

# Photochromism of Metal–Organic Frameworks Based on Carbazole-dicarboxylic Acid and Bipyridine: Sensing Adjustment by Controlling Strut-to-strut Energy Transfer

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Table S1. Crystallographic data and structure refinement details of **1** and **2**.

MOF	<b>1</b>	<b>2</b>
formula	C <sub>31</sub> H <sub>26</sub> N <sub>4</sub> O <sub>5.5</sub> Zn	C <sub>33</sub> H <sub>27</sub> N <sub>4</sub> O <sub>7</sub> Zn
Formula weight	607.93	657.00
Temperature/K	293.15	293.15
Radiation	MoK $\alpha$ ( $\lambda$ = 0.71073)	MoK $\alpha$ ( $\lambda$ = 0.71073)
Crystal system	triclinic	triclinic
Space group	P-1	P-1
a/Å	10.4072(8)	10.6378(6)
b/Å	11.4334(8)	12.1483(6)
c/Å	12.9954(9)	13.0565(6)
$\alpha$ /°	99.827(3)	71.249(2)
$\beta$ /°	98.033(3)	83.003(2)
$\gamma$ /°	113.779(2)	73.420(2)
Volume/Å <sup>3</sup>	1356.47(17)	1530.48(14)
Z	2	2
$\rho_{\text{calc}}$ (g/cm <sup>3</sup> )	1.488	1.4255
Reflections collected	21149	16214
Independent reflections	6235	6969
F(000)	628.0	678.9

GOF	1.030	1.047
$R_1( >2\sigma(I) )^a$	0.0471	0.0416
$wR_2( >2\sigma(I) )^b$	0.1299	0.1041

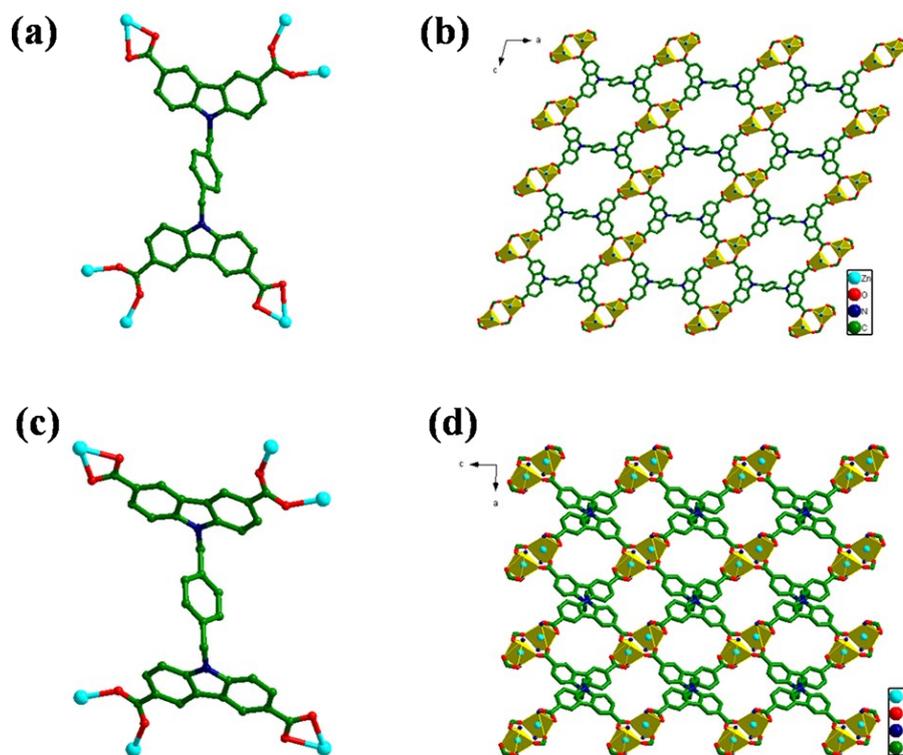


Fig. S1 (a) (b) The coordination mode of  $L^{4-}$  and the 2D structure of **1** along the b axis.

