Reversible photo/thermoswitchable dual-color fluorescence through single-crystal-to-single-crystal transformation

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Experiments.

Materials and Physical Measurements. All the reagents used in this work are purchased from Alfa without any purification. X-ray powder diffraction were collected by a Bruker AXSD8 Discover powder diffractometer at 40 kV, 40 mA for Cu Kα, (λ = 1.5406Å). The simulated powder patterns were calculated by Mercury 1.4. The purity of the bulk products were determined by comparison of the simulated and experimental PXRD patterns. The fluorescence property were measured by fluorospectro photometer F7000, absolute PL quantum yield spectrometer C11347 and compact fluorescence lifetime spectrometer C11367.

Synthesis of 1. A 5mL DMF and 1ml H_2O mixture solution of $ZnNO_3 \cdot 6H_2O$ (2 mmol), 1,4-bis[2-(pyridin-4-yl)ethenyl]benzene (2 mmol) and 2-aminoterephthalic acid (2 mmol) was sealed in a Teflon reactor, and heated at 115˚C for 3 days, and then cooled to room temperature at 3˚C/h. Subsequently, red block crystals were obtained in 90% yield based on Zn. Elemental analysis is found to be C/52.69, H/3.26, N/6.10. where the corresponding expected value is calculated to be C/52.73, H/3.24, N/6.15.

Synthesis of 2. The crystal of **1** is explored by UV (365 nm) irradiation for 4 h, then we obtained polymer **2.**

X-ray Crystallography. X-ray diffraction data of **1** and **2** were collected respectively at room temperature on a Bruker-AXS SMART Breeze CCD diffractometer using graphite monochromated MoKα radiation (λ=0.71073 Å). The data reduction included a correction for Lorentz and polarization effects, with an applied multi-scan absorption correction (SADABS). The crystal structure was solved and refined using the SHELXTL program suite. Direct methods yielded all non-hydrogen atoms, which were refined with anisotropic thermal parameters. All hydrogen atom positions were calculated geometrically and were riding on their respective atoms. CCDC 1515067-1515068 contains the supplementary crystallographic data of **1** and **2**. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

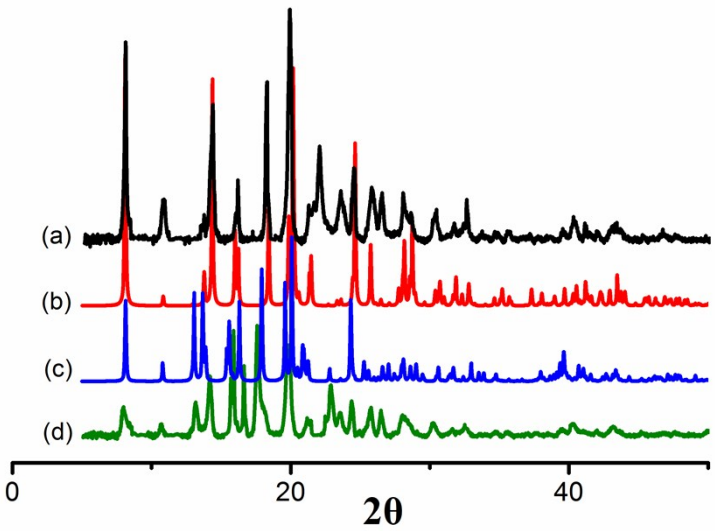
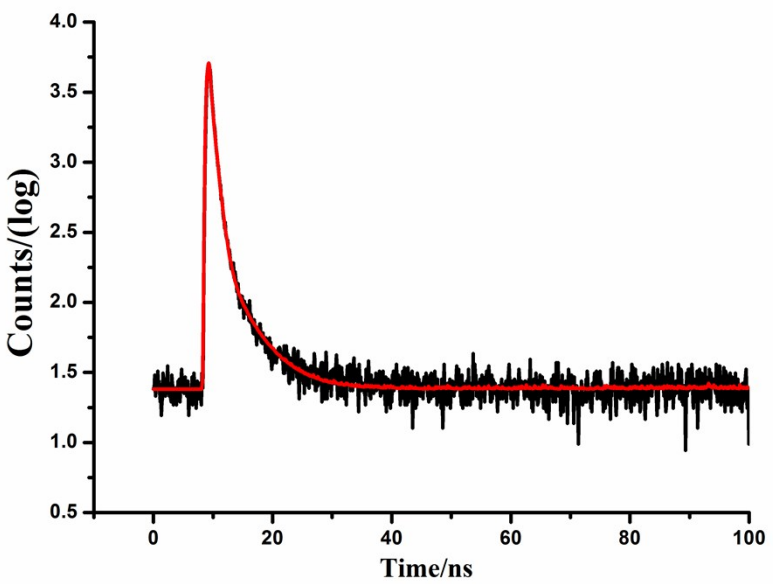


Fig. S1 The experimental XRD pattern(a) and the simulated XRD pattern from single crystal data(b) for crystal **1**, as well as simulated (c) and experimental (d) PXRD patterns for crystal **2.**

a)



b)

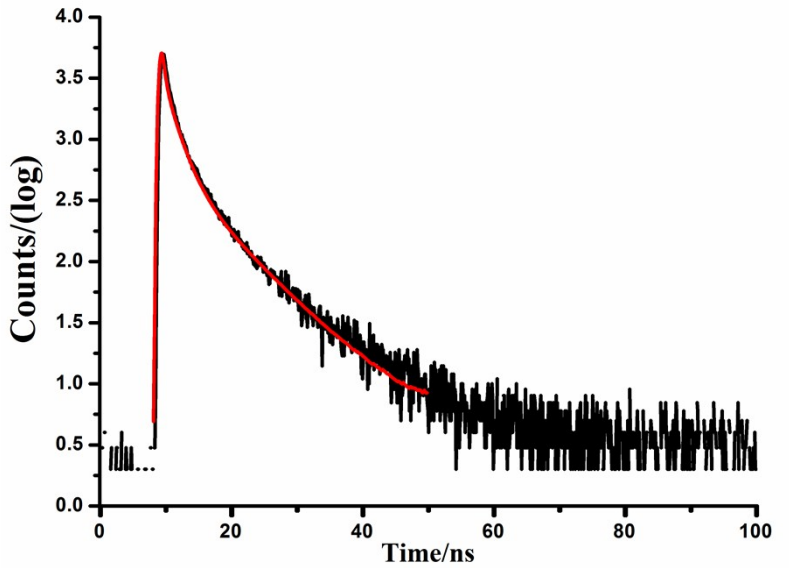


Fig. S2 Fluorescence lifetime decay spectra (black line) with fitting (red line) of **1**(a) and **2**(b).