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Electronic Supplementary Information for

Functionalization of a stable AIE-based hydrogen-bonded organic framework for white light-emitting diodes

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Experiment Section

Materials and Measurements. All the chemicals were obtained from commercial sources and used without further purification. Hexabromobenzene was purchased from Tokyo Chemical Industry Co., Ltd. (TCI, Shanghai, China). Ethyl 4-Ethynylbenzoate, $Pd(PPh_3)_4$ and CuI were purchased from Sun Chemical Technology Co., Ltd. (Shanghai, China). Triethylamine was purchased from Macklin Biochemical Co., Ltd. (Shanghai, China). Organic fluorescent dye DSMI was purchased from Excition (Shanghai, China).

Powder X-ray diffraction (PXRD) patterns were measured by a PANalytical X'Pert Pro X-ray diffractometer with Cu-Kα radiation (λ = 1.54 Å), scanning over the range of 2-45° (2θ) at a rate of 5°/min. Excitation and emission spectra were performed on a Hitachi F-4600 fluorescence spectrometer. A xenon lamp serves as the excitation source. The fluorescence micrographs were taken on an Olympus IX71 inverted fluorescence microscope. UV-vis spectra were collected on a UV-2600 spectrometer (Shimadzu Corp, Japan). Fluorescence lifetime was evaluated on Edinburgh FLS920 and an external laser was used as a light source. The excited white light of a WLED assembly (23 mA, 3 V, 460 nm LED chip coated with 0.22 wt% HOF-76⊃DSMI) was collected by the fiber optic spectrometer (PG2000-Pro, Ideaoptics Instruments) at room temperature.

Preparation of HOF-76⊃DSMI and fabrication of WLED. At first, a series of DSMI aqueous solutions were prepared in the molar ration varied from 1.67 μM to 167 μM. 6 mg activated HOF-76 was added into a 20 mL glass bottle containing 3 ml different concentrations of DSMI aqueous solution and balanced for 3 days, respectively. Afterward, the obtained phosphors were filtered, then washed thoroughly with H_2O and ethanol at least six times to remove the DMSI molecules absorbed on the surface of HOF-76. The prototype WLED was fabricated by coating the phosphors on a commercial 460 nm blue LED chip.

Energy transfer efficiency calculations. The energy transfer efficiency (η) can be calculated by the following equation:

$$\eta = 1 - \tau_{dsmi}/\tau_0 \tag{1}$$

Where τ_0 and τ_{dsmi} represent the exciton relaxation time constant of pure HOF-76 in the presence and absence of DSMI, respectively.

Average lifetime calculations. The crystal shows the behavior of bi-exponential decay (τ_1 and τ_2). Average lifetime τ is calculated according to the formula:

$$\tau = (B_1 \tau_1^2 + B_2 \tau_2^2)/(B_1 \tau_1 + B_2 \tau_2) \tag{2}$$

B_1 and B_2 represent the pre-exponential factors in front of τ_1 and τ_2 respectively, which are obtained during fitting the decay curve.

Table S1. The photophysical properties of HOF-76 and HOF-76⊃DSMI materials.

Sample	τ_1 (ns)	τ_2 (ns)	τ (ns)	η (%)	Quantum yield
HOF-76	5.63	14.94	13.69	–	9.76%
HOF-76⊃DSMI (0.03 wt% DSMI)	6.44	13.82	12.40	9.4	8.41%
HOF-76⊃DSMI (0.04 wt% DSMI)	6.03	13.52	12.12	11.47	7.93%
HOF-76⊃DSMI (0.07 wt% DSMI)	5.18	11.20	10.12	26.07	7.3%
HOF-76⊃DSMI (0.15 wt% DSMI)	5.07	10.85	9.31	31.99	6.37%
HOF-76⊃DSMI (0.22 wt% DSMI)	4.52	11.16	9.43	31.10	5.62%
HOF-76⊃DSMI (0.29 wt% DSMI)	3.97	9.83	8.50	37.91	4.91%
HOF-76⊃DSMI (0.46 wt% DSMI)	3.63	11.21	9.93	27.46	4.21%
HOF-76⊃DSMI (0.78 wt% DSMI)	3.75	10.24	8.78	35.86	3.27%
HOF-76⊃DSMI (1.10 wt% DSMI)	3.00	10.03	8.72	36.30	2.48%
HOF-76⊃DSMI (1.42 wt% DSMI)	3.36	9.97	8.05	41.20	2.63%

