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Supporting Information

Encapsulation of Stimuli-Responsive Dyes into Metal-Organic Frameworks for High-Efficiency Dynamic Multi-Color Emission

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1. Materials

2-(3,3-dimethyl-3H-indol-2-yl)-5-(piperidin-1-yl)naphtho[1,2-d]oxazole (USTS-3, $C_{26}H_{25}N_3O$) and 2-(3,3-dimethyl-3H-indol-2-yl)-5-morpholinonaphtho [1,2-d]oxazole (USTS-4, $C_{25}H_{23}N_3O_2$) are two solvatofluorochromic dye which were synthesized by our research group. Znic acetate ($Zn(OAc)_2$, AR, 99.1%) was purchased from Bide Pharmatech Ltd. 4,5-Dichloroimidazole (dcIm, AR, 97%) was purchased from Damas-beta. Petroleum ether with a boiling range of 60-90 °C (PE, AR), dichloromethane (DCM, 99.5%, AR), ethyl acetate (EA, 99.5%, AR), acetone (Me_2CO, 99.0%, AR), acetonitrile (CH_3CN, 99.5%, AR), methanol (MeOH, 99.5%, AR) and dimethyl sulfoxide (DMSO, 99.0%, AR) was purchased from Shanghai Titan Scientific Co., Ltd. All chemicals were used as received without further purification.

2. Synthesis

Synthesis of ZIF-71. Crystalline ZIF-71 powder was synthesized by reacting $Zn(OAc)_2$ with dcIm in methanol solution at room temperature. Under stirring, 9 mL of a clear methanol solution containing 0.24 mmol $Zn(OAc)_2$ was rapidly poured into 9 mL of methanol solution containing 0.96 mmol dcIm. The mixed solution immediately turned milky-white turbid from colorless and transparent. After stirring at room temperature for 24 h, centrifugation was performed at 8000 rpm to remove excess reactants. The sample was then sonicated in methanol for 10 min and washed twice with methanol, followed by vacuum drying at 60 °C for 12 h.

Synthesis of USTS-3/4$_n$@ZIF-71. The preparation procedure of USTS-3/4$_n$@ZIF-71 is similar to that of pure ZIF-71, except that different amounts of USTS-3 and USTS-4 methanol solutions are added to 9 mL of methanol solution containing 0.96 mmol dcIm. The detailed synthetic procedure is described as follows: A 9 mL methanol clear solution of 0.24 mmol of zinc acetate was rapidly poured into a 9 mL methanol solution of 0.96 mmol of dcIm and different amounts of USTS-3/4 solution (0.5 mmol/L; I: 1 mL, II: 2 mL, III: 4 mL, IV: 5 mL) under stirring. The mixed solution immediately changed from clear to turbid. The purification procedure of USTS-3/4$_n$@ZIF-71 is consistent with that of pure ZIF-71.

Synthesis of Prodan@ZIF-71. The procedure for preparing Prodan@ZIF-71 was the same, except that USTS-3/4 is replaced with Prodan.

Synthesis of USTS-3$_I$@NKU-110. 0.5 mmol $Zn(NO_3)_2 \cdot 6H_2O$, 0.2 mmol H_2PyC and 0.25 mmol H_3BTC were added into a mixed solvent containing 5 mL DMF and 5 mL DMA, and ultrasonicated until full dissolution. The resulting solution was transferred into a 20 mL glass vial, sealed and heated at 95 °C for 72 h. After natural cooling to room temperature, beige crystalline powder was collected. The product was washed sequentially with DMF and EtOH for

two times each, and finally dried under vacuum at 60 °C for 12 h.

3. Structural and morphological characterization

Powder X-ray diffraction measurements were carried out on a diffractometer (D8 ADVANCE, Bruker, German) using Cu-Kα (λ = 1.54056 Å) radiation operated at 40 kV and 40 mA. Scanning electron microscopy (SEM) was characterized on a JSM-IT800SHL at 10 kV.

4. Photophysical Characterizations

UV−vis absorption spectra were recorded using a SHIMADZU UV-2600 UV-Vis-NIR spectrophotometer. Steady photoluminescence (PL) spectra of all samples were performed on a SHIMADZU RF-6000 fluorescence spectrophotometer. The photoluminescence quantum yield and fluorescence lifetime of USTS-3/4_n@ZIF-71 were characterized using an Edinburgh FLS1000 spectrometer equipped with a time-correlated single-photon counting (TCSPC) module and an integrating sphere accessory.

5. Supplementary Figures

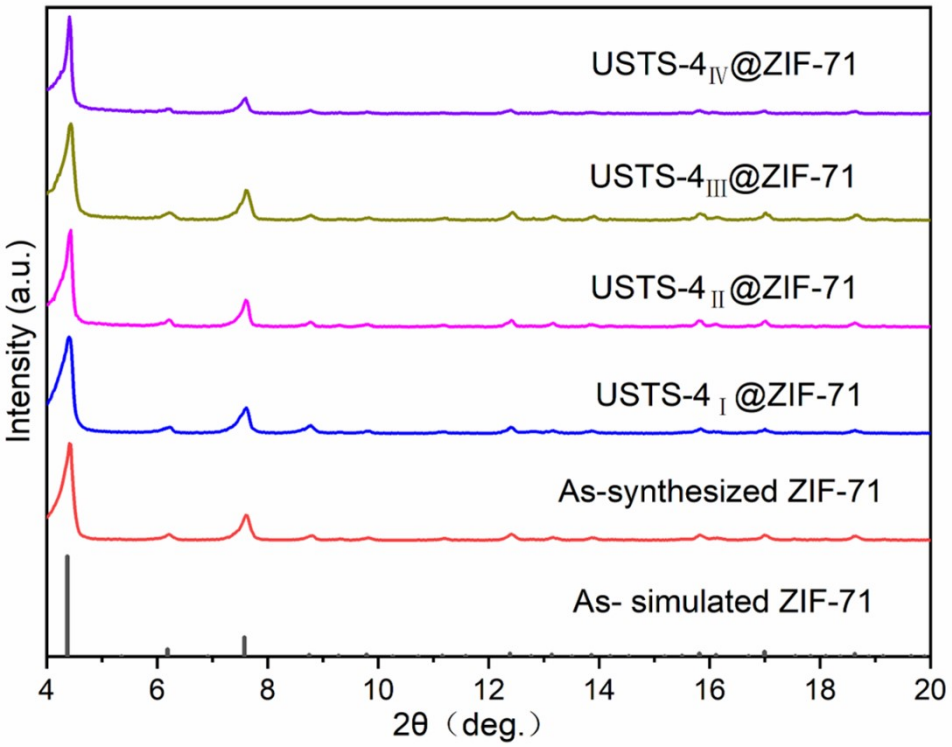

Fig. S1 Simulated crystallographic diffraction pattern of ZIF-71 and X-ray powder diffraction (PXRD) patterns of the as-prepared ZIF-71 and USTS-4@ZIF-71 with different loaded concentrations of USTS-4.

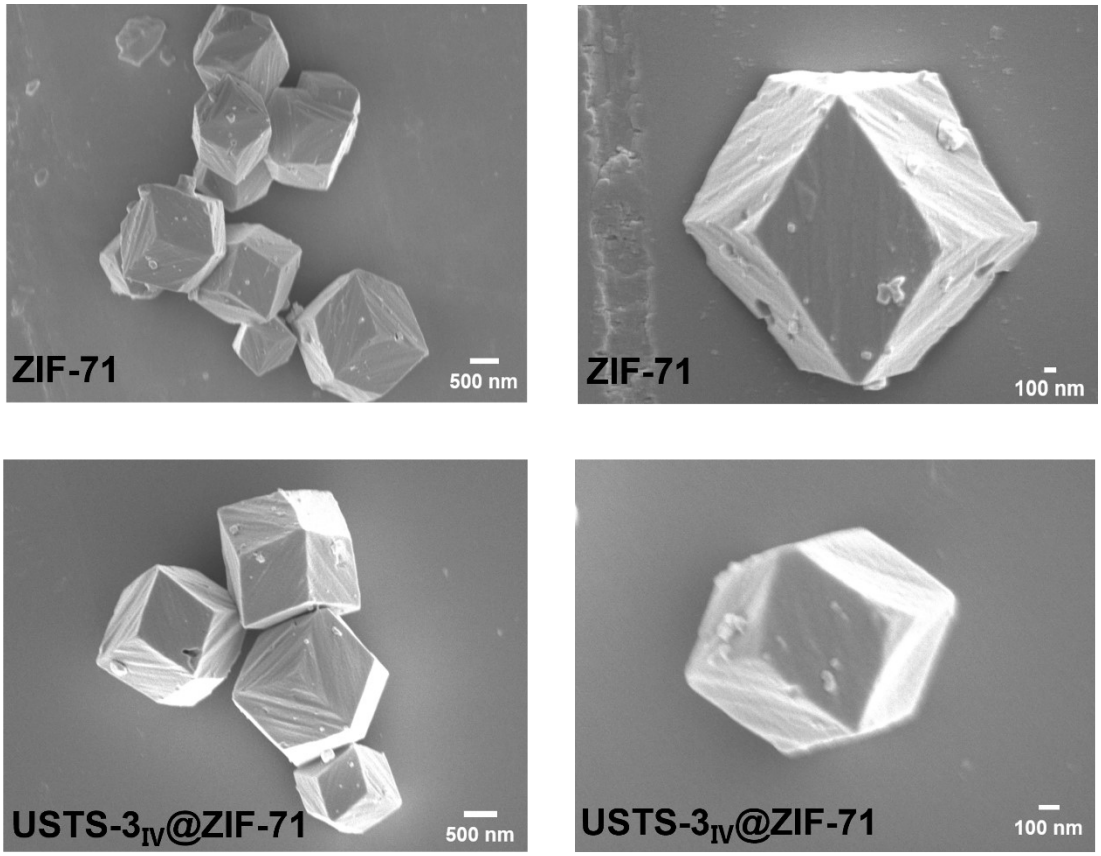

Fig. S2 SEM micrographs of submicron-sized ZIF-71 and USTS-3_{IV}@ZIF-71 crystals.

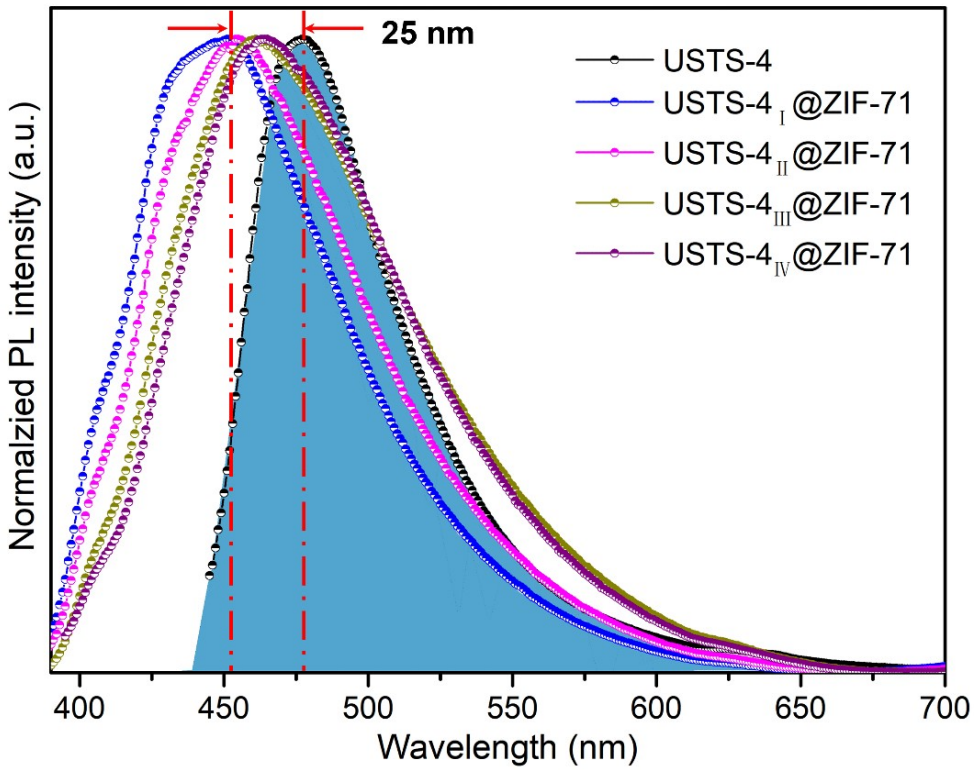

Fig. S3 Solid-state fluorescence spectra of USTS-4@ZIF-71 with different USTS-4 loadings.

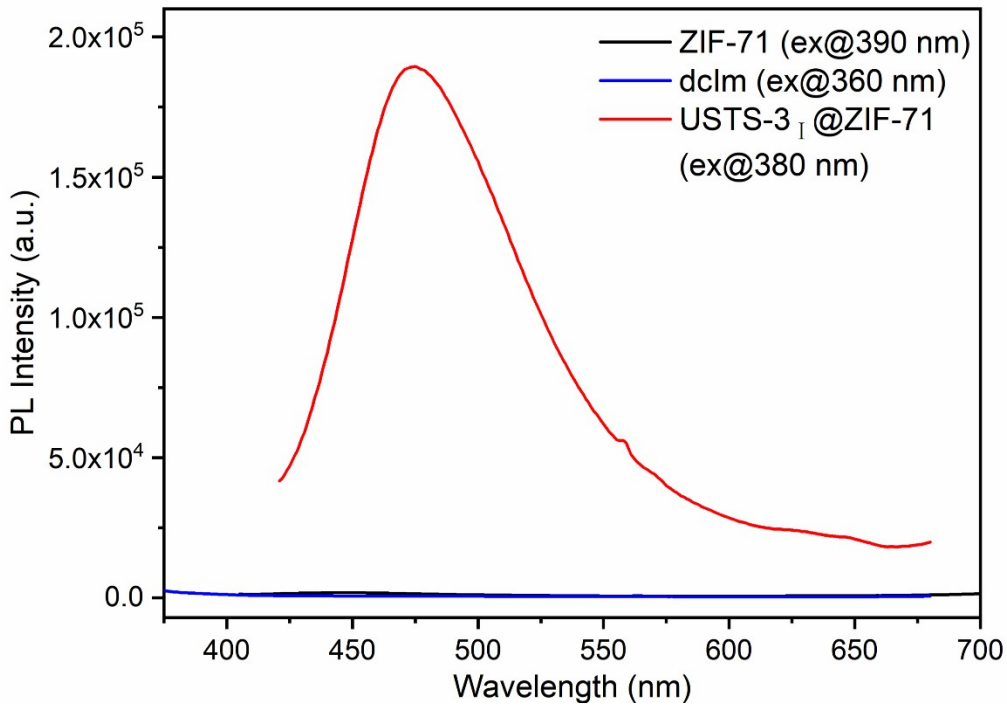

Fig. S4 FL spectra of ZIF-71, dcIm and USTS-3_I@ZIF-71.

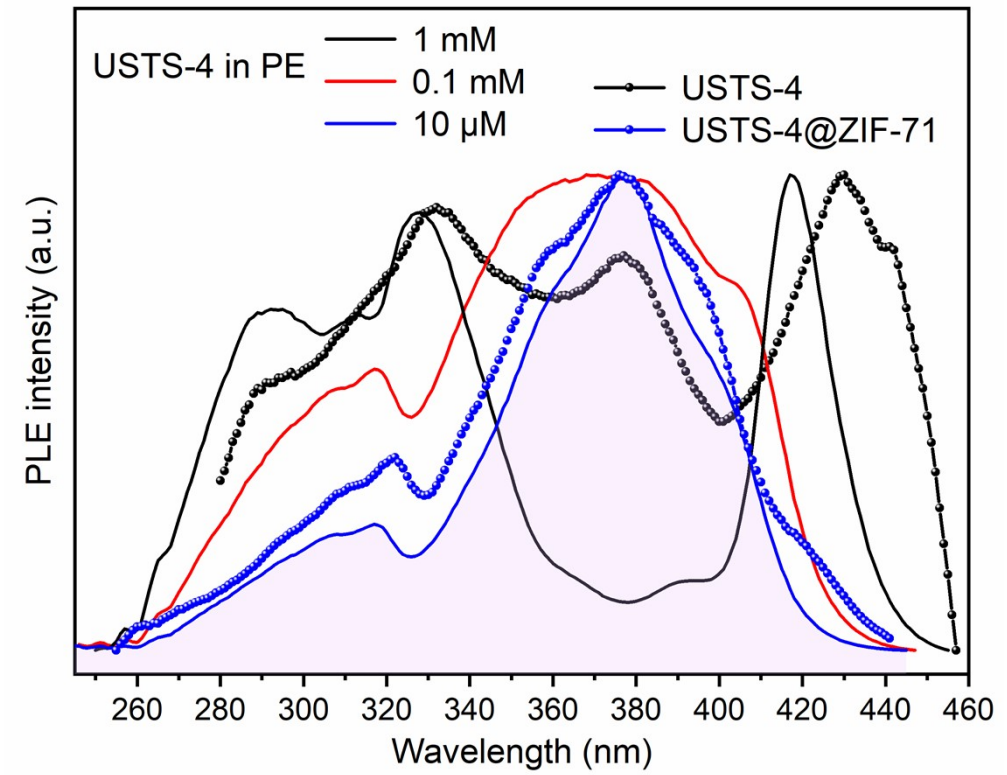

Fig. S5 Typical excitation spectra of USTS-4 in PE solution at various concentrations, pure USTS-4 powder, and USTS-4@ZIF-71.

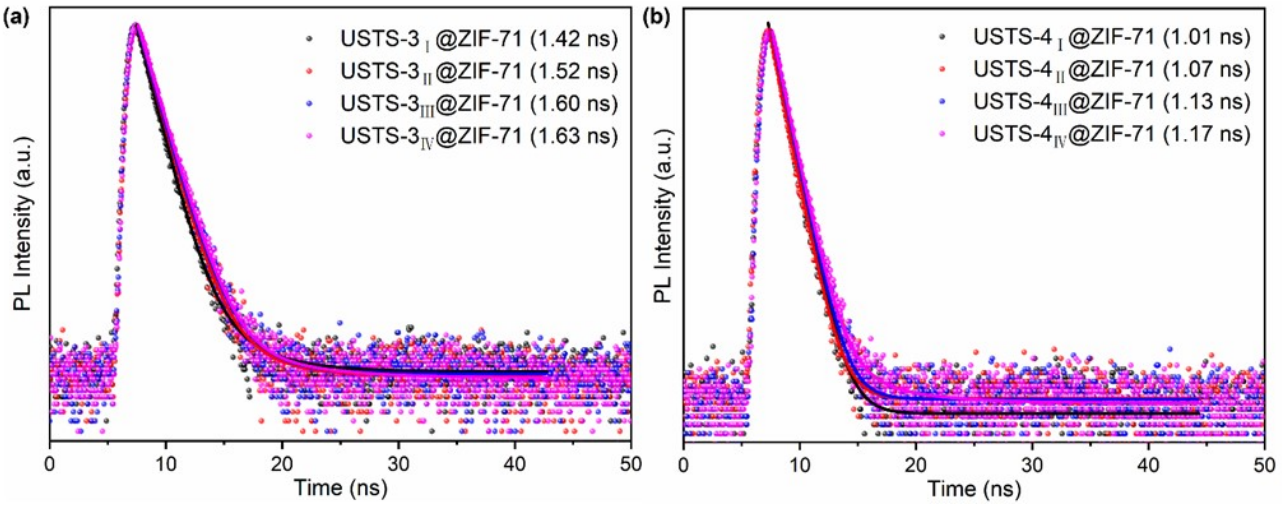

Fig. S6 PL lifetime of USTS-3/4$_n$@ZIF-71 measured under 365 nm wavelength excitation.

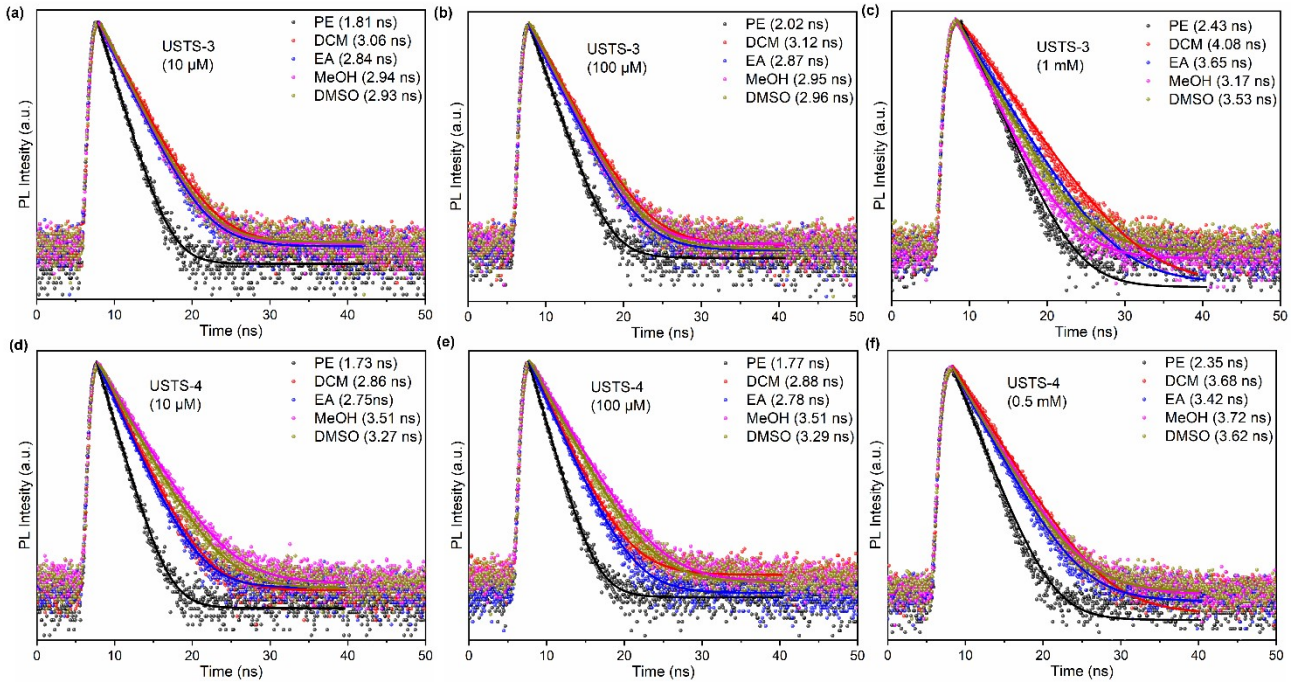

Fig. S7 PL lifetime of USTS-3 (a, c, e) and USTS-4 (b, d, f) in different solvents with a concentration of 10 μM, 100 μM and 1/0.5 mM measured under 365 nm wavelength excitation.

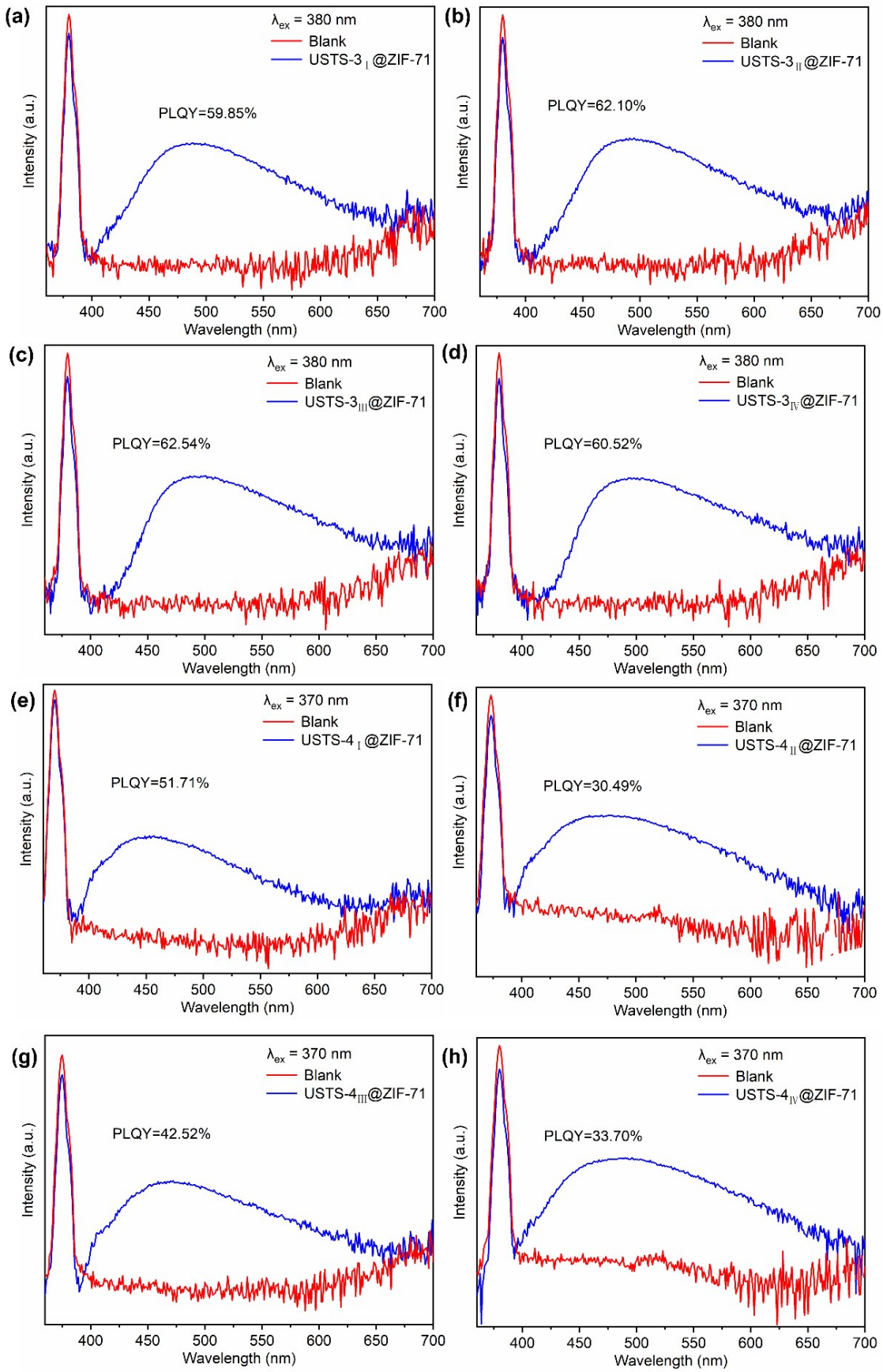

Fig. S8 Photoluminescence quantum yields of USTS-3@ZIF-71 (a-d) and USTS-4@ZIF-71 (e-h).

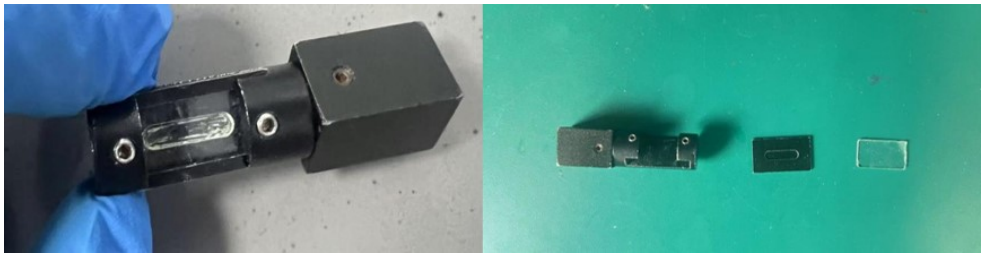

Fig. S9 Fixture for micro-powder fluorescence testing.

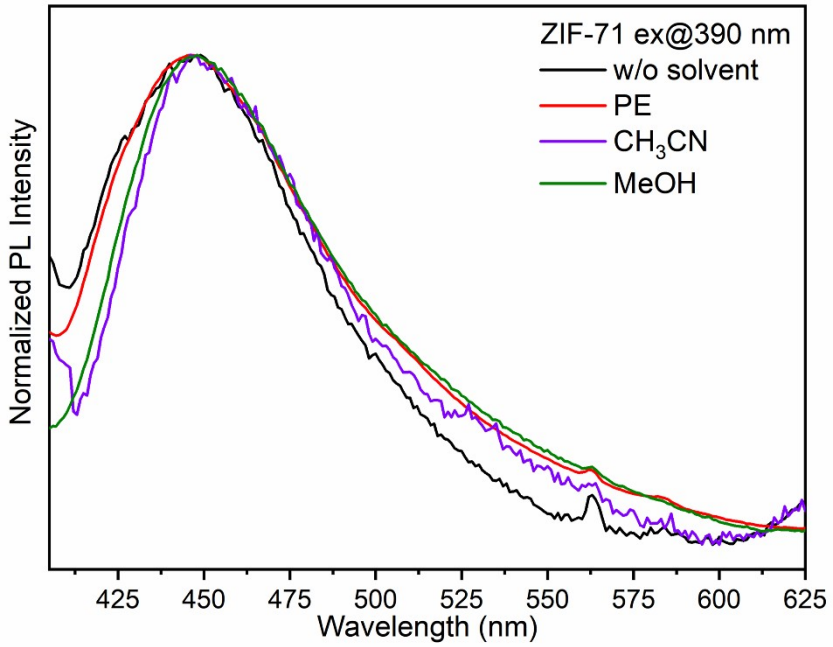

Fig. S10 Solvent polarity-dependent PL spectra of ZIF-71 in various solvents.

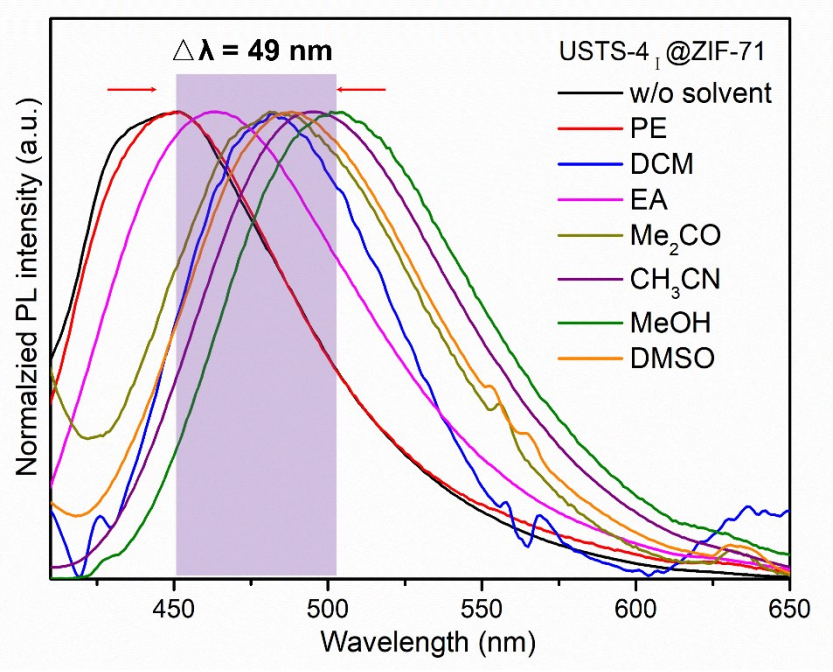

Fig. S11 Solvent polarity-dependent PL spectra of USTS-4$_I$@ZIF-71 in various solvents.

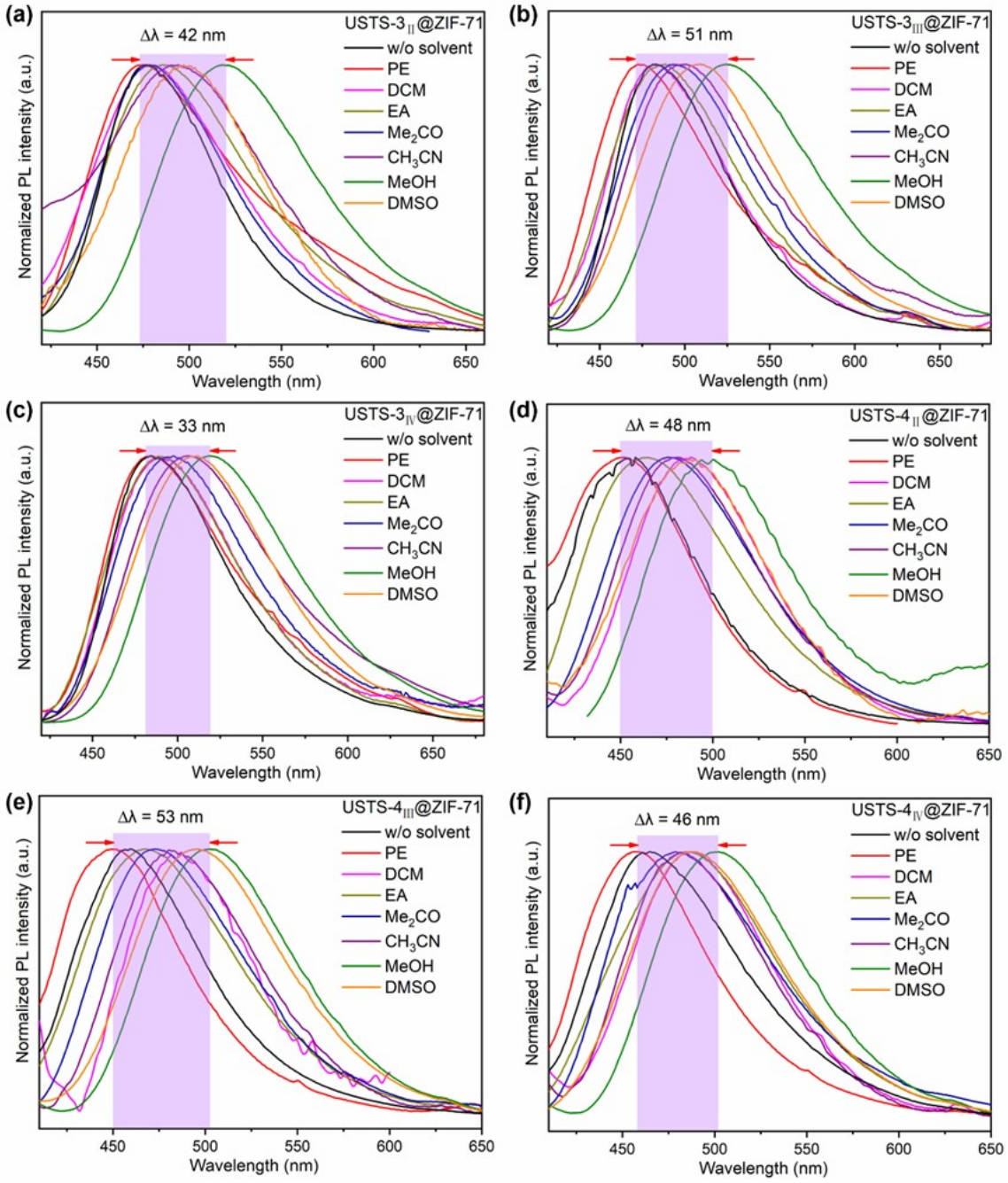

Fig. S12 Solvent polarity-dependent fluorescence spectra of USTS-3_{II-IV}@ZIF-71(a-c) and USTS-4_{II-IV}@ZIF-71 (d-f) in various solvents.

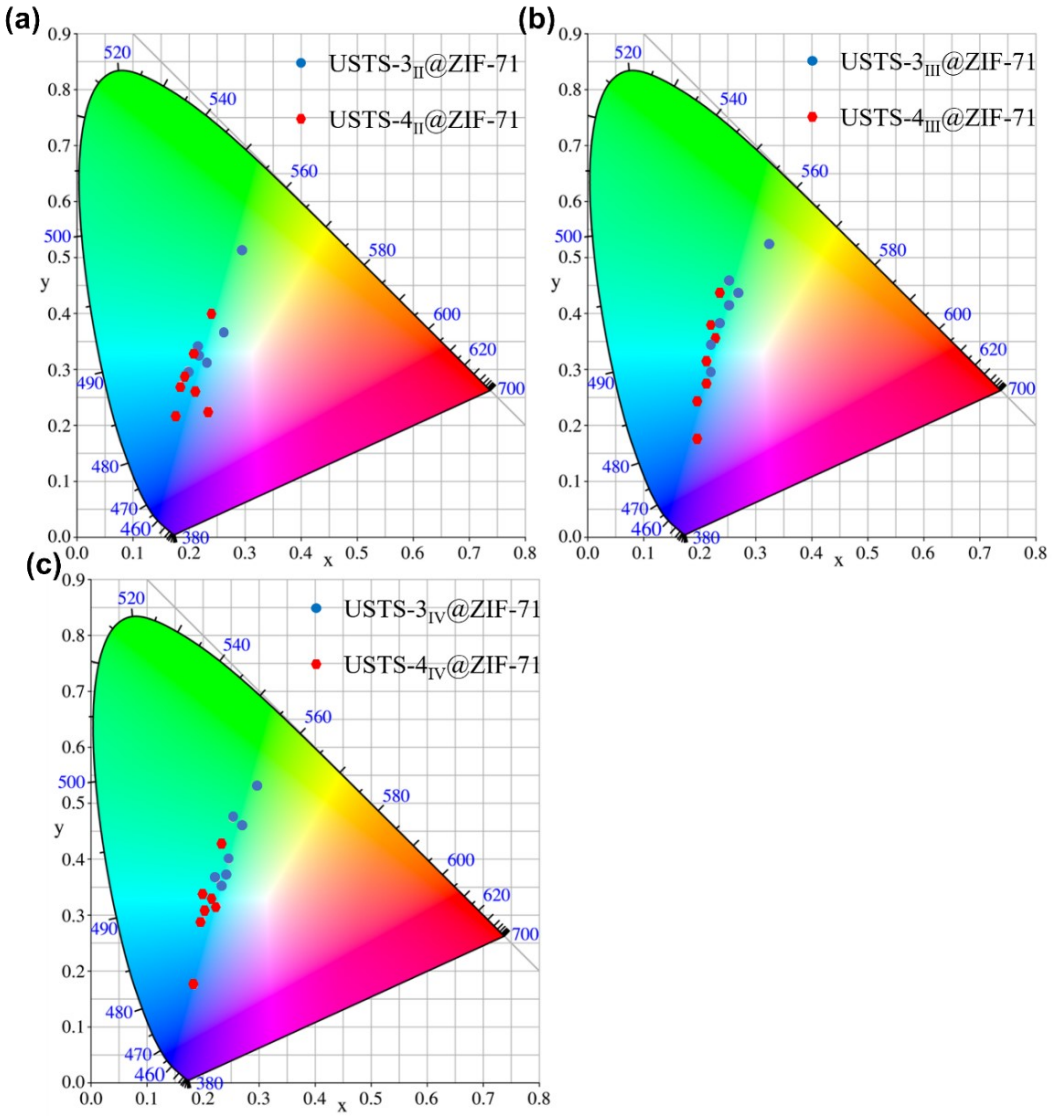

Fig. S13 CIE chromaticity coordinates of USTS-3_{II}/USTS-4_{II}@ZIF-71 (a), USTS-3_{III}/USTS-4_{III}@ZIF-71 (b), and USTS-3_{IV}/USTS-4_{IV}@ZIF-71 (c), which were calculated from the photoluminescence (PL) spectra of samples treated with different solvents, respectively.

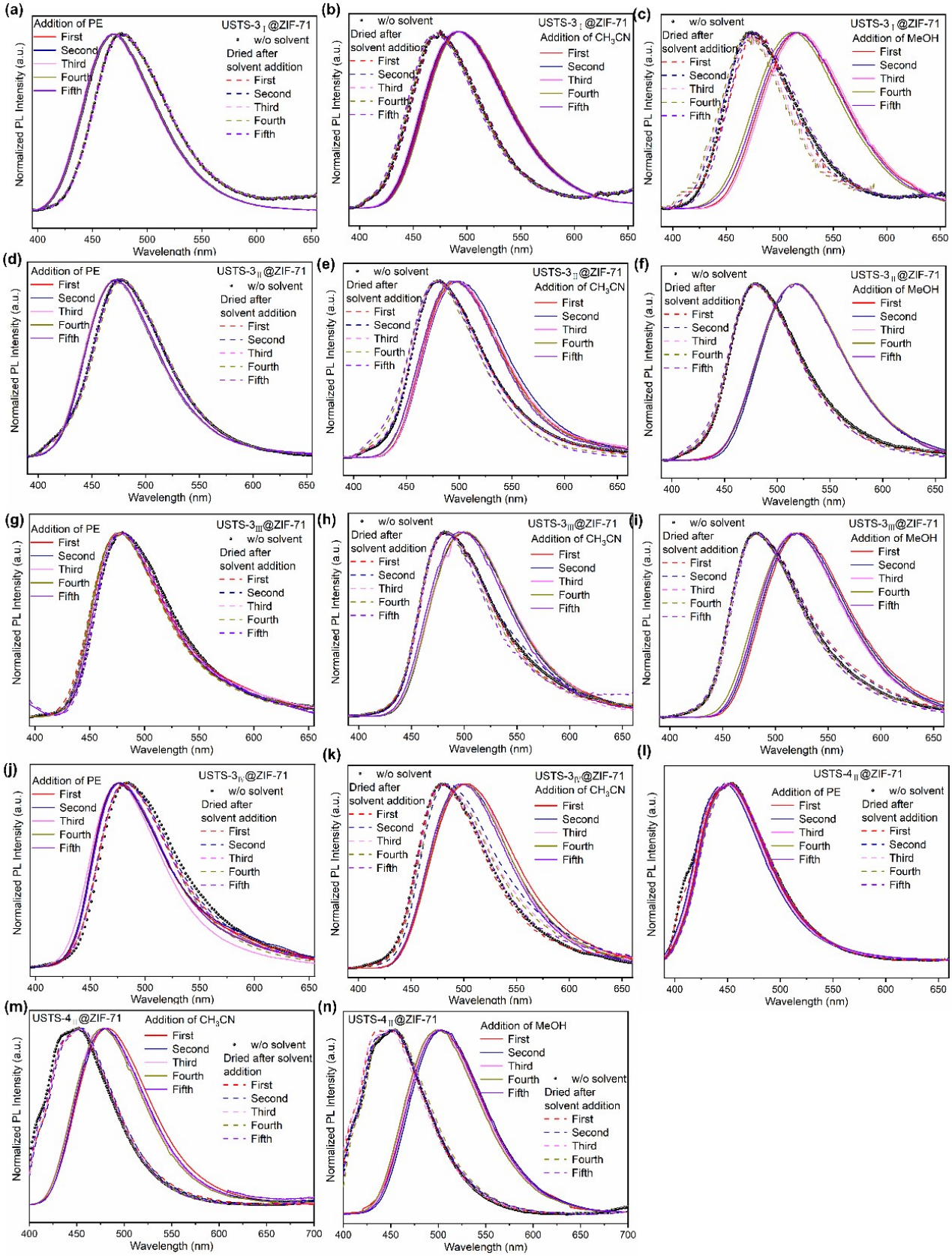

Fig. S14 Fluorescence switching of USTS-$3_{I\text{-}IV}$@ZIF-71 (a-k) and USTS-4_{II}@ZIF-71 (l-n) upon different solvents absorption and desorption (ex@375 nm).

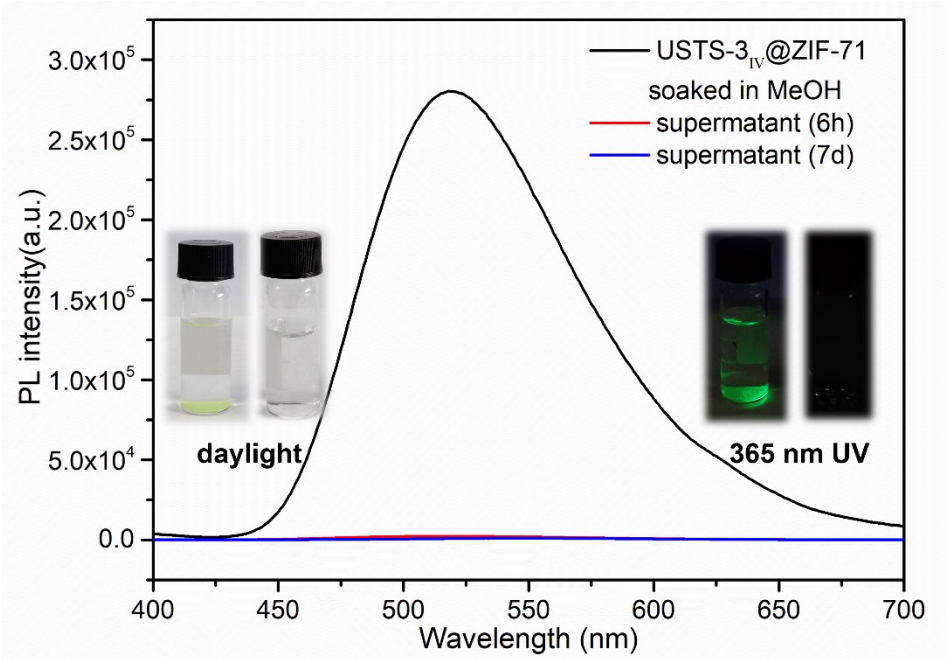

Fig. S15 FL spectra of USTS-3_{IV}@ZIF-71 soaked in MeOH and the corresponding supernatant after 7 days (inset: photographs of MeOH-soaked USTS-3_{IV}@ZIF-71 under daylight and 365 nm UV light).

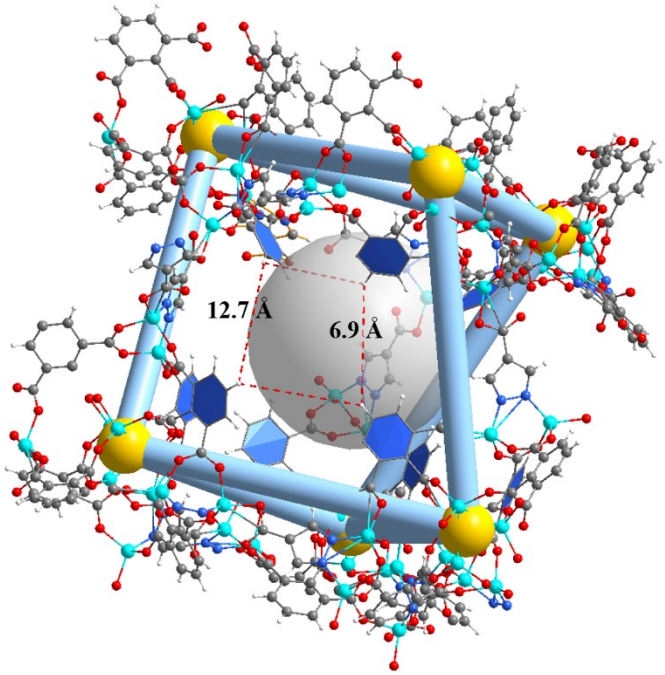

Fig. S16 Single crystal structure of NKU-110 with dangling ligands in the inner cage.

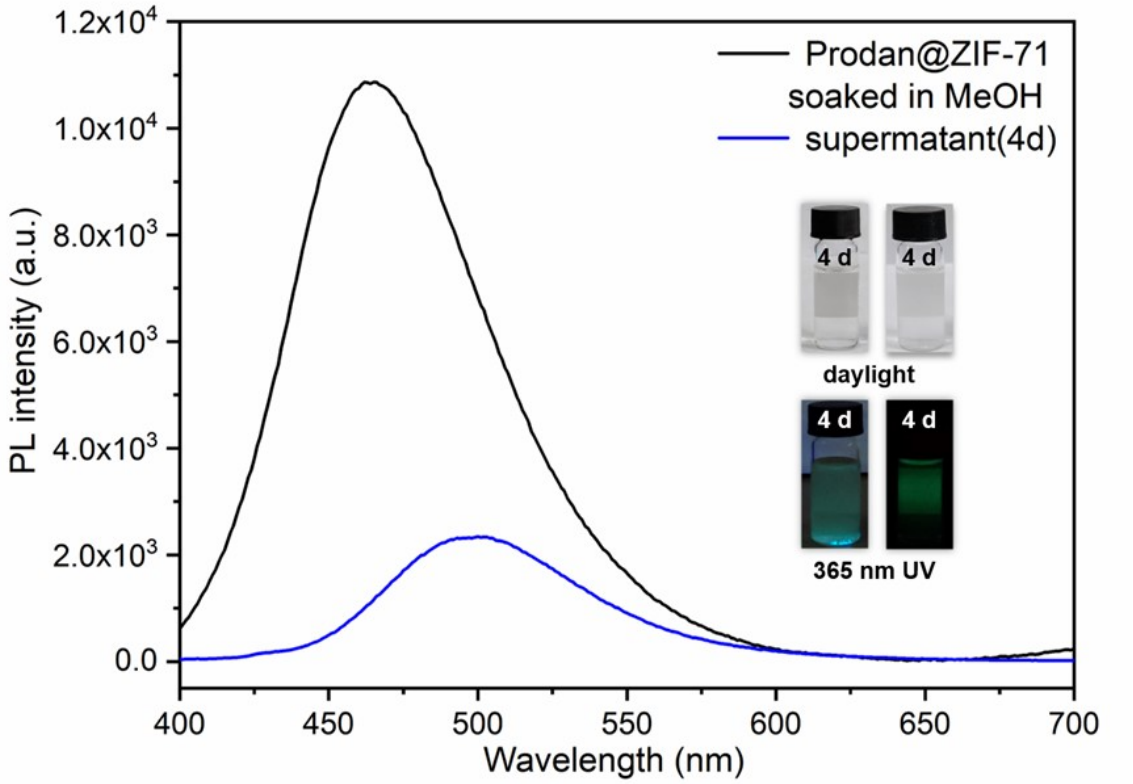

Fig. S17 FL spectra of Prodan@ZIF-71 soaked in MeOH and supernatant after 4 days (inset: photographs of MeOH-soaked Prodan@ZIF-71 under daylight and 365 nm UV light).

