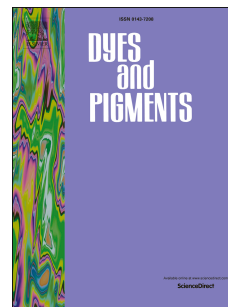


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# Optical anti-counterfeiting of a single molecule by two solvents based on intra- and intermolecular excited state proton transfer mechanisms

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## Abstract

Organic dye molecules with excited state proton transfer property gain huge scientific interest owing to the design flexibility and functional diversity. However, the anti-counterfeiting of a single dye molecule through intra- and intermolecular excited state proton transfer (ESIPT and ESPT) has yet to be achieved. This study demonstrates a simple and efficient approach to realize the anti-counterfeiting of a single dye molecule in a PMMA film. We control the 1-hydroxypyrene-2-carbaldehyde (HP) to be fluorescent or not through two different solvents based on ESIPT and ESPT mechanisms. Furthermore, we investigate the detailed information of excited-state dynamics for HP in two solvents, aiming at exploring the mechanisms of totally different luminescence property, through the femtosecond transient absorption spectroscopy. Meanwhile, the theoretical TDDFT research sheds light on the correlation between molecular structure and luminescence character. Specifically, the fluorescence of the molecule in acetonitrile is quenched by an ESIPT (127 fs) induced intersystem crossing (11.8 ps) whereas the ESPT (195 fs) and following aldehyde group rotation (26.5 ps) make the molecule to exhibit a strong luminescence property in dimethyl sulfoxide. The results are promising and offer new avenues to realize the greener and sustainable anti-counterfeiting of a single dye molecule.

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