Electronic Supplementary Material (ESI) for Soft Matter.

SUPPORTING INFORMATION

A new strategy for constructing artificial light-harvesting systems: supramolecular self-assembly gels with AIE properties

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Experimental section

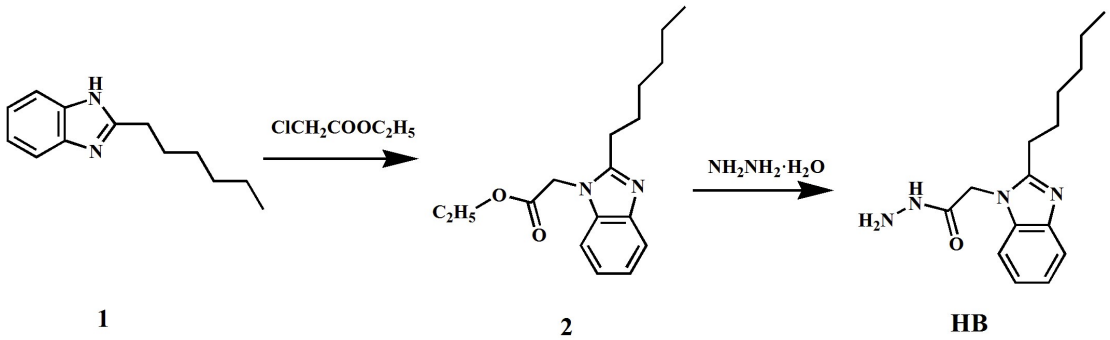
Materials

Unless otherwise noted, all reactions were performed in air atmosphere. The commercially available reagents and solvents were used as received unless otherwise specified purification.

Characterizations

All yields were given as isolated yields. The ^{1}H and ^{13}C NMR spectra were recorded on a Bruker 400 MHz spectrometer. The infrared spectra were recorded on a Thermo Scientific Nicolet iS5 FT-IR spectrophotometer. The absorption spectra were measured with a Shimadzu UV-3600 spectrometer and fluorescence spectra were recorded with a Shimadzu RF-5301PC spectrometer. Transmission electron microscopy (TEM) images were acquired by a FEI Tecnai F20 transmission electron microscope at 200 kV. Scanning electron microscopy (SEM) micrographs were recorded on Zeiss Gemini300 microscope. The quantum yields were carried out on a FLS980 instrument with the integrating sphere. Fluorescence micrographs (FOM) of the samples were performed with Olympus IX 71. The fluorescence lifetimes were measured employing a time-correlated single-photon counting (TCSPC) spectrometer (Edinburgh, FLS 980).

Synthesis



Scheme S1 The synthetic route of **HB**

2-hexyl benzimidazole (1) [1,2] were prepared according to the literature method.

Synthesis of HB

2-hexyl benzimidazole (1) (0.05 mol), ethyl chloroacetate (0.08 mol) and K_2CO_3 (0.10 mol) were dissolved in appropriate absolute acetone and stirred at 60 ℃ for 12 h. After cooling to room temperature, the reaction mixture was filtered. From the clear filtrate，excess acetone was removed by distillation and then was dispersed in distilled water. Afterwards, the solution was filtered and dried to obtain a dry solid product. After further purification, the residue was recrystallized from ethyl acetate to obtain ethyl-(2-hexyl-1H-benzimidazol-1-yl)acetate (2). Yield: 12.25 g (85%). Ethyl-(2-hexyl-1H-benzimidazol-1-yl)acetate (2) (0.038 mol) and hydrazine hydrate (99%) (2 mL, 0.04 mol) were dissolved in appropriate absolute ethanol and stirred at 80 ℃ for 10 h. The solution was evaporated under reduced pressure, and the residue was dispersed in excess of water. Afterwards, the solid separated was filtered and the crude product was recrystallized from ethanol to give 2-(2-hexyl-1H-benzimidazol-1-yl) acethydrazide (**HB**). Yield: 9.38 g (90%). ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 9.51 (s, 1H), 7.54-7.56 (dd, *J* = 2.68, 1.84 Hz, 2H), 7.39-7.41 (dd, *J* = 1.90, 0.74 Hz, 2H), 7.14-7.16 (m, *J* = 28.00 Hz, 2H), 4.80 (s, 2H), 4.34 (s, 2H), 2.80-2.84 (t, *J* = 15.35 Hz, 2H), 1.74-1.83 (m, *J* = 30.44 Hz, 2H), 1.38-1.43 (m, *J* = 18.97 Hz, 2H), 1.31-1.34 (m, *J* = 14.53 Hz, 2H), 0.87-0.91 (t, *J* = 14.38 Hz, 3H); ^{13}C NMR (400 MHz, DMSO-d_6) δ (ppm): 165.64, 155.58, 142.13, 135.51, 121.12, 120.90, 117.67, 109.40, 44.19, 30.74, 28.43, 26.21, 21.80, 14.05.

