Supporting Information

Supramolecular isomer-dependent photochromism and emission color tuning of bipyridinium salts

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Additional characterization data and structural figures

Fig. S1 a) A 1D hydrogen-bonded helical chain in A1. b) A 1D hydrogen-bonded zigzag chain in A2. The hydrogen atoms are omitted for clarity. The dashed lines represent hydrogen bonds.

Fig. S2 Left: The topology of 1D channel in A2. Right: 1D meso-helical water chain confined in the channel of A2. The HBpybc+ ligands are simplified as yellow stick. The hydrogen bond distances are in angstrom unit.
**Fig. S3** The ESR spectra of A1 (black) and A2 (red) after irradiation.

**Fig. S4** The distance and orientation between the donor and acceptor in A1 (upper) and A2 (bottom).
Fig. S5 $^1$H NMR (400 MHz, D$_2$O) for A1 (upper) and A2 (bottom), respectively.
**Fig. S6** Normalized fluorescence emission spectra of A1 to show a large blue-shift of the peak position (from 524 nm to 443 nm) with decreasing solvent polarity from water (black) to THF-water (volume ratio: 4:1) mixture (green). Excitation wavelength: 360 nm.

**Fig. S7** Calculated XRPD pattern from the single crystal structural data of A1 (black), experimental pattern for the colored samples of A1 after irradiation (green), and initial sample of A1 (red).

**Fig. S8** Calculated XRPD pattern from the single crystal structural data of A2 (black), experimental pattern for the colored samples of A2 after irradiation (green), and initial sample of A2 (red).
**Fig. S9** Excitation spectral change of A1 in the solid state upon irradiation with a xenon lamp.

**Fig. S10** IR spectra of A1 (black) and A2 (red). The bands appearing around 1695 cm\(^{-1}\) are attributed to the characteristic asymmetric C=O stretching vibration of the carboxylic group in monoprotonated HBpybc\(^+\).