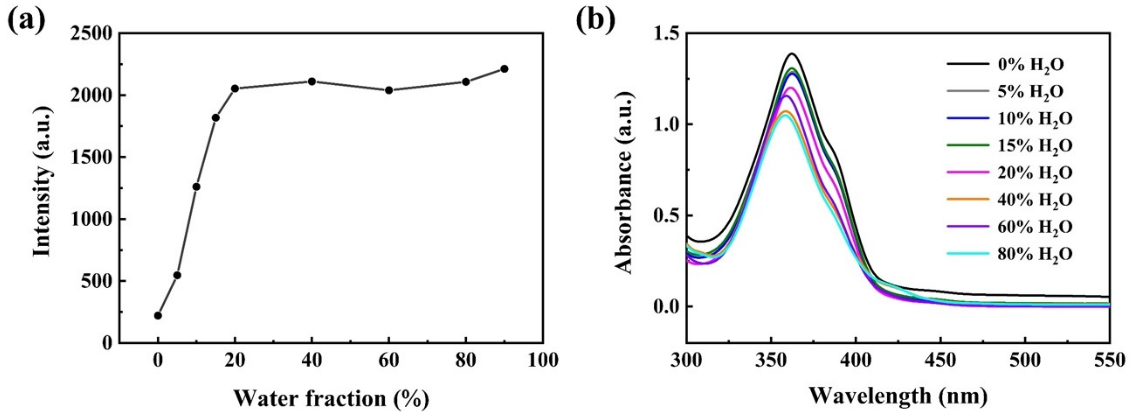

Fig. S1. (a) PL intensity of HCEB versus solvent composition of DMSO/water mixture. (b) The UV-vis absorption spectra of HCEB in mixture of DMSO/water with different water fractions (10 μM).

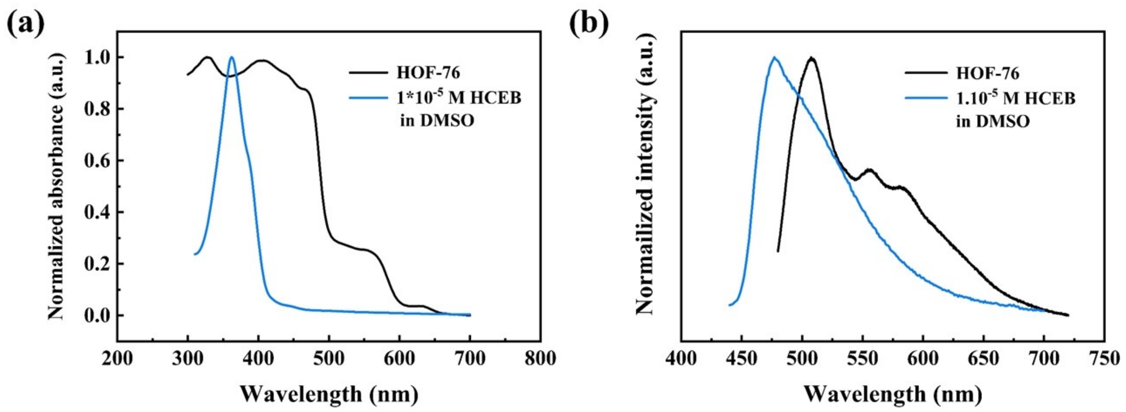

Fig. S2. (a) UV-vis absorption spectra of HOF-76 and HCEB at concentration of ~10^{-5} M in DMSO at room temperature. (b) Emission spectra of HOF-76 and HCEB at concentration of ~10^{-5} M in DMSO at 80 K.