(c) (d) The coordination mode of  $L^{4-}$  and the 2D structure of **2** along the b axis.

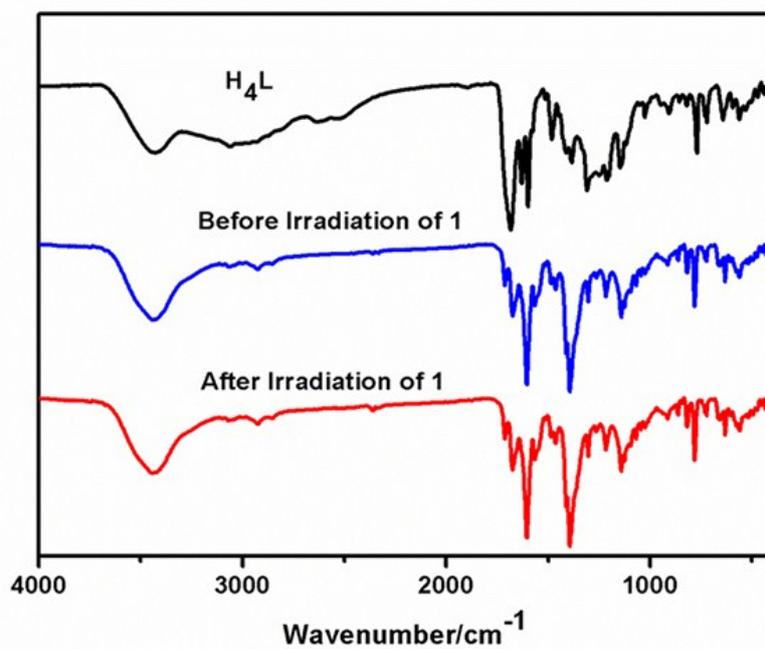


Fig. S2 IR spectra of H<sub>4</sub>L ligand, before and after irradiated for **1**.

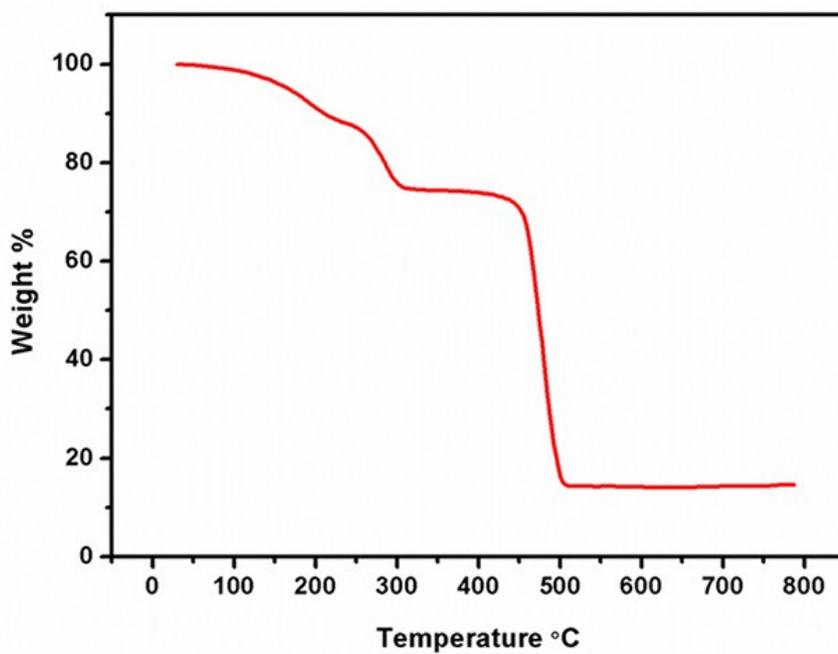


Fig. S3 TGA curve of **1**.

