Electronic Supplementary Information (ESI)

Oxidation-enhanced emission: exploring novel AIEgens from thieno[3,2-b]thiophene S,S-dioxide

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General Information

All other chemicals and reagents were purchased from commercial sources and used as received without further purification. ^{1}H and ^{13}C NMR spectra were measured on a Bruker AV 500 spectrometer in appropriated deuterated solution at room temperature. High resolution mass spectra (HRMS) were recorded on a GCT premier CAB048 mass spectrometer operating in MALDI-TOF mode. Single crystal X-ray diffraction intensity data were collected at 173 K on a Bruker–Nonices Smart Apex CCD diffractometer with graphite monochromated MoKα radiation. Processing of the intensity data was carried out using the SAINT and SADABS routines, and the structure and refinement were conducted using the SHELTL suite of X-ray programs (version 6.10). UV-vis absorption spectra were measured on a Shimadzu UV-2600 spectrophotometer. Photoluminescence spectra were recorded on a Horiba Fluoromax-4 spectrofluorometer. Solution fluorescence quantum yields were measured using a Hamamatsu absolute PL quantum yield spectrometer C11347

Quantaurus_QY. Fluorescence lifetimes were determined with a Hamamatsu C11367-11 Quantaurus-Tau time-resolved spectrometer. The frontier orbitals of the molecules based on the ground state geometries are calculated at B3LYP/6-31G (d, p) by Gaussian 09 program. The cyclic voltammetry measurement was conducted on a CHI610E A14297 in dichloromethane with 0.1 M tetrabutylammonium hexafluorophosphate as the supporting electrolyte at a scan rate of 100 mV s^{-1}, using platinum as the working electrode, saturated calomel electrode (SCE) as the reference electrode, and platinum wire counter electrode. The SCE reference electrode was calibrated using the ferrocene/ferrocenium (Fc/Fc^{+}) redox couple as an external standard.

Additional Data

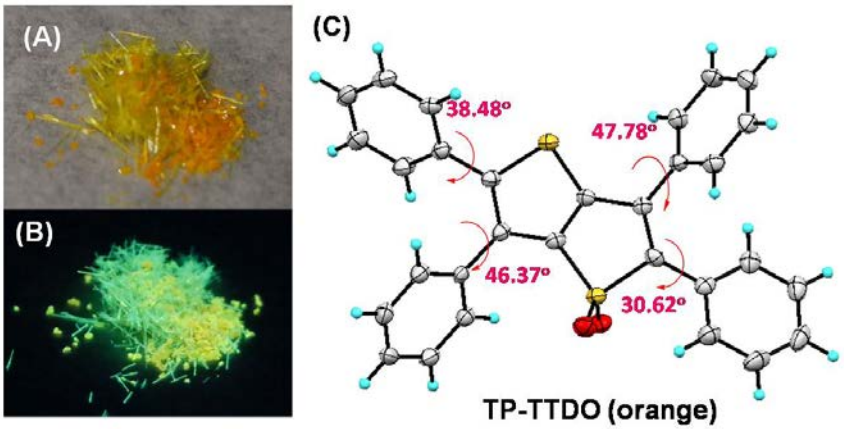

Fig. S1 Photos of green needle crystals and orange block crystals of TP-TTDO, taken under (A) daylight and (B) UV excitation. (C) ORTEP drawing of the crystal structure of TP-TTDO in orange block crystals.

