Deformation-induced phosphorescence shift in a 2D elastically flexible organic single crystal: Role of chalcogen-centered weak interactions

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Molecular single crystals that can be mechanically reconfigured without losing the long-range intrinsic order are part of the core research in materials science and crystal engineering [1-2]. In particular, flexible as well as luminescent organic crystals are one of the promising choices of materials for smart photonic devices [3-4]. However, the adjustment in phosphorescence peak as a function of the flexibility of a crystal has never been reported.

We demonstrate two-dimensional (2D) and one-dimensional (1D) macroscopic elastic deformability, under mechanical stress, in elastically flexible single crystals of dibenzothiophene, and its brominated derivative, respectively [5]. Unlike the presence of dual fluorescence (FL) and room temperature phosphorescence (RTP) in dibenzothiophene single crystals, the derivative was found to show only RTP. Interestingly, upon elastic deformation, single crystals of the dual emissive dibenzothiophene show a noticeable blue shift (~20 nm) of RTP emission (Fig. 1) when compared to their pristine crystals (straight and naturally bent). However, their FL peaks remain nearly unchanged irrespective of the crystal deformation. A hierarchy of structure-elastic functionality to RTP modulation has been quantitatively mapped by rationalizing the role of chalcogen-involved weak interactions.

Figure 1. RTP emission spectra, showing a hypsochromic shift of the RTP emission peak (563 nm to 543 nm) for an elastically bent single crystal (blue spectrum) of dibenzothiophene and corresponding CIE color coordinates for the RTP emission of dibenzothiophene crystals. Single crystals were excited at λex = 300 nm, using a xenon lamp for emission measurements.

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