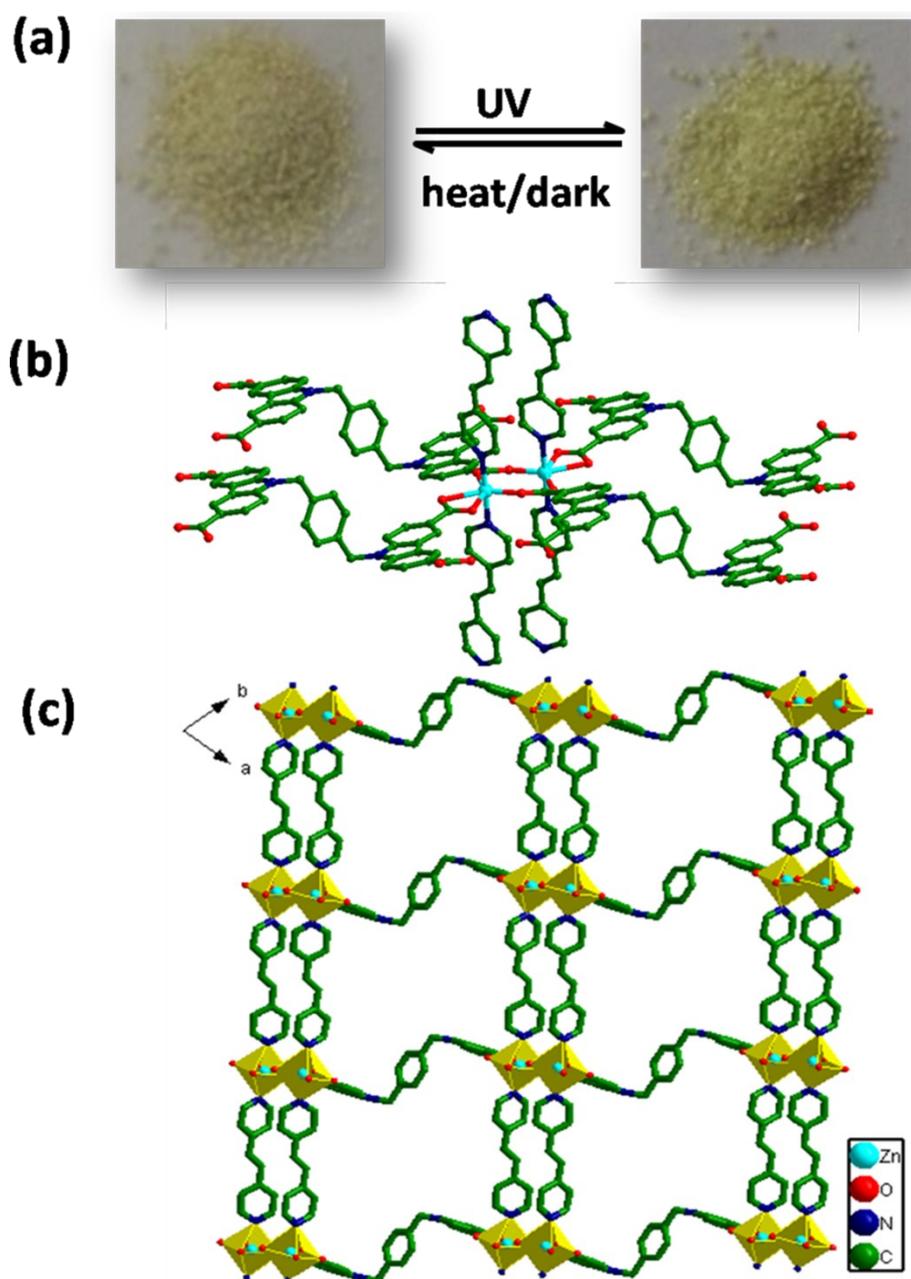


Fig. S4 (a) Single crystal photo of **2** displaying the photochromic behaviour. (b) 2D sheet of **2**. (c) The 2D structure is connected with bpe molecules along the *b* axis to form the 3D structure. The solvent molecules and all hydrogen atoms are omitted for clarity.