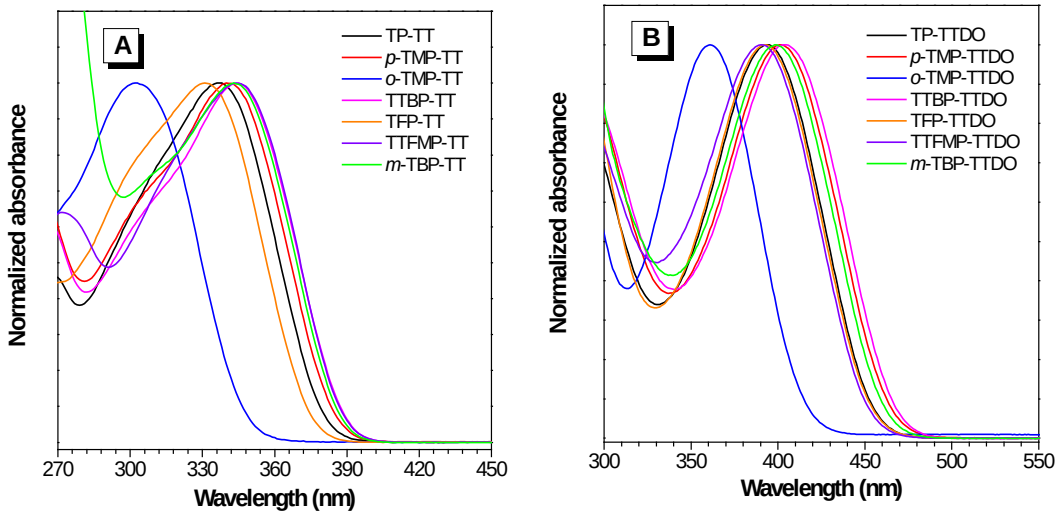

Fig. S2 Absorption spectra of luminogens based on (A) thieno[3,2-b]thiophene and (B) thieno[3,2-b]thiophene S,S-dioxide in THF solutions (10 μM).

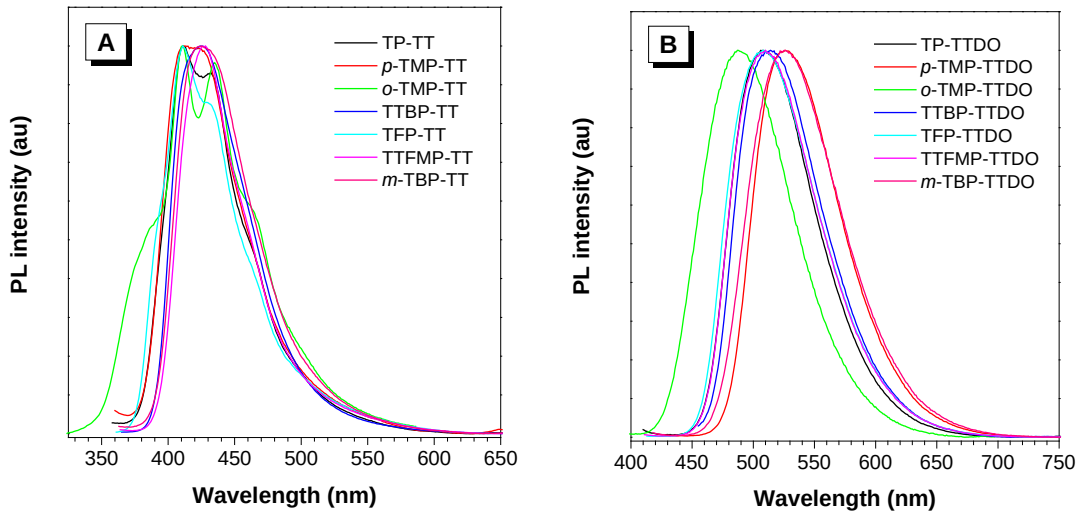

Fig. S3 Photoluminescence (PL) spectra of the solid films of luminogens based on (A) thieno[3,2-b]thiophene and (B) thieno[3,2-b]thiophene S,S-dioxide.