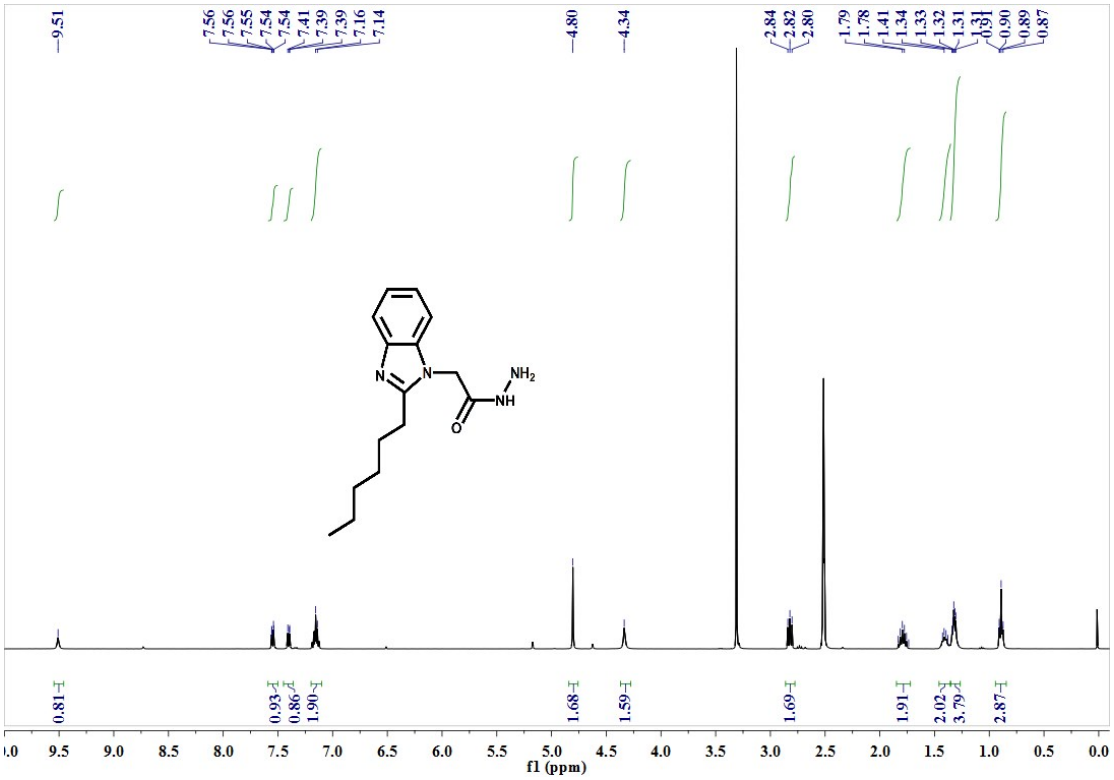


Fig. S1 ^{1}H NMR (400 MHz) spectrum of **HB** in DMSO-d_6 at 30°C

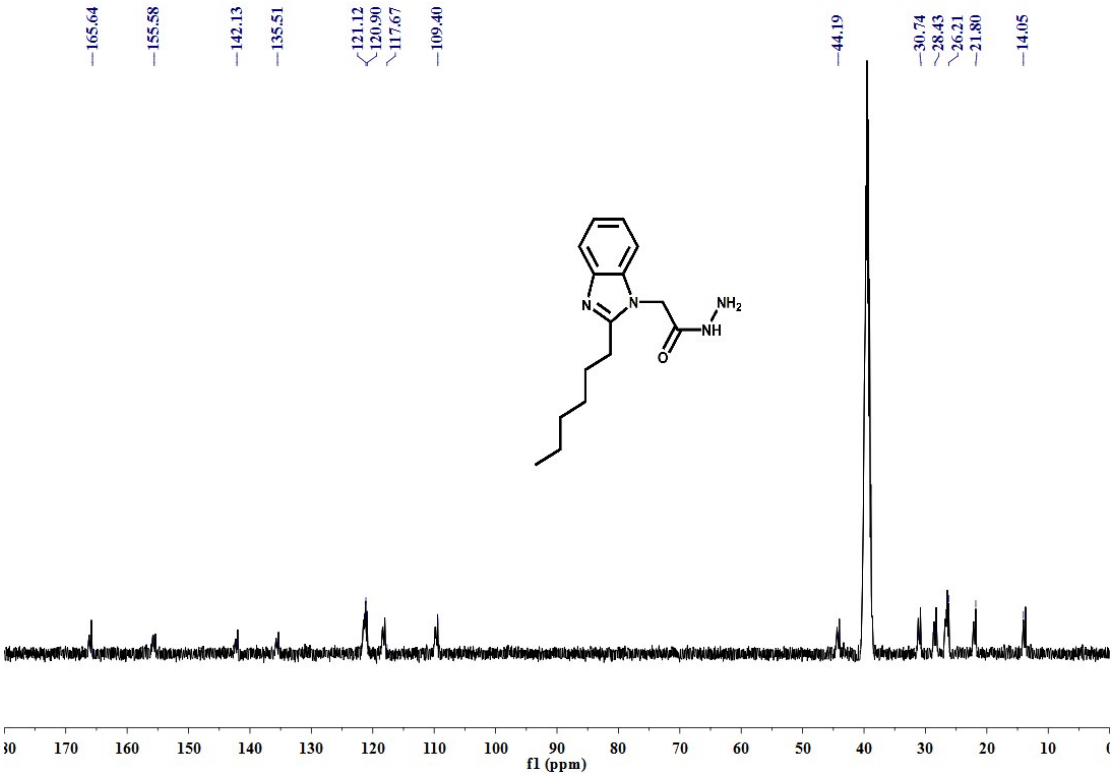


Fig. S2 ^{13}C NMR (400 MHz) spectrum of **HB** in DMSO-d_6 at 30°C

T_{sg} (gel−sol transition temperature)

A capped vial containing the gel was immersed in an oil bath. With the increase of temperature, once gel moving was observed upon the tilting of the vial, an average temperature of three such measurements was defined as the sol-gel transition.

Characterization of HB

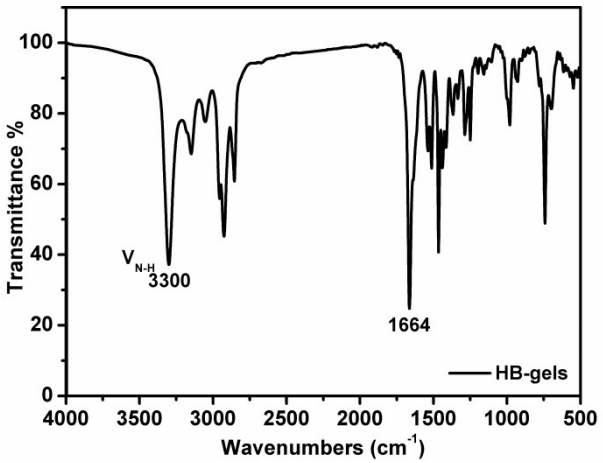


Fig. S3 FT-IR spectra of the xerogel **HB** (0.6 %)