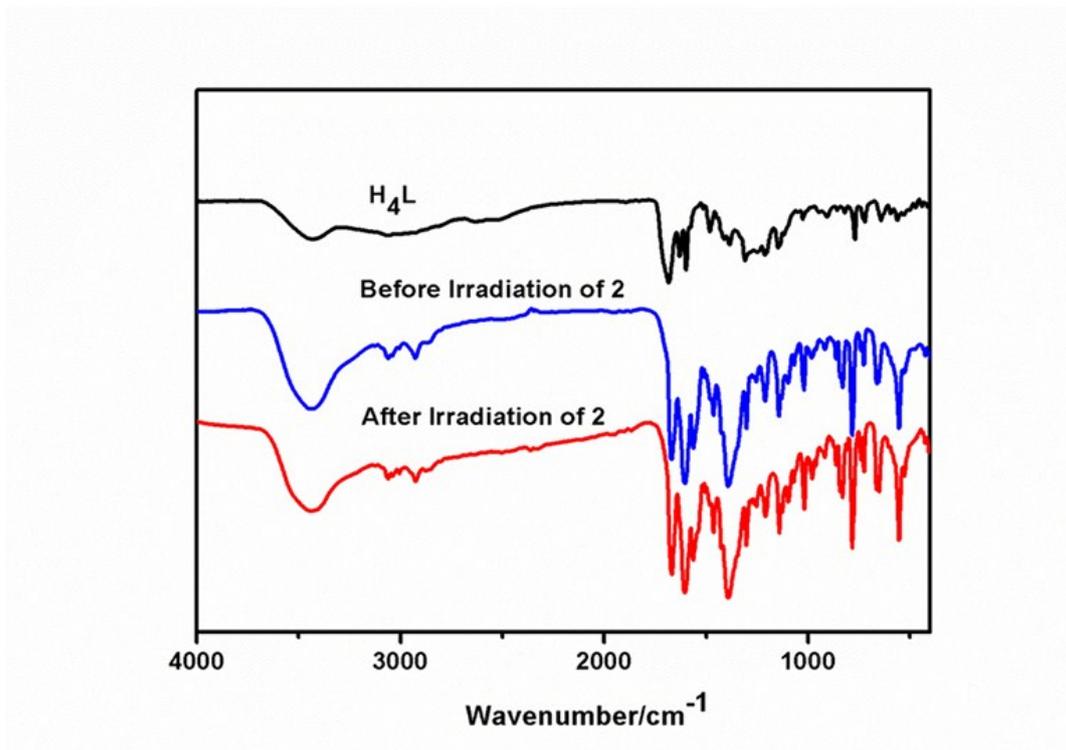


Fig. S5 IR spectra of H<sub>4</sub>L ligand, before and after irradiated for 2.

