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Key features for efficient long-lived room temperature persistent luminescence of organic molecular crystals

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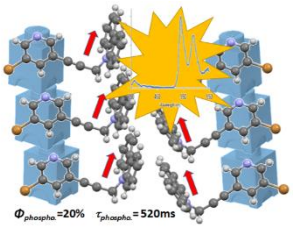
Abstract:

Room-temperature long-lived persistent luminescence from metal-free organic materials has recently attracted renewed attention from fundamental and application point of view.[1-3] This afterglow luminescence has gained increasing interest as a viable alternative to well-studied inorganic phosphorescence based on toxic, rare, and expensive elements. However, the realization of organic systems, mostly molecular crystals, with long-lived emission remains a formidable challenge, since the features of the persistent luminescence strongly depend on the electronic properties of the molecular components and on their molecular packing in the crystal.

Here, a new strategy is developed by rationally designing molecular 'phosphors' incorporating and combining for the first time a bridge for σ-conjugation between the D and A units and a structure-directing unit for H-bond-directed supramolecular self-assembly.[4] Quantum chemical calculations highlight the critical role played by the two degrees of freedom of the σ-conjugated bridge, on the chromophore optical properties. The molecular crystals exhibit room-temperature 'phosphorescence' quantum yields up to 20% and lifetimes up to 520 ms. On the other hand, the crystal structures establish the existence of an unprecedented well-organization of the emitters into two-dimensional (2D) rectangular 'columnar-like' supramolecular structure stabilized by intermolecular H-bonding. We also elucidate the underlying spin-and photo-physics of ultralong-lived light emission by demonstrating that the 'doping' by an isomer plays a crucial role.[5]



'Columnar-like' supramolecular structure stabilized by intermolecular H-bonding as structural key parameter.[4]

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