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Aggregation-Induced Red-NIR Emission Organic Nanoparticles as Effective and Photostable Fluorescent Probe for Bioimaging

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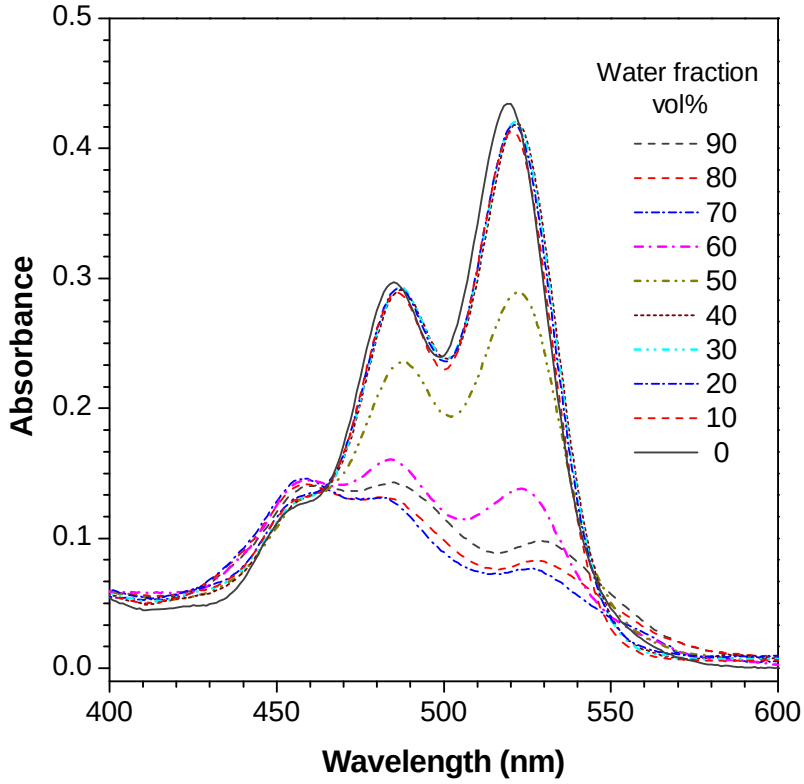

Figure S1. Absorption spectra of DBrPBI in THF/H_2O mixtures. Concentration of DBrPBI:10 μM.

The absorption spectrum of the intermediate DBrPBI in THF shows a peak at 520 nm and two shoulders around 485 and 454 nm, which assigned to 0-0, 0-1 and 0-2 electronic transitions, respectively. With addition of water, which is a poor solvent for DBrPBI, the molecules began aggregating due to the limited solubility, resulting dramatic changes in the absorption features. The 0-0 and 0-1 electronic transitions decreased gradually with the increasing volume fraction of water (f_w). When $f_w < 50\%$, 0-0 transition is dominant and when $f_w \geq 50\%$, the 0-1 and 0-2 transitions are more intense than 0-0 transition. These spectra changes indicate molecular aggregated strongly by π-π stacking.[1-3] As a result, the emission intensity decreased significantly in the mixed solvents as demonstrated by Figure 1A in main text. When f_w is over 80%, the emission spectra are nearly parallel to the abscissa.

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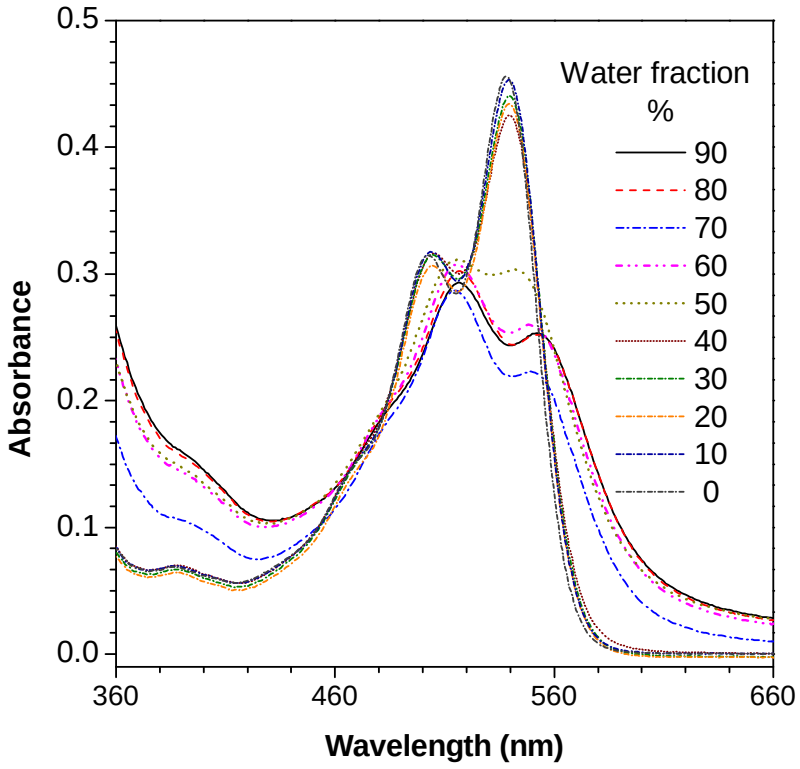

Figure S2. Absorption spectra of BTPEPBI in THF/H_2O mixtures. Concentration of BTPEPBI:10 μM.