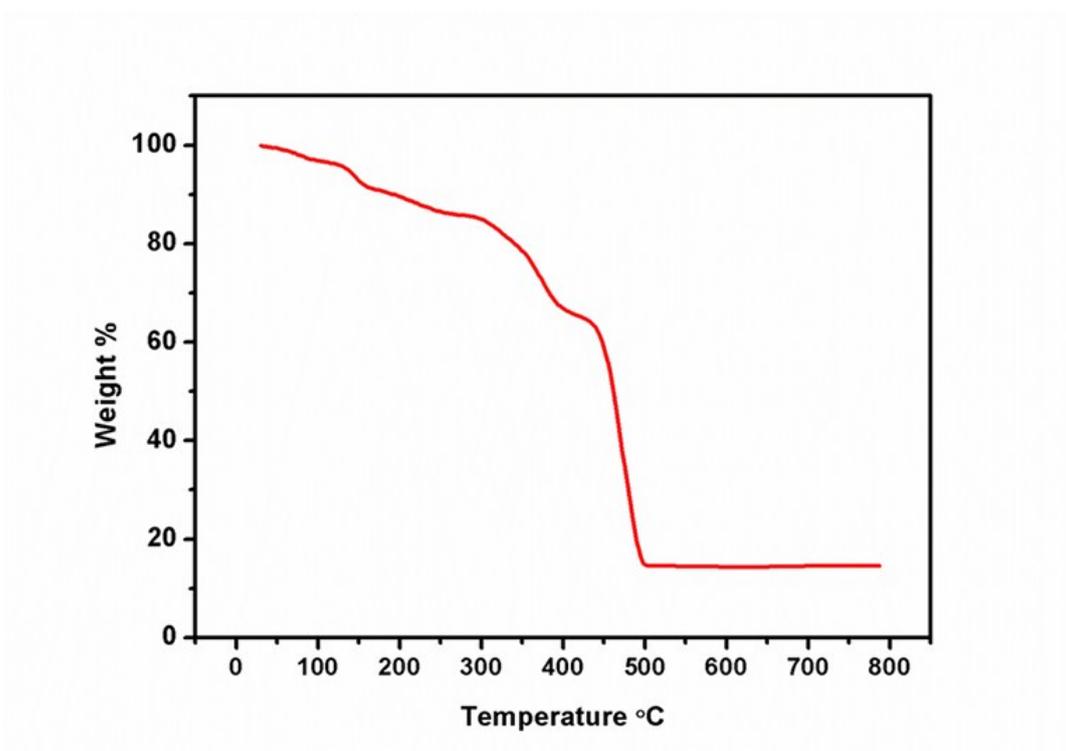


Fig. S6 TGA curve of 2.

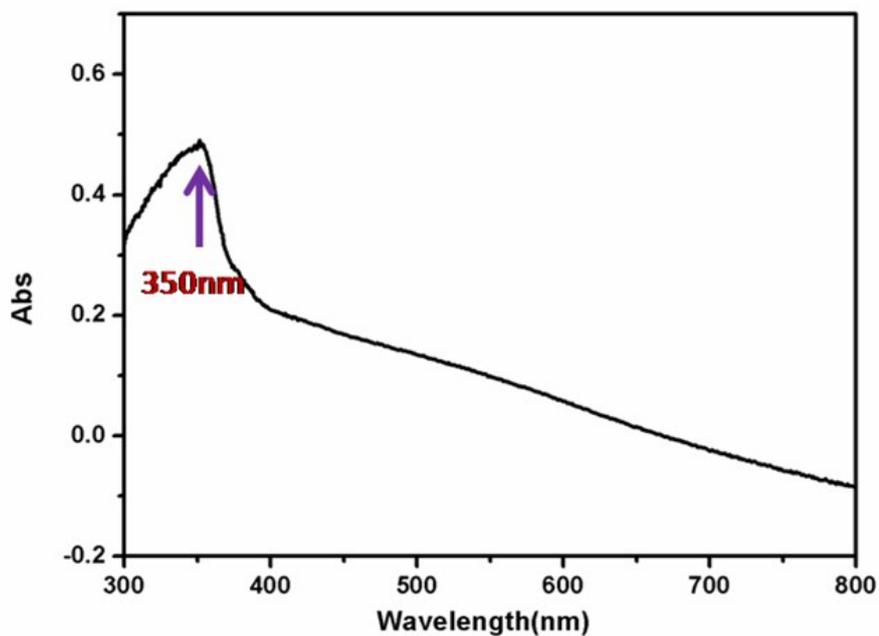


Fig. S7 The UV-vis reflectance spectroscopy of H<sub>4</sub>L.

