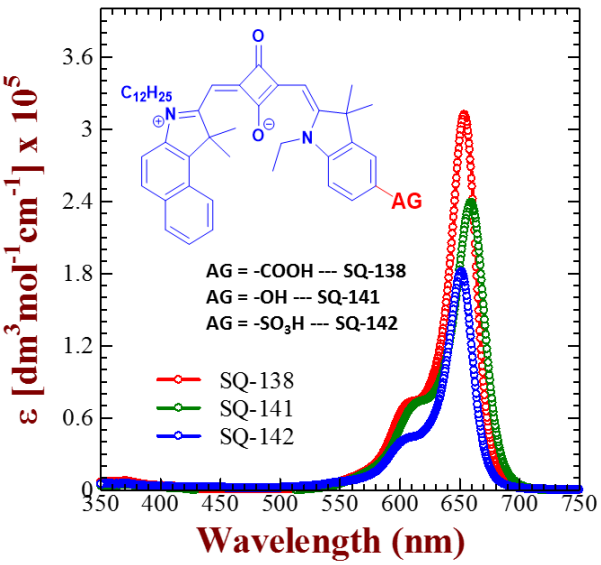

Figure 1. Chemical structure and electronic absorption spectra in ethanol solution for different squaraine dyes.

Results: Electronic absorption spectra of the dyes in ethanol solutions as shown in the Fig. 1 reveals that dyes exhibit sharp and intense light absorption mainly in the far-red (550 nm-700 nm) wavelength region with very high molar extinction coefficients. Rate of dye adsorption on the mesoporous TiO2 was found to be **SQ-138>SQ-142>>SQ-141**. Results pertaining to the nature of anchoring group upon various photophysical parameters like, absorption, emission, HOMO energy, LUMO energy, band gap and adsorption behavior on the mesoporous TiO_2 will be discussed in detail.