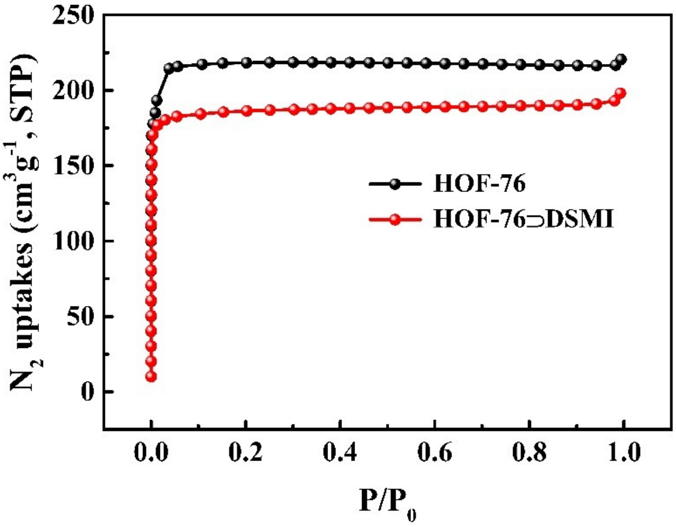

Fig. S3. N_2 adsorption isotherms (77 K) of activated HOF-76 and HOF-76⊃DSMI@0.22 wt%.

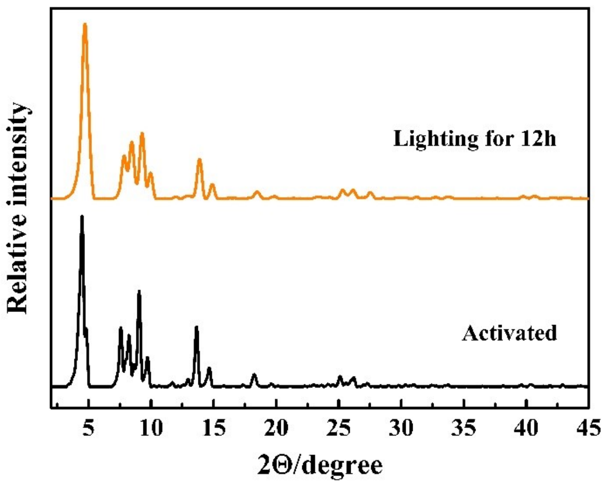

Fig. S4. Powder X-ray diffraction patterns of HOF-76⊃DSMI. The crystallinity can still be maintained after lighting for 12 h.

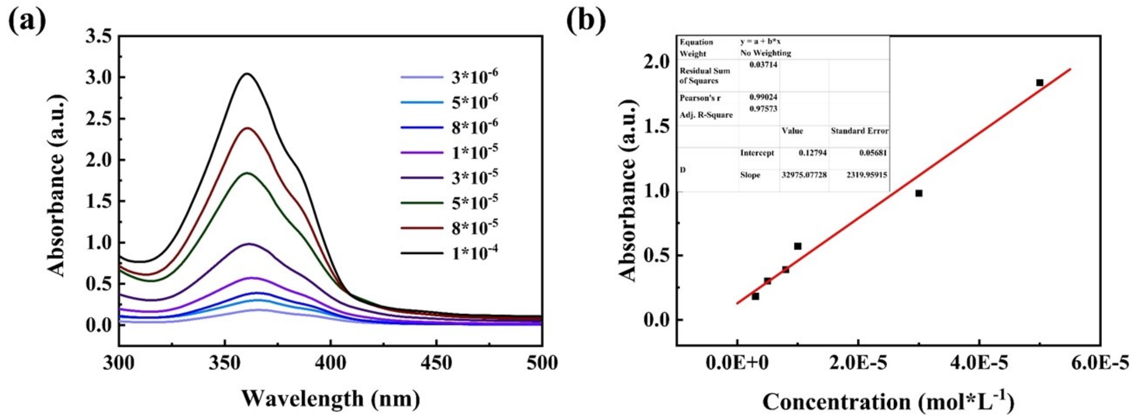

Fig. S5. (a) The UV-vis absorption spectra of HCEB in DMF dilute solution with different concentrations. (b) The intensity-concentration relationship of HCEB in DMF solution.

