Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

New functionalized thioxanthone derivatives as Type I photoinitiators for polymerization under UV-Vis LEDs

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Figures and Tables

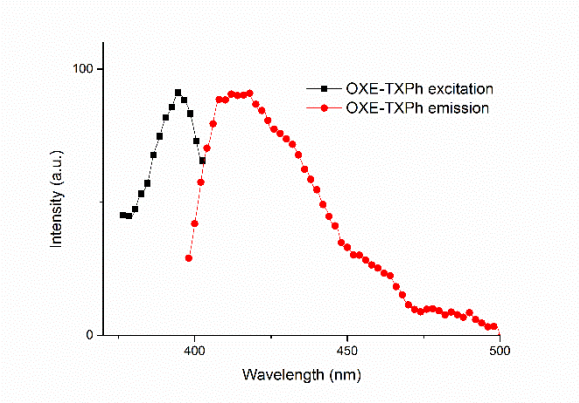

Fig. s1 Fluorescence excitation and emission spectra of OXE-TXPh in acetonitrile (10^{-5} M) at room tempreture, and 385 nm and 407 nm are the maximum fluorescence excitation and emission

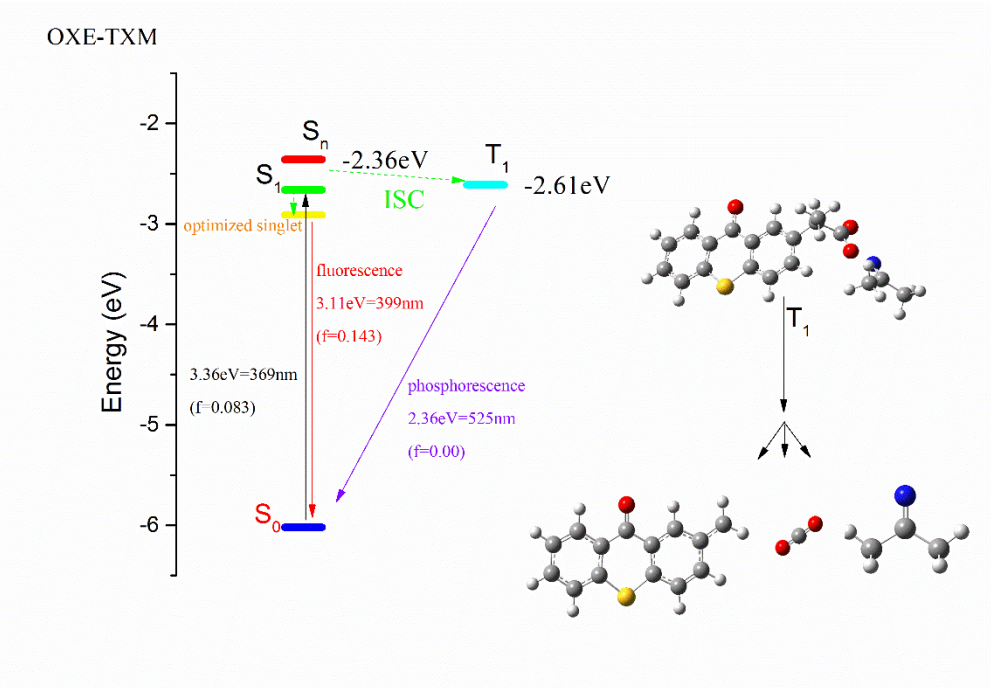

Fig. s2 Jabłoński-type diagram of possible processes from the excited states of OXE-TXM after TD-DFT calculation based on the B3LYP/6-311G(d) level implemented Gaussian 09 to optimize the ground state and the excited states.

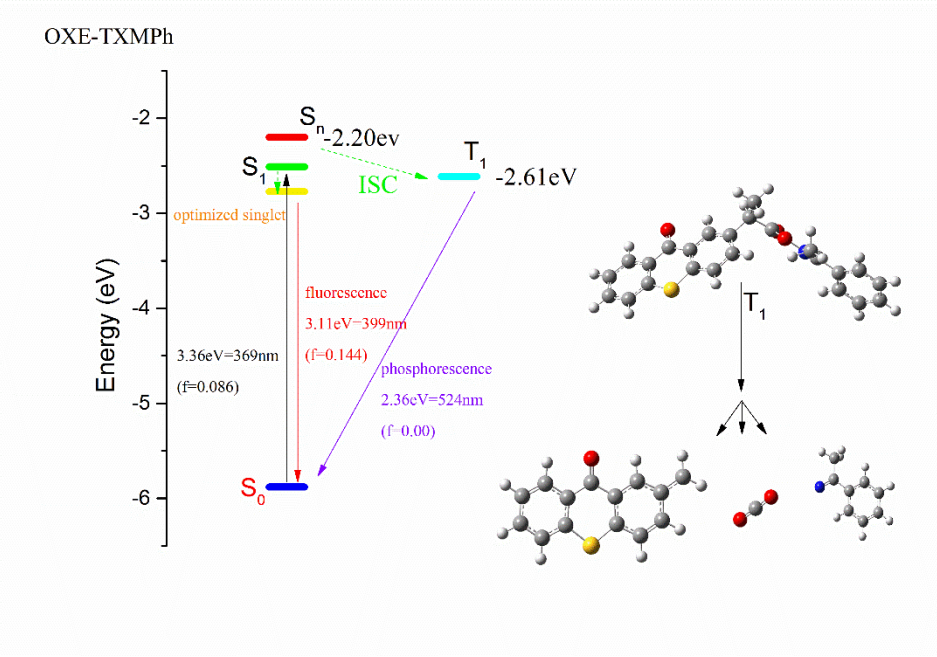

Fig. s3 Jabłoński-type diagram of possible processes from the excited states of OXE-TXMPh after TD-DFT calculation based on the B3LYP/6-311G(d) level implemented Gaussian 09 to optimize the ground state and the excited states.