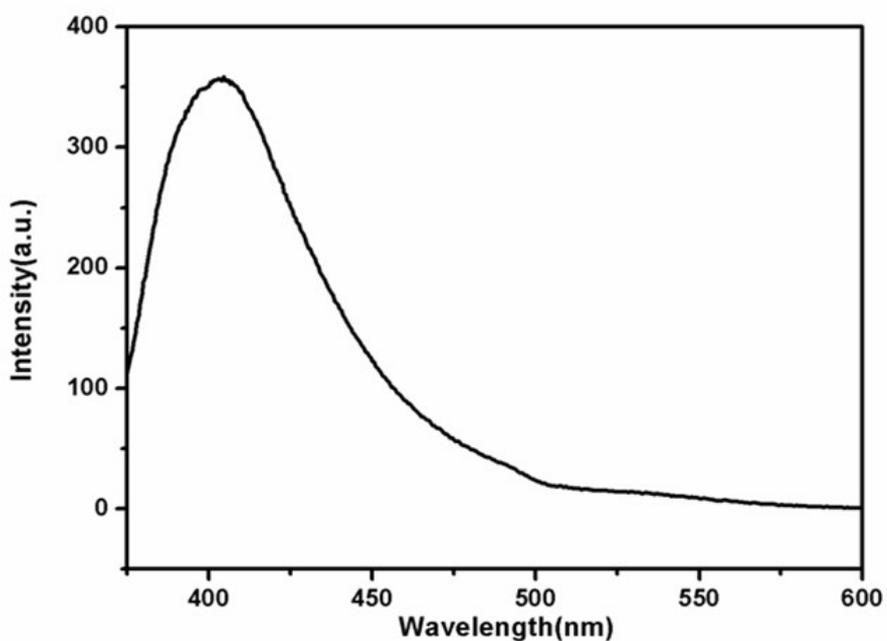


Fig. S8 The fluorescence spectra of H<sub>4</sub>L.

When H<sub>4</sub>L was irradiated with UV light, photochromism was not observed and its UV-vis reflectance spectroscopy and fluorescence spectra also did not change. H<sub>4</sub>L is non photochromic.

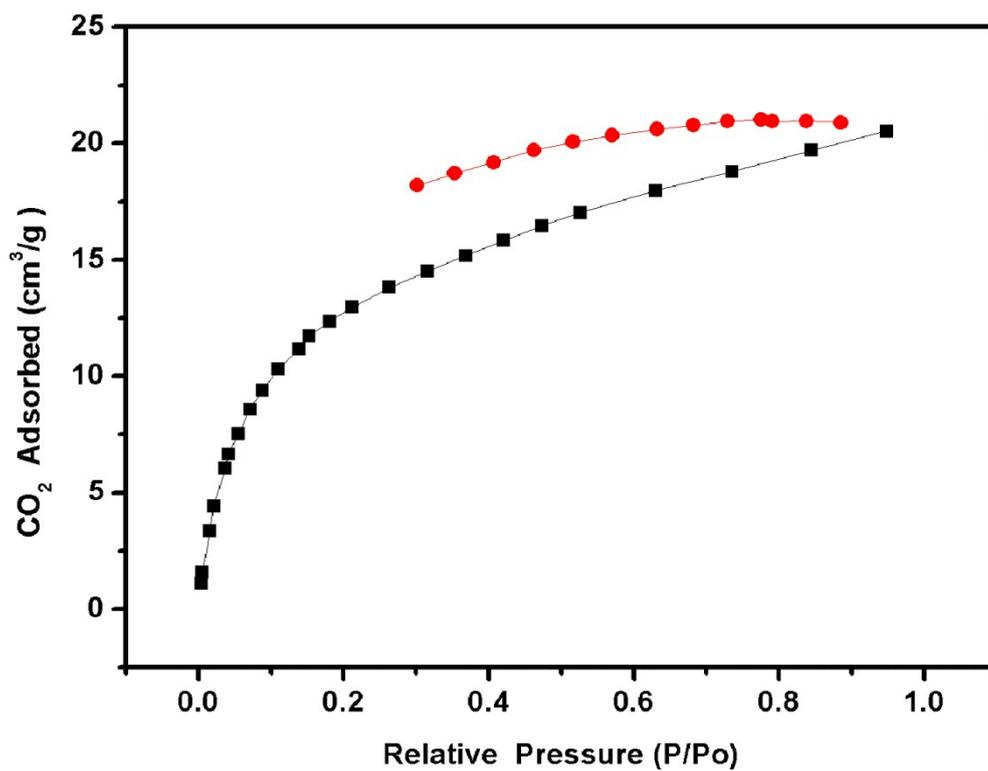


Fig. S9 The CO<sub>2</sub> isotherms at 273 K of **1**.