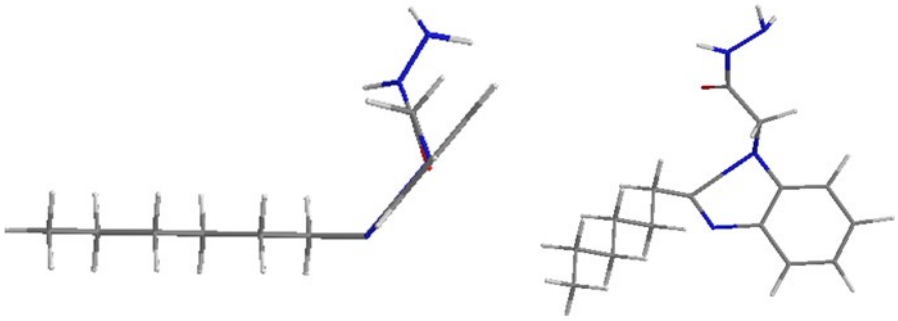


Fig. S4 Sticks structures of **HB** in the side view and front view, respectively

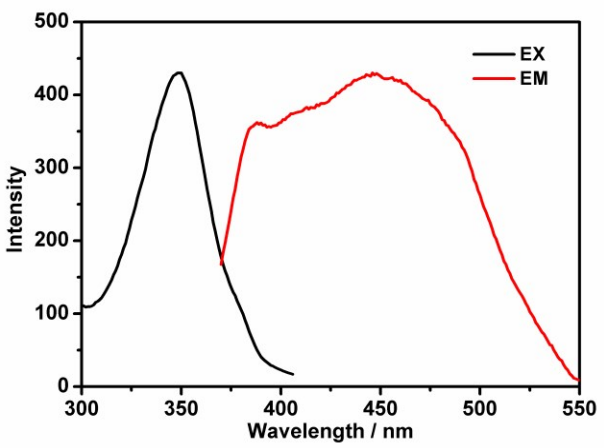


Fig. S5 Excitation and emission spectra of **HB**

Table S1 Key parameters of excitation and emission spectra of **HB**

maximum of HB' peak		
excitation spectra of HB (λ_{ex})	**emission spectra of solution** (λ_{em})	**emission spectra of gel** (λ_{em})
350 nm	480 nm	450 nm

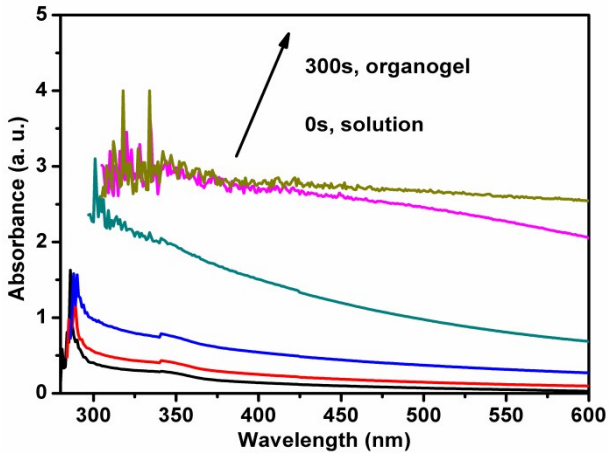


Fig. S6 Time-dependent UV-Vis absorption spectra of organogel **HB** (0.3%, in mixed solutions) during the gelation process

Characterization of HB/RhB

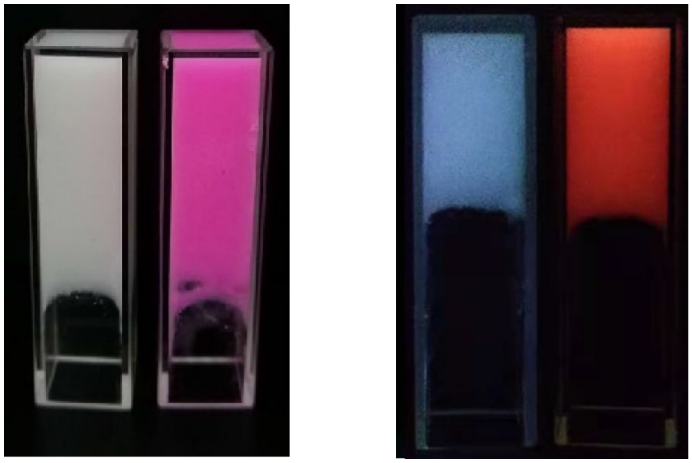


Fig. S7 Photographs of **HB** and **HB**/**RhB** under ambient light and illumination at 365 nm ([**HB**] = 0.024 M, [**RhB**] = 0.061 mM)