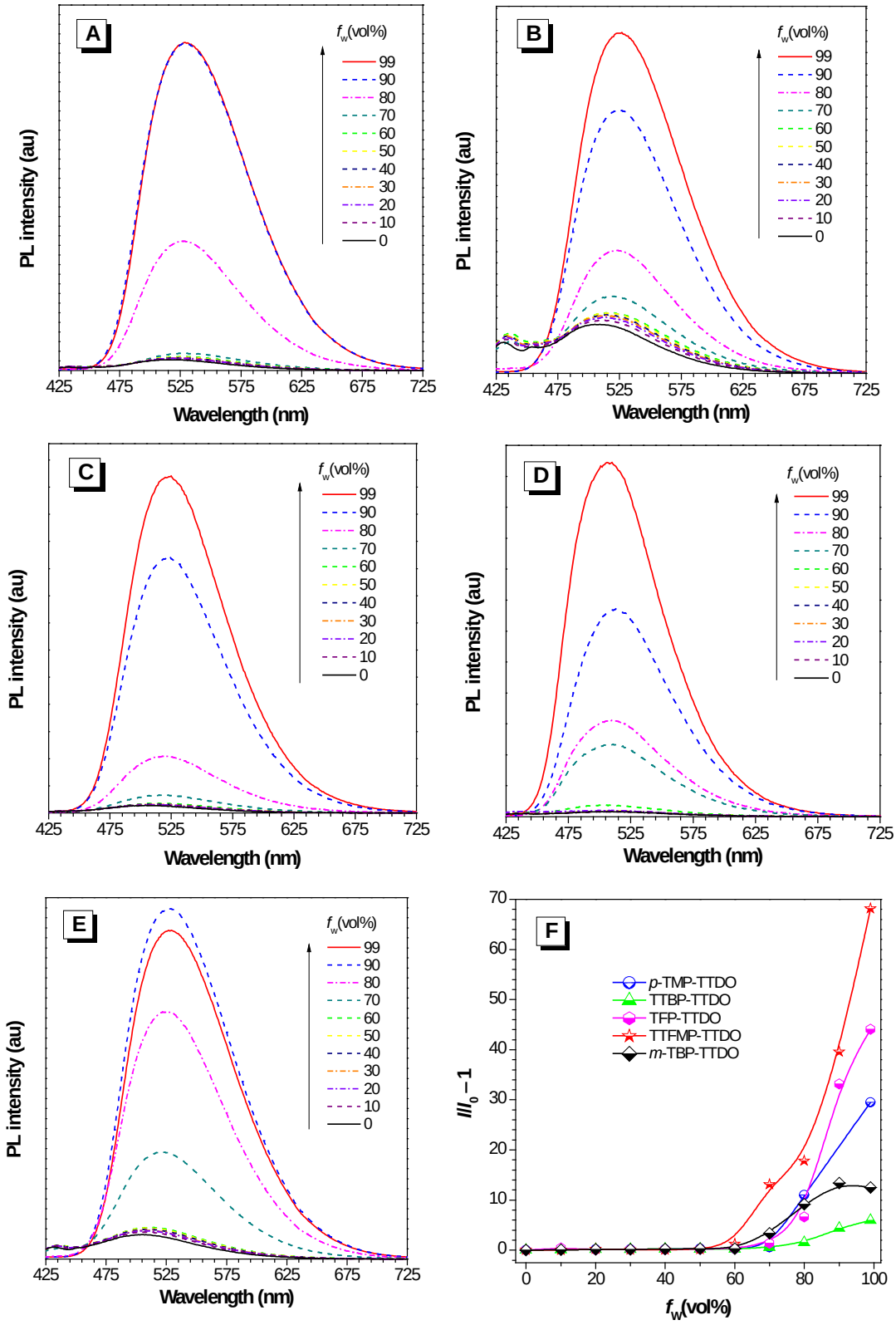

Fig. S4 PL spectra of (A) *p*-TMP-TTDO, (B) TTBP-TTDO, (C) TFP-TTDO, (D) TFMP-TTDO and (E) *m*-TBP-TTDO in THF/water mixtures with different water fractions (f_w). (F) Plots of $I/I_0 - 1$ versus the f_w; I_0 is the PL intensity in pure THF.

