

Dynamic molecular crystals for organic optoelectronics

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Dynamic molecular crystals represent a compelling class of smart materials poised to revolutionize organic optoelectronics. These crystalline organic solids challenge the traditional notion of crystals as rigid and static by demonstrating capabilities such as *bending*, *twisting*, *shape memory*, and *self-healing*.¹⁻³ Integrating dynamic materials with rich *optical* and *charge transport* functionalities will be ideal candidates for flexible, responsive, durable, and sustainable optoelectronic device architectures, *viz.*, organic field effect transistors (OFETs), organic light emitting diodes (OLEDs), and smart sensors. By leveraging *non-covalent interactions* (e.g., π - π stacking, van der Waals forces, hydrogen bonding) and *quantum mechanical principles*, we engineer crystal architectures capable of harvesting triplet excitons through *phosphorescence* and *thermally activated delayed fluorescence* (TADF) (Figure 1).⁴⁻⁶ Our work explores the rational design of organic molecular crystals that exhibit dynamic mechanical responses while maintaining high photoluminescence quantum yield (PLQY) and tuneable emission characteristics. Moreover, dynamic materials with high charge carrier mobility⁷ are particularly promising for applications in OFETs, photodetectors, and flexible electronics. We also examine *polymorphic* and *co-crystalline* systems where dynamic phase transitions induce mechanical reconfiguration.⁸⁻¹¹ Highlighting recent advances in *crystal adaptronics*,¹⁻³ we demonstrate how these soft, yet robust, molecular solids enable next-generation applications, including optical waveguides and stimuli-responsive actuators. This poster will emphasise the synergy between crystal engineering and photophysical/charge transport behaviours, offering a strategy for integrating organic crystalline materials into real-world optoelectronic devices.

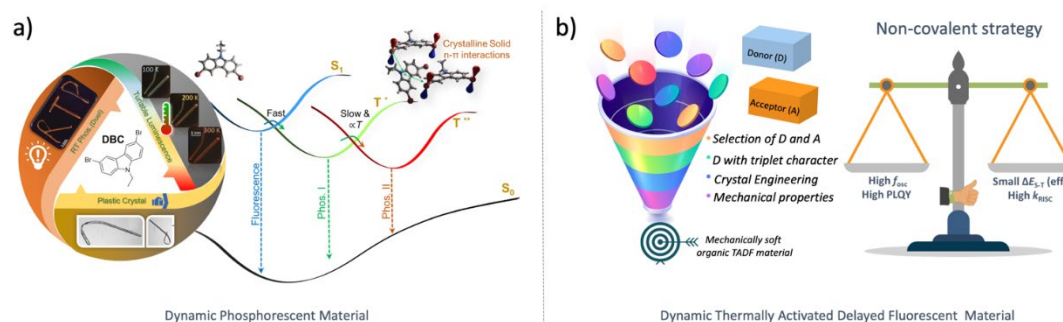


Figure 1. Schematic summary of the findings: **a)** graphical representation of the dynamic phosphorescent material, **b)** simplified diagram representing our non-covalent donor-acceptor design strategy for dynamic TADF material.

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