

# Large-Stokes-shifted Dual Photoluminescence of Thianthrene-containing Imide Compounds and Polyimides Undergoing Transient Conformational Changes

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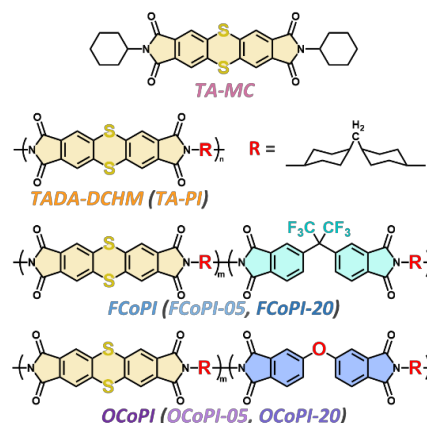
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**Topic:** Photoluminescence, Dual-emission, Polyimide, Thianthrene, Conformation change,

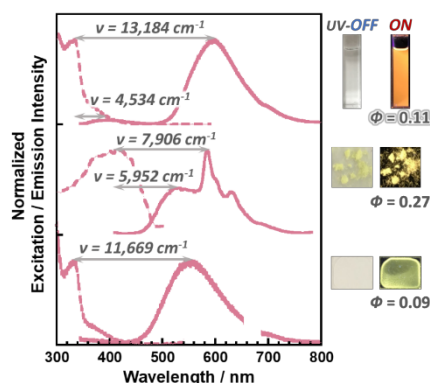
**Abstract:** Highly luminescent polyimides (HL-PI)[1] are expected to be applied to solar wavelength converters (SWC) which should have high optical transparency in the visible region and intense photoluminescence (PL) at longer wavelengths with a large Stokes shift (SS).[2] Phosphorescence (PH) induced via intersystem crossing (ISC) between the excited singlet ( $S_1$ ) and triplet states ( $T_1$ ) leads PL at longer wavelengths than fluorescence (FL). Thianthrene (TA), consisting of a ring structure with two sulfur atoms, may have a large spin-orbit coupling (SOC) not only by the heavy-atom effect of sulfurs but also by the transient conformational changes in the excited state.[3] In this study, we synthesized a dianhydride having a thianthrene moiety in the core (TADA) and prepared a model compound (TA-MC), homo-PI (TA-PI), and coPIs (FCoPI, OCoPI) (Fig. 1) and investigated their dual PL properties. Under UV-irradiation in solution, V-shaped TA in the ground state ( $S_0$ ) undergoes a transient conformational change to a planar conformation in the  $S_1$  state, exhibiting bright orange FL with a very large SS of  $13184\text{ cm}^{-1}$  (Fig. 2), while the  $T_1$  state generated via ISC exhibits PH in the same wavelength range. In contrast, in solids, the conformational change is restricted and ISC is enhanced, intense yellowish PH emission was observed for TA-MC in crystalline powder and dispersed in PMMA. The dual FL and PH emissions of TA-containing imides and PIs would be useful to make a way to design guidelines for novel HL-PIs applicable to the SWCs with efficient and large-SS PLs.

## References:

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- [3] H. Liu, Y. Gao, J. Cao, T. Li, Y. Wen, Y. Ge, L. Zhang, G. Pan, T.



**Fig. 1** Chemical structures of TA-MC, TA-PI, FCoPI, and OCoPI.



**Fig. 2** Excitation/emission spectra and photos of TA-MC in  $\text{CHCl}_3$ , crystalline state, and dispersed in PMMA.