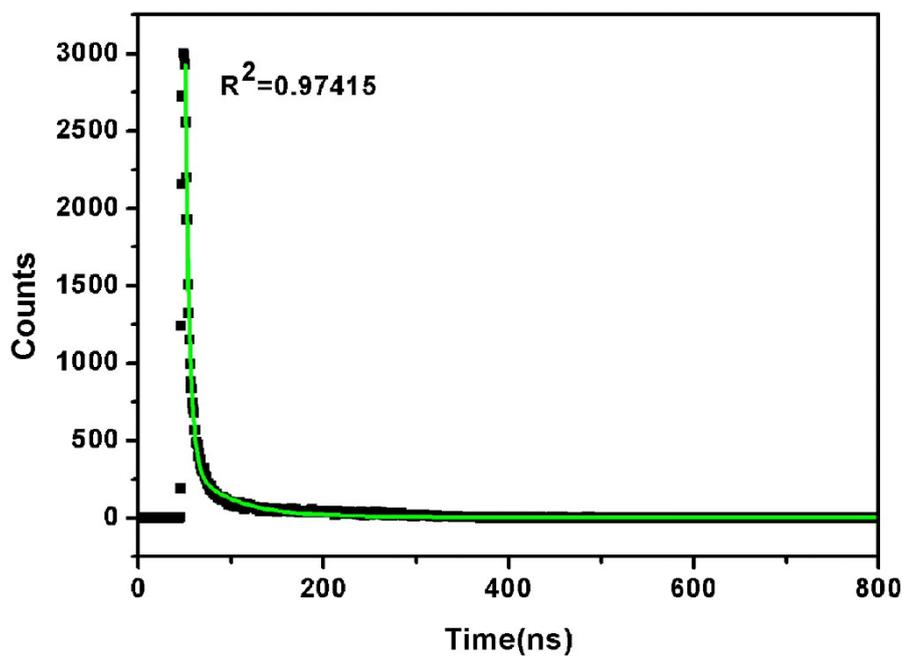


Fig. S10 The lifetime decay profile and fit residual of **1** before illumination.

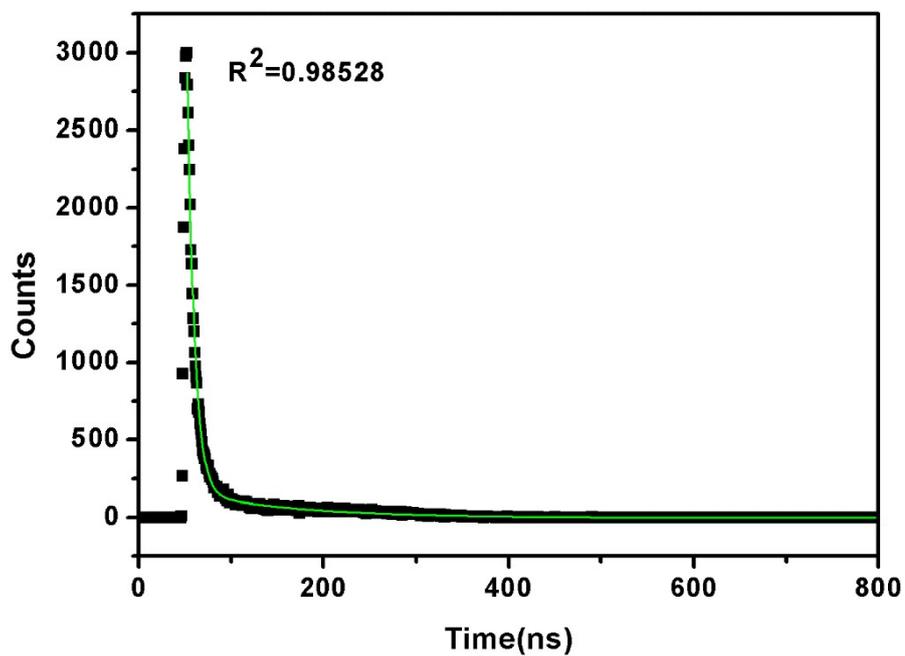


Fig. S11 The lifetime decay profile and fit residual of **1** after illumination.