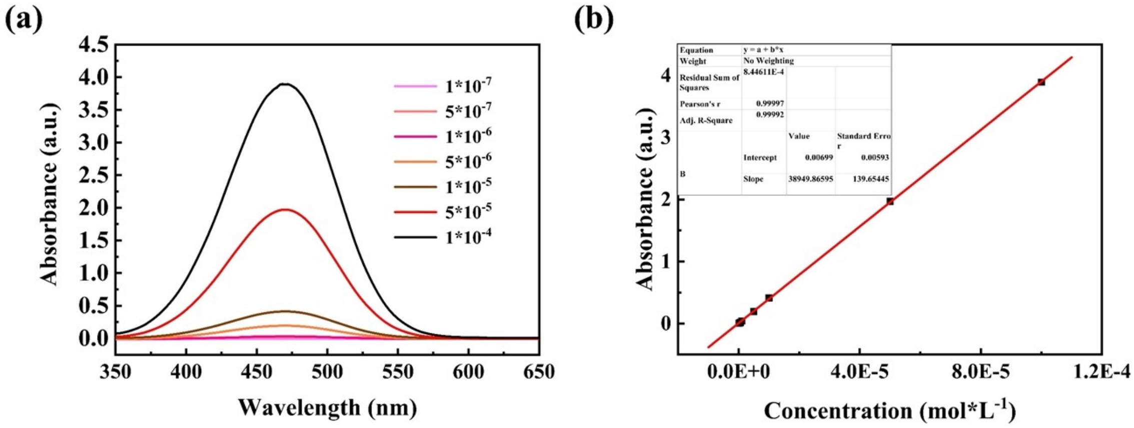

Fig. S6. (a) The UV-vis absorption spectra of DSMI in DMF dilute solution with different concentrations. (b) The intensity-concentration relationship of DSMI in DMF solution.

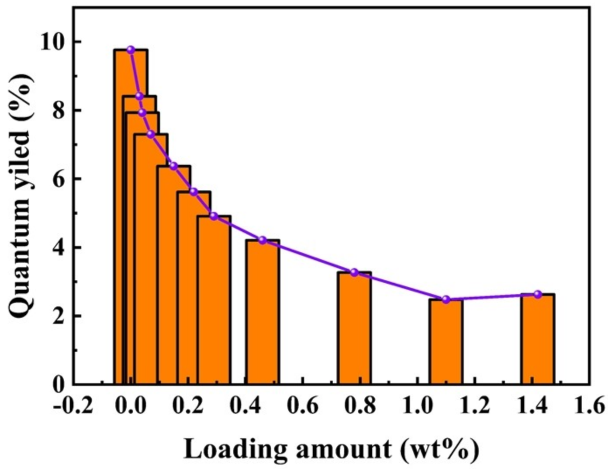

Fig. S7. Quantum yield of HOF-76⊃DSMI with different dye loading amount.

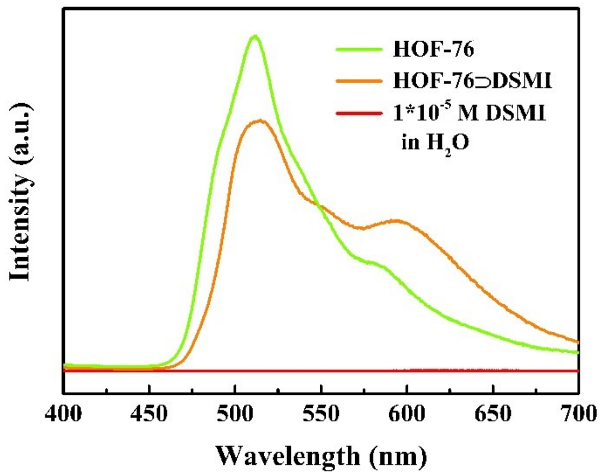

Fig. S8. The emission spectrum of HOF-76, dilute solution of DSMI and HOF-76⊃DSMI at the excitation of 365 nm, which further effectively prove the energy transfer between the host HOF-76 framework and guest DSMI molecules.