BTPEPBI in THF/water mixture solvent shows absorption features with a peak at 539 nm and a pronounced shoulder at 503 nm. The change in their relative intensity is a marker of intermolecular interaction. Similar to the variation of absorption features of DBrPBI, addition of water in THF can cause evident variation of absorption features. When f_w< 50%, 0-0 transition is dominant when $f_w \geq$ 50%, the 0-1 transition is prominent. These spectral changes indicate the formation of aggregates.

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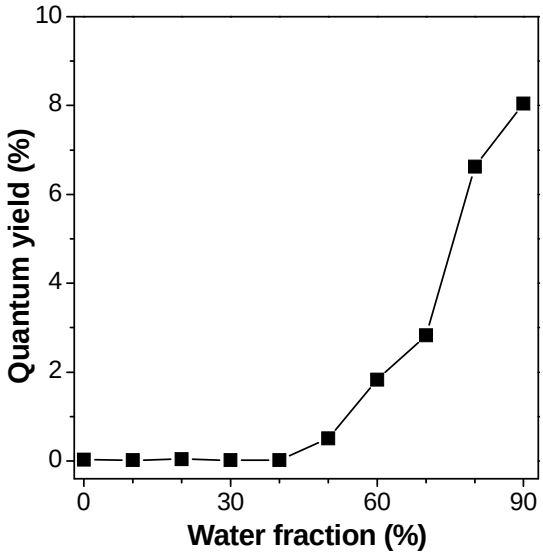

Figure S3. Variation of Φ_F of BTPEPBI in THF/H_2O mixture with water fraction. The Φ_F values were estimated using Rhodamine 6G in ethanol as the standard (Φ_F = 95%).

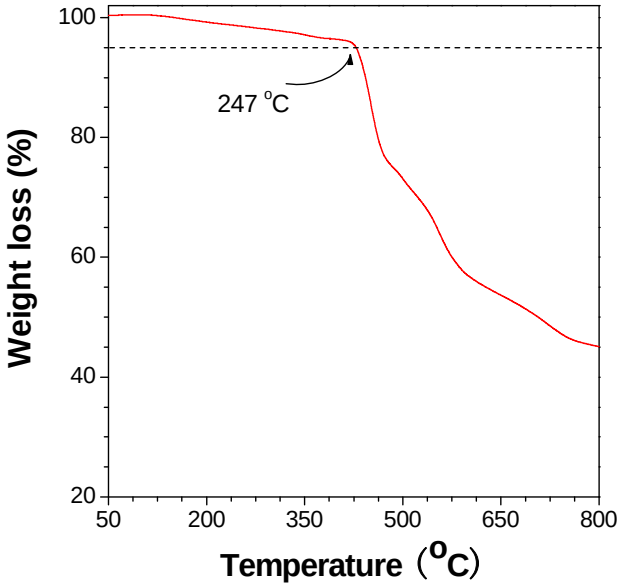

Figure S4. Thermal gravimetry analysis curve of BTPEPBI recorded under nitrogen at a heating rate of 20 °C min^{-1}.

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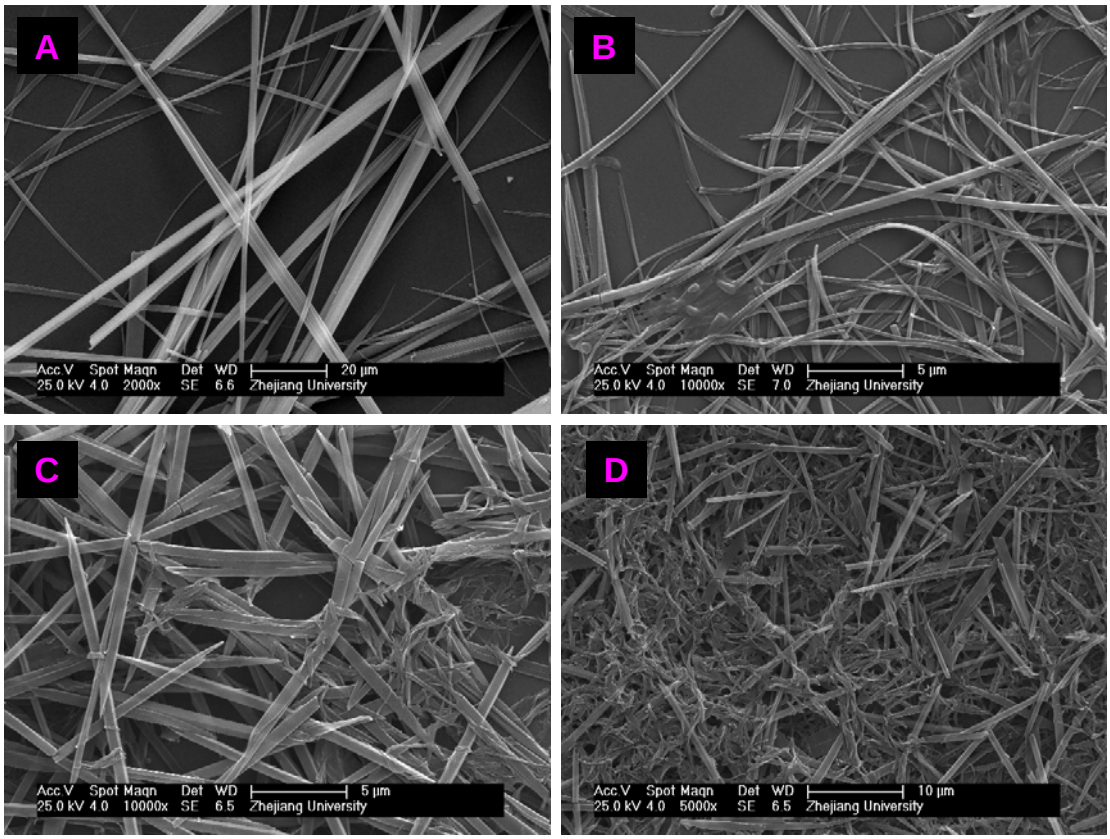

