

INVESTIGATIONS OF PHOTOPHYSICAL PROPERTIES OF DERIVATIVES OF PHENOTHIAZINE AND DIFFERENTLY MODIFIED 3,5-DICYANOPYRIDINE FOR DOWN-CONVERTING WHITE LIGHT-EMITTING DIODES

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Single-molecular white organic emitters are highly desirable for down-converting white light-emitting diodes (WLEDs) [1]. However, most reported organic compounds generally emit one colour, and the few examples of single-molecular white emitters exhibit low photoluminescence quantum yields (PLQYs), subpar colour quality, or complex molecular structures that hinder their practical applications [2]. For instance, we previously reported a single molecule white light emitter showing CIE 1931 coordinates of (0.26, 0.31) and PLQY of 33% [3]. Considering the low quality of the white light from existing emitters, there remains a need to develop novel single-molecular white emitters with high PLQYs, stable colour coordinates, and colour rendering index (CRI) values, as well as simple structures that can be easily incorporated into solid films. In this work, we investigated the photophysical properties of three newly developed derivatives of phenothiazine and 3,5-dicyanopyridine aiming to obtain single-molecular white emitters for WLEDs. Powders of phenothiazine and 3,5-dicyanopyridine derivatives were investigated before and after they underwent different external stimuli, including grinding, solvent-fuming, heating and melting. The target compounds exhibit attractive mechanochromic properties, facilitating the tuning of emissions from deep blue to red. Their mechanochromic properties were elucidated by various conformational states that enable single-molecule white emissions with PLQYs of 9.63%. Derivatives of phenothiazine and 3,5-dicyanopyridine were used as emitters in down-converting WLEDs. In the best case, fabricated WLEDs were characterised by power efficiency of 6.1 lm/W and white emission with CRI of 78 and CIE 1931 coordinates (0.34, 0.32).

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[1] M. Zhang et al., Efficient single-molecular white-light emission for iridium-based photoluminescent and electroluminescent white OLEDs, (*Cell Rep Phys Sci*, vol. 4, no. 12, p. 101684, Dec. 2023).

[2] Z. He et al., White light emission from a single organic molecule with dual phosphorescence at room temperature (*Nature Communications*, vol. 8, no. 1, pp. 1–8, Sep. 2017).

[3] F. Khan, L. Volyniuk, M. Ghasemi, D. Volyniuk, J. V. Grazulevicius, and R. Misra, "Efficient monomolecular white emission of phenothiazine boronic ester derivatives with room temperature phosphorescence" (*J Mater Chem C Mater*, vol. 10, no. 28, pp. 10347–10355, Jun. 2022).