Energy-transfer efficiency (Φ_{ET})

Energy-transfer efficiency, Φ_{ET}, the fraction of the absorbed energy that is transferred to the acceptor is experimentally measured as a ratio of the fluorescence intensities of the donor in the absence and presence of the acceptor (I_D and I_{DA}).[3]

$$\Phi_{ET}=1-I_{DA}/I_D$$

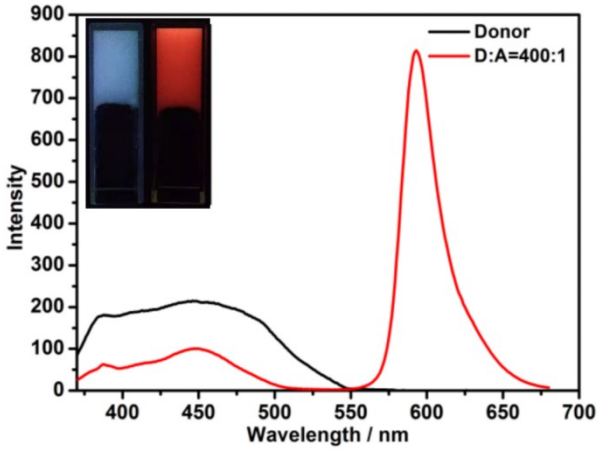


Fig. S8 Fluorescence spectra of **HB** and **HB**/**RhB** assembly (λ_{ex} = 350 nm). Inset: photographs of **HB** and **HB**/**RhB** under UV light (365 nm) ([**HB**] = 0.024 M, [**RhB**] = 0.061 mM)

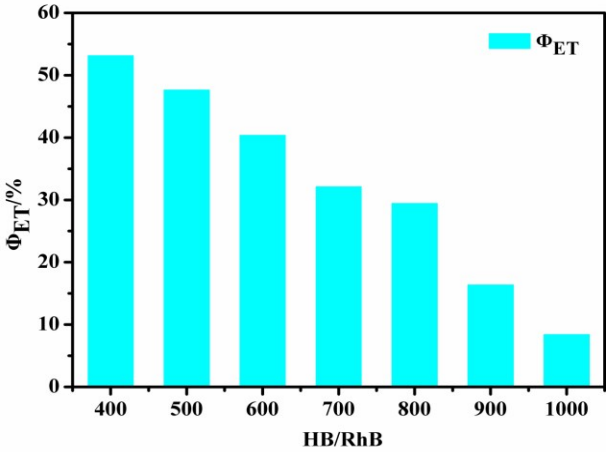
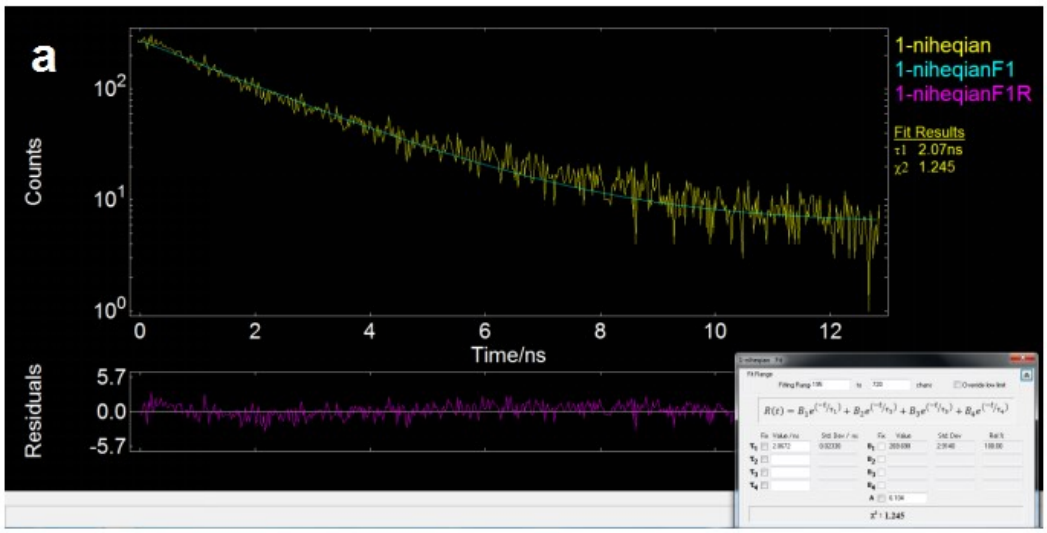


