# **Electronic Supplementary Information**

## Excitation-light-responsive phosphorescent color changes in

## **β-cyclodextrin inclusion complex**

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#### Materials and physical measurements:

All reagents were commercially available and used without further purification. The FT-IR spectra (KBr disk, 4000–400 cm<sup>-1</sup>) were recorded on a Bruker EQUINOX55 FT-IR spectrophotometer. Microanalytical data (C, H and N) were collected on Vario ELIII elemental analyzer. The solid photoluminescence (PL) spectra and the decay lifetimes were determined at room temperature on a Fluorolog-3-TAU fluorescence spectrophotometer. The CIE-1931 chromaticity coordinates were calculated using a ColorCoordinate.exe program. The same results can also be obtained using a gocie.exe program from <u>http://www.geocities.com/</u>krjustin/gocie.html. Reflectance diffusion spectra were recorded in the solid state at room temperature on a DUV–3700 UV/vis/NIR spectrometer. Thermogravimetric analyses were performed under N<sub>2</sub> atmosphere with a heating rate of 10 °C min<sup>-1</sup> with a Shimadzu TGA-50H thermogravimetric analyzer. Powder X-ray diffraction (PXRD) patterns were collected on a Philips X'pert PRO SUPER diffractometer operating with nickel-filtered Cu-K\alpha radiation ( $\lambda = 1.540598$  Å).

### Preparation of β-CD inclusion complex:

2-(imidazo[1,2-a]pyridin-2-yl)-2-oxoacetic acid radical (1) was synthesized according to previous procedure.<sup>S1</sup>

A solution of 1 (0.056 g, 0.27 mmol) in water (1 mL) was added to a solution of  $\beta$ -CD (0.61g, 0.54 mmol) in water (10 mL), and the resulting solution was stirred overnight at room temperature. The resulting white precipitate was filtered, washed with ethanol, and then dried in air at room temperature to afford white powder of 1@CD.

After dried at 80 °C under vacuum condition for 8 h, 1@CD was then determined by elemental analysis (EA). The determined EA data for 1@CD are: C (42.17%), H (7.12%) and N (0.051%). Very low N content and high H content in 1@CD sample indicate it is not 1 itself. Moreover, the existence of N element in sample implies it is not also  $\beta$ -CD itself. When 1@CD is considered as a 2:1 inclusion complex and containing 16 hydrated water molecules, the calculated composition of 1@CD ([C<sub>93</sub>H<sub>146</sub>N<sub>2</sub>O<sub>73</sub>]•16H<sub>2</sub>O) is: C (40.61%), H (6.48%) and N (1.02%), which is slightly close to the determined EA data.



**Fig. S1** IR spectra of pristine  $\beta$ -CD hydrate (a), **1@CD** (b), and **1** (c) showing the N-H stretching band at 3178 cm<sup>-1</sup> of radical **1** (dotted line, Fig. S1c).



Fig. S2 Molecular size of radical 1 based on crystal structure.<sup>S1</sup>



Fig. S3 TGA curves of 1, 1@CD and pristine  $\beta$ -CD hydrate determined under nitrogen atmosphere, and 1@CD determined under air atmosphere.

The 10% remains of CD (up to 800 °C) might be ascribed to somewhat amorphous carbon formed via thermal pyrolysis of CD under nitrogen atmosphere. From Fig. S3, one can find 1 even has 55 % remains up to 800 °C, also probably attributable to the formation of amorphous carbon under nitrogen atmosphere. However, under air atmosphere, 1@CD can be completely decomposed to 0 % even at 600 °C (Fig. S3). Under nitrogen atmosphere, thermal pyrolysis of 1 leading to amorphous carbon is interesting, and deserves to further investigate in future.



Fig. S4 The PXRD patterns of pristine  $\beta$ -CD hydrate and 1@CD.



Fig. S5 Schematic representation of packing structure of channel-type  $\beta$ -CD crystal.<sup>S2</sup>



Fig. S6 PL spectrum of 1 in the dilute  $H_2O$  solution.



Fig. S7 The diffuse reflective spectra of 1 and 1@CD collected in the solid state at room temperature.



Fig. S8 Room-temperature solid excitation spectra of 1 and 1@CD at emission wavelength of 482 and 450 nm, respectively.



**Fig. S9** The decay lifetime curves of **1** and **1@CD** in the solid state. The inset shows the decay lifetime curves of **1@CD** at emission wavelengths of 425, 450 and 500 nm, respectively. The lifetime ( $\tau$ ) is defined as the time in which the emission intensity decays to 1/e of the initial intensity (I<sub>o</sub>), where e is the natural log constant and is equal to 2.718. (I = I<sub>o</sub>e<sup>-(t/ $\tau$ )</sup> =>  $\tau$  = t => I = (1/e) I<sub>o</sub>).<sup>S3</sup>



Fig. S10 CIE chromaticity diagrams for 1@CD by variation of excitation light under same determining conditions.



**Fig. S11** Room-temperature solid-state PL spectra of **1** by variation of excitation light under same determining conditions.

#### Reference

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