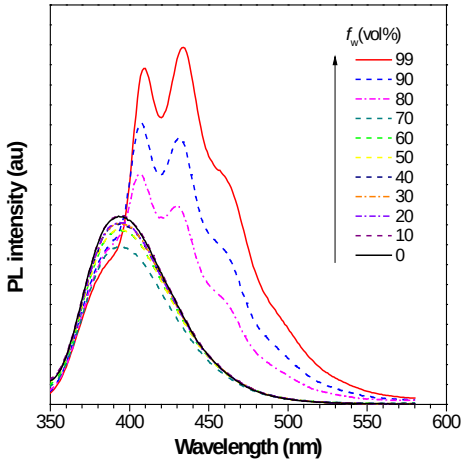

Fig. S5 PL spectra of *o*-TMP-TT in THF/water mixtures with different water fractions (f_w).

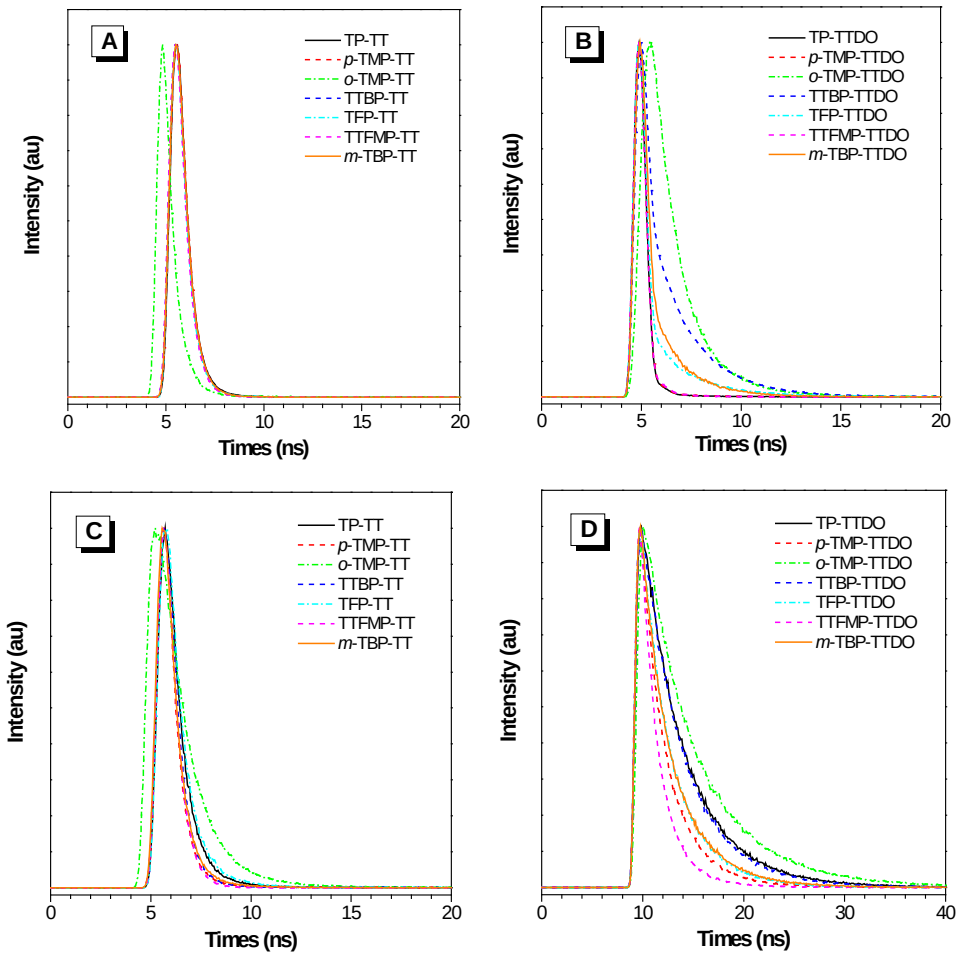

Fig. S6 Time-resolved fluorescence decay curves: (A) and (C) thieno[3,2-b]thiophene-based luminogens in THF solutions and solid films, respectively. (B) and (D) thieno[3,2-b]thiophene S,S-dioxide-based luminogens in THF solutions and solid films, respectively.