Fig. S9 Energy transfer efficiency at different **HB**/**RhB** ratios

Fluorescence lifetime measurements



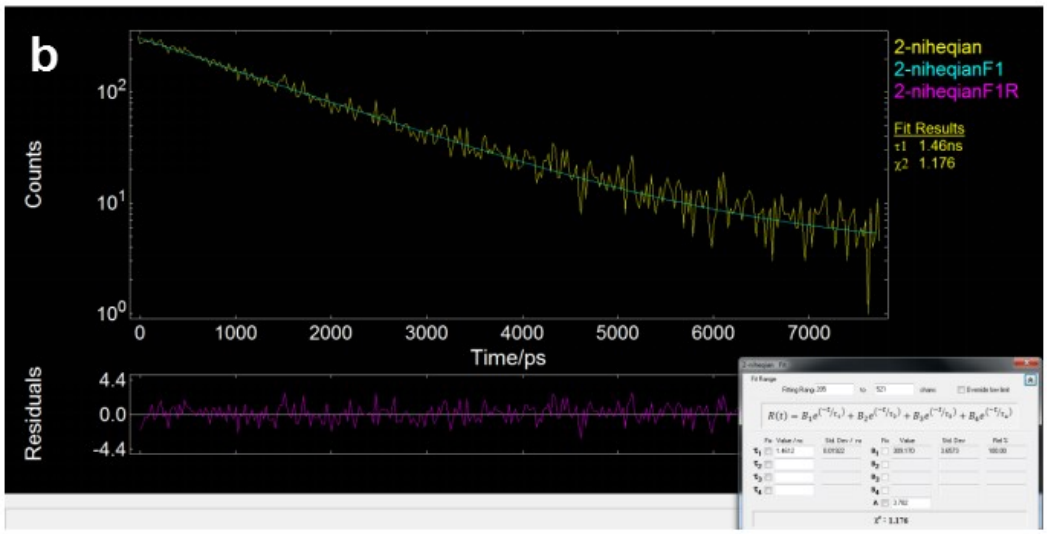


Fig. S10 Fluorescence decay profiles of (a) HB assembly monitored at 450 nm upon excitation at 350 nm, and (b) HB/RhB assembly monitored at 590 nm upon excitation at 350 nm in mixed solutions ([HB] = 0.024 M, [RhB] = 0.061 mM)

Table S2 Fluorescence lifetimes of HB assembly and HB/RhB assembly monitored at 450 nm upon excitation at 350 nm ([HB] = 0.024 M, [RhB] = 0.061 mM)

Sample	**τ** / ns	χ^2
HB [**HB**] =0.024 M	2.07	1.245
HB/RhB ([**HB**] = 0.024 M, [**RhB**] = 0.061 mM)	1.46	1.176

References

1. W. O. Pool, H. J. Harwood, A. W. Ralston, J. Am. Chem. Soc. 1937, 59 (1), 178-179.
2. Y. M. Zhang, Q. Lin, T. B. Wei, X. P. Qin, Y. Li, Chem Commun., 2009, 6074–6076.
3. (a) J. J. Li, Y. Chen, J. Yu, N. Cheng, Y. Liu, Adv. Mater. 2017, 29, 1701905; (b) S. Guo, Y. Song, Y. He, X. Y. Hu, L.Wang, Angew. Chem. Int. Ed. 2018, 57, 3163; (c) M. Hao, G. P. Sun, M. Z. Zuo, Z. Q. Xu, Y. Chen, X. Y. Hu, L. Y.Wang, Angew. Chem. Int. Ed. 2019, 58, 2.