

# TADF EMISSION WAVELENGTH INSTABILITY DUE TO CONFORMATIONAL DISORDER

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Organic light emitting diodes attracts a lot of interest due to vibrant colors, flexible, cheap and lightweight applications. However due to spin statistics 75% of electrically injected charge ends up in non-emissive “dark” triplet states. Thermally activated delayed fluorescence (TADF) is the most promising pathway for triplet harvesting since TADF compounds are cheaper and much more stable than rare-earth metals based phosphorescent emitters.

TADF molecules are usually constructed from donor (D) and acceptor (A) moieties twisted by large dihedral angles to reduce spatial overlap of HOMO–LUMO electron orbitals and minimize  $\Delta E_{ST}$ , which is important to utilize non-emissive triplet states [1]. However, large steric hindrance between D and A units reduces the vibronic coupling between localized (<sup>3</sup>LE) and charge transfer (<sup>3</sup>CT) triplet states, which is mandatory for efficient rISC, therefore some lability of molecular core is required [2]. In dilute solutions, minor dispersion of D–A twist angles may be observed, having negligible effect on excited state relaxation. In solid films molecules are frozen in large variation of geometrical conformations with different <sup>1</sup>CT energies and  $\Delta E_{ST}$  gaps, causing temporal shifts of prompt and delayed fluorescence and resulting in multiexponential emission decay with prolonged lifetime [3, 4]. The impact of conformational disorder to TADF properties in solid films, its relation to rISC rate and methods to reduce it, despite its importance, still are scarcely studied.

In this work we investigate the conformational disorder in solid films of phenothiazine-pyrimidine TADF compounds (Fig. 1) and its relation to emission properties. Compounds were designed to have different lability of molecular core and different reverse intersystem crossing (rISC) rate. Phenothiazine electron-donor unit was selected for its ability to form several conformations, increasing the number of possible molecular core arrangements in solid state. We have shown, that variations of molecular core rigidity had only minor impact on conformational disorder and emission properties, while the rISC rate was found to have the crucial importance to TADF properties. The long rISC resulted in emission wavelength redshift.

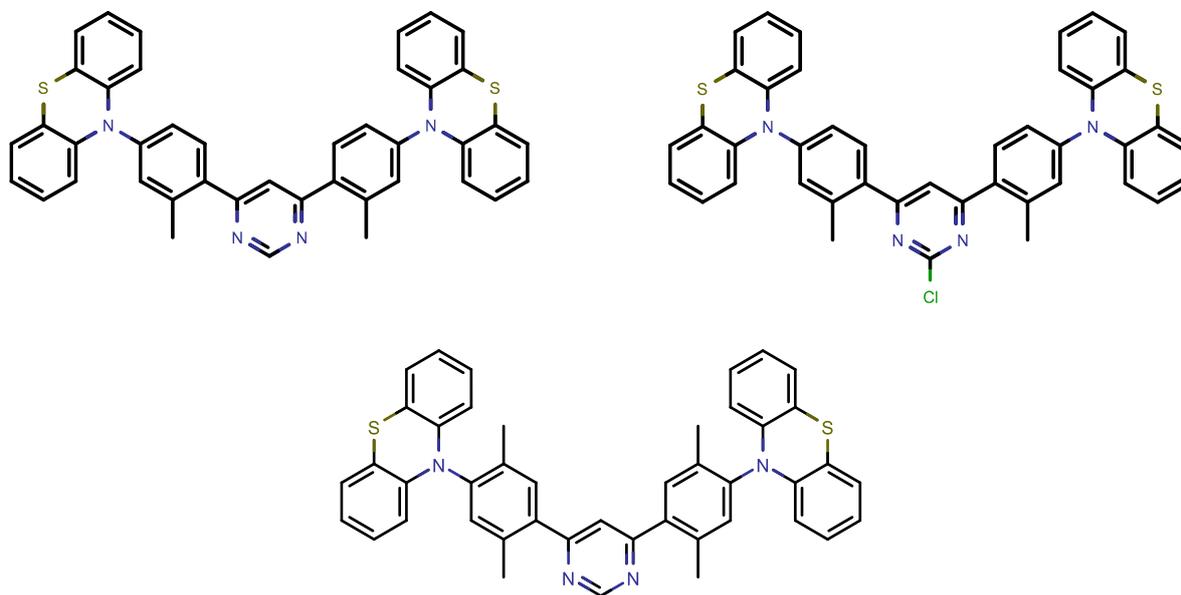


Fig. 1. Phenothiazine-pyrimidine TADF compounds analyzed in this work

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[4] T. Serevičius et al., Room temperature phosphorescence vs. thermally activated delayed fluorescence in carbazole–pyrimidine cored compounds, *Journal of Materials Chemistry C*, 2018, **6**, 11128–11136