

Understanding Organic Cocrystals for Room Temperature Phosphorescence

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ABSTRACT

Organic co-crystals offer a versatile platform for designing efficient room temperature phosphorescence (RTP) materials. Despite the growing number of reported organic co-crystals with RTP, there is a lack of understanding regarding how to exploit specific intermolecular interactions to achieve and enhance phosphorescence. Different strategies such as crystallisation, H-aggregation, and the heavy atom effect allow obtaining organic RTP with significant excited state lifetimes.¹ Recently, Abe *et al.*² used the heavy atom effect and rigid environment strategies to modulate the RTP in co-crystals of DITFB with Chry, Pyr, and Phen (Figure 1). To understand how specific intermolecular interactions and crystal packing affect the excited state mechanisms, we investigated the nature of the electronic transitions and the effects of the spin-orbit couplings in these co-crystals. Our calculations provide information about how to control photophysical properties in these systems through specific intermolecular interactions, which have an impact on the rational design of organic materials with a broad range of applications.

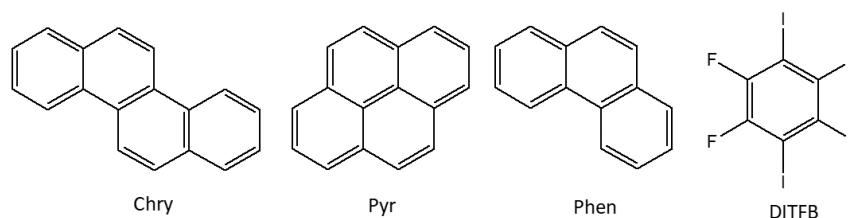


Figure 1: Components of the co-crystals with RTP under study

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- [1] Singh, M.; Liu, K.; Qu, S.; Ma, H.; Shi, H.; An, Z.; Huang, W. Recent Advances of Cocrystals with Room Temperature Phosphorescence. *Adv. Optical Mater.* **2021**, *9*, 2002197.
- [2] Abe, A.; Goushi, K.; Mamada, M.; Adachi, C. Organic Binary and Ternary Cocrystal Engineering Based on Halogen Bonding Aimed at Room-Temperature Phosphorescence. *Adv. Mater.* **2023**, 2211160.