Electronic Supplementary Information

J-aggregation of a squaraine dye and its application in organic photovoltaic cells

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Fig. S1 UV-visible (UV-vis) absorption and photoluminescence (PL) spectra of SQ film spin-coated from chloroform solution. Peaks 1-4 were obtained from absorption spectrum de-convoluted via multi-peak fitting.
**Fig. S2** UV-visible (UV-vis) absorption and photoluminescence (PL) spectra of SQ solution ($1 \times 10^{-5}$ M) in dichloromethane (DCM), chloroform (CF), chlorobenzene (CB) and o-dichlorobenzene (ODCB), respectively.
Fig. S3 Cyclic voltammetry (CV) curve of SQ. The electrochemical potential was internally calibrated against the standard ferrocene/ferrocenium redox couple (Fc/Fc⁺). From the values of oxidation potential onset (E_{ox}) and reduction potential onset (E_{red}) referenced to the internal standard Fc/Fc⁺, the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) were calculated according to the equations HOMO = −(E_{ox} + 4.76) (eV) and LUMO = −(E_{red} + 4.76) (eV), where E_{ox} and E_{red} are oxidation potential onset and reduction potential onset versus Fe/Fe⁺, respectively.
**Fig. S4** Ball-and-stick structure of SQ molecule in a single crystal, atoms of C, O, N and H are shown in grey, red, blue and olive, respectively.
Fig. S5 In-plane (left) and out-of-plane (right) X-ray diffraction (XRD) patterns of SQ films spin-coated from chloroform (CF) and o-dichlorobenzene (ODCB) solution.
Fig. S6 Atom force microscopy (AFM) images (3-dimensional) of SQ films spin coated from different solvents: dichloromethane (DCM), chloroform (CF), chlorobenzene (CB) and o-dichlorobenzene (ODCB), respectively.