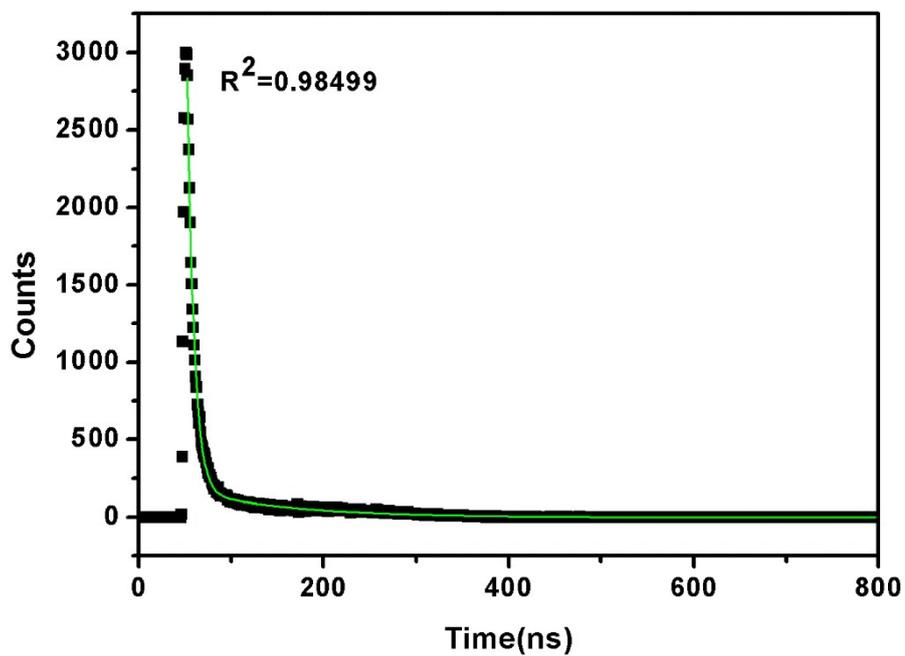


Fig. S12 The lifetime decay profile and fit residual of **2** before illumination.

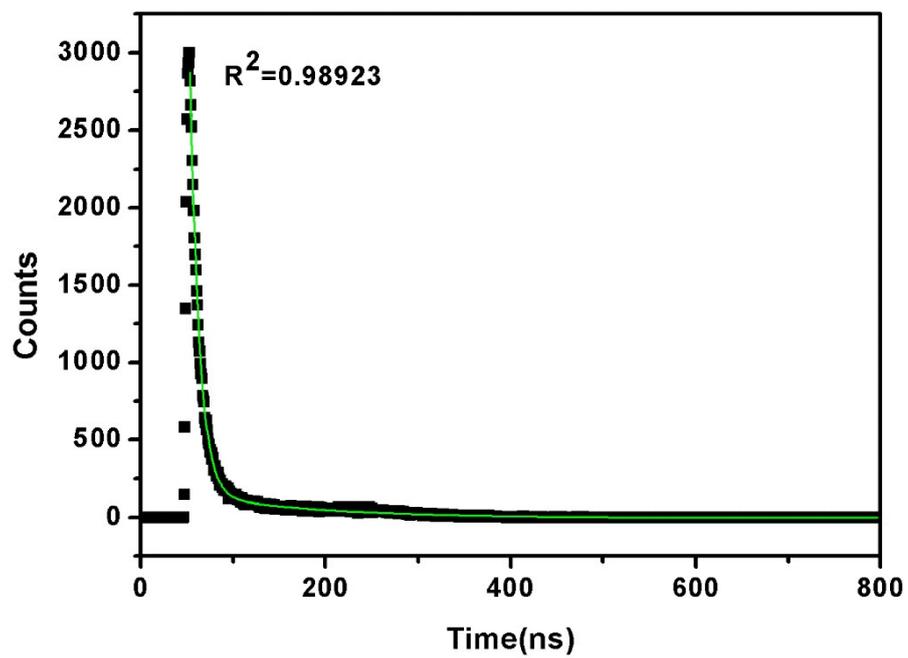


Fig. S13 The lifetime decay profile and fit residual of **2** after illumination.