Figure S5. Typical SEM images showing the morphology of aggregates formed by BTPEPBI in THF/H_2O mixtures with f_w of 30%, 40%, 50% and 60%, respectively.

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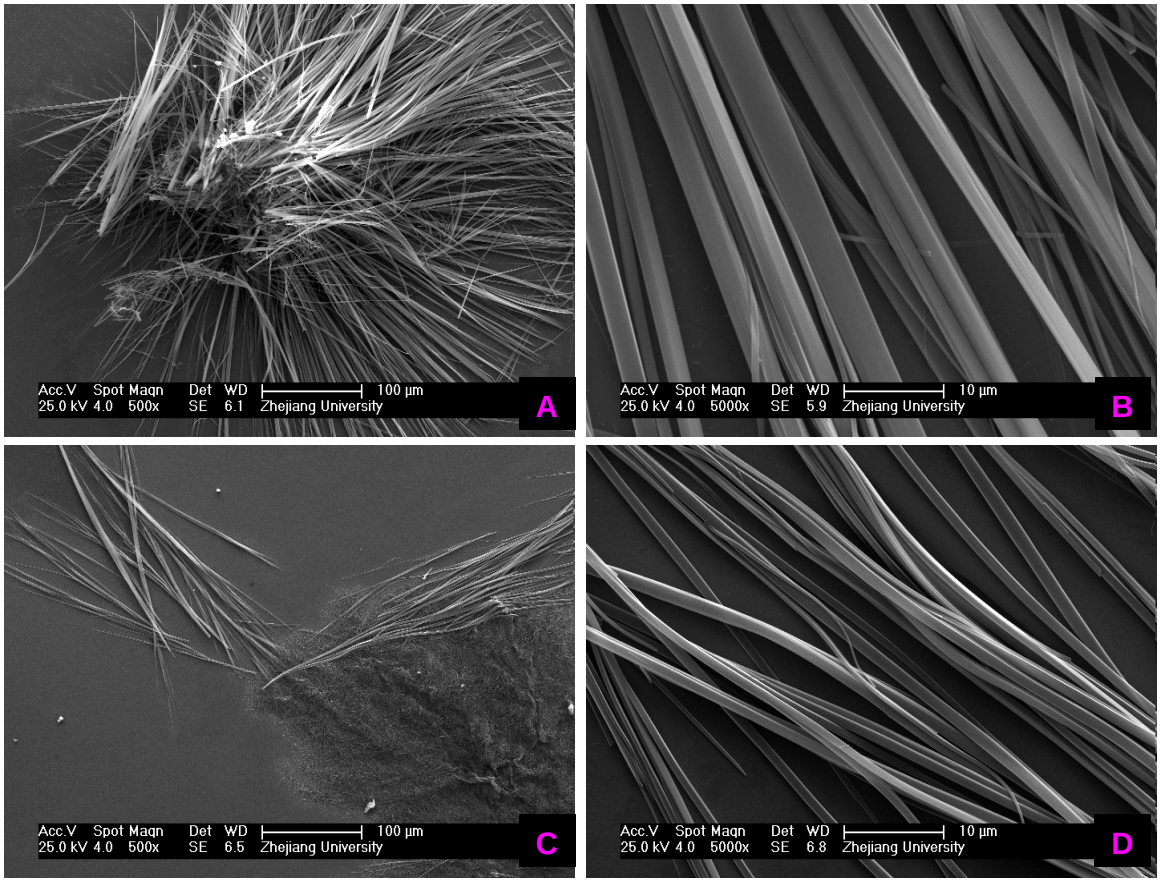

Figure S6. (A) and (C) are typical SEM images showing the morphology of aggregates formed by BTPEPBI in dichloromethane/methanol mixtures with $f_{methanol}$ of 60% and 80%, respectively; images (B) and (D) are magnified views of the aggregates formed by BTPEPBI in dichloromethane/methanol mixtures with $f_{methanol}$ of 60% and 80%, respectively.

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