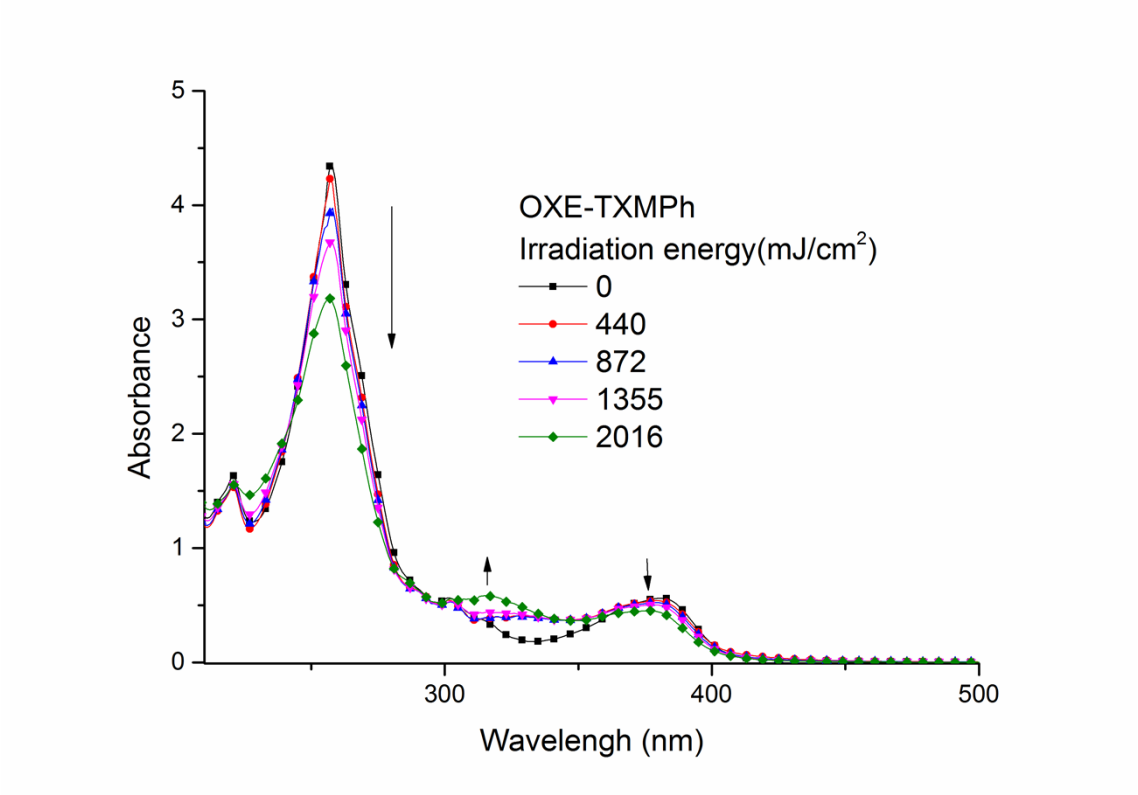

Fig. s4 UV-vis spectra changes of OXE-TXMPh solution (10^{-4} M) irradiated with an 365 nm LED at different light doses.

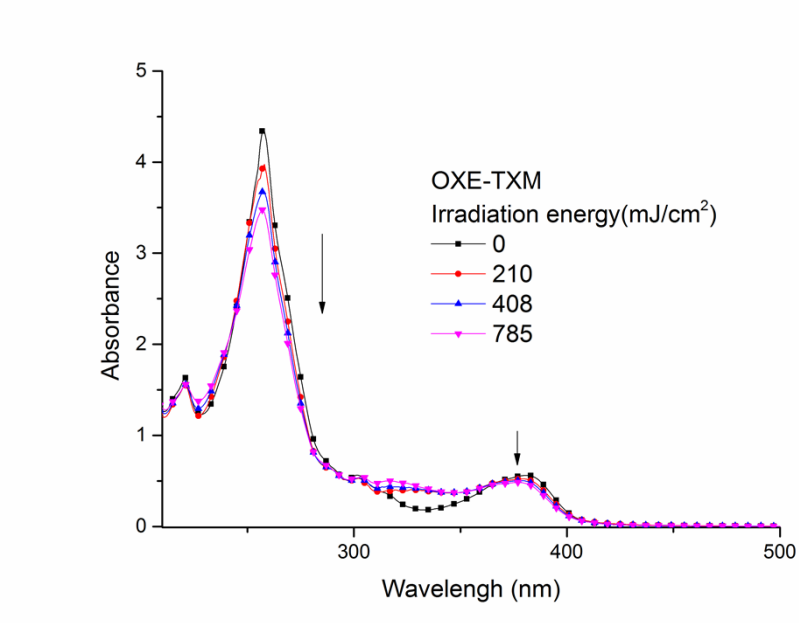

Fig. s5 UV-vis spectra changes of OXE-TXM solution (10^{-4} M) irradiated with an 365 nm LED at different light doses.irradiate 365 nm light

Table s1 Energies of excited triplet state relative to the singlet ground state of oxime esters and bond dissociation energy (N-O), as computed by TD-DFT/B3LYP/6-311G(d) method in acetonitrile.

	E_{rel} of S_1 (eV)	E_{rel} of T_1 (eV)	*BDE* (kJ mol^{-1})
OXE-TXM	3.12	2.61	85
OXE-TXPh	3.36	3.78	63
OXE-TXMPh	3.36	2.61	64