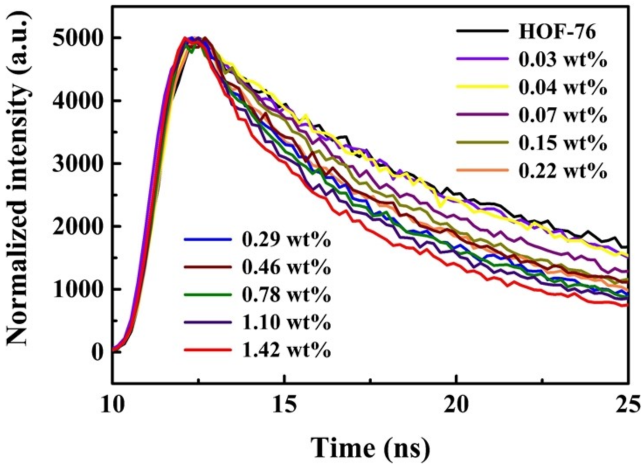

Fig. S9. Time-resolved PL decay curves of HOF-76 and HOF-76⊃DSMI with different concentration of DSMI at 510 nm excited by 470 nm continuous laser.

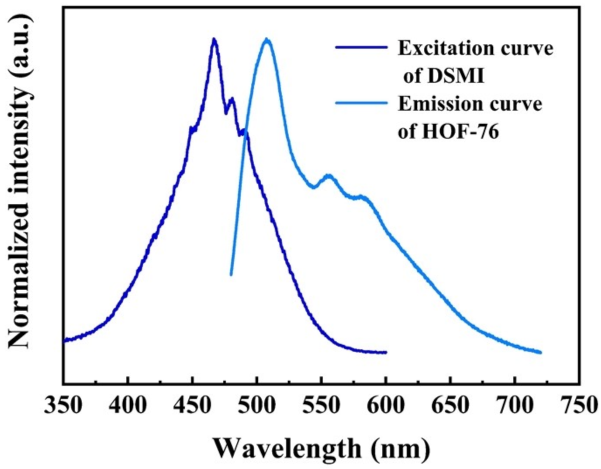

Fig. S10. The excitation spectrum of DSMI and the emission spectrum of HOF-76.

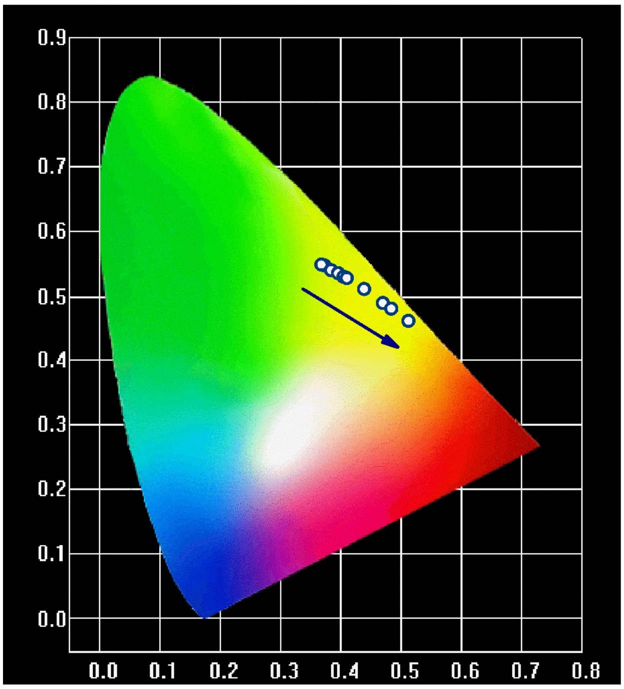

Fig. S11. CIE chromaticity coordinates of HOF-76⊃DSMI with different loading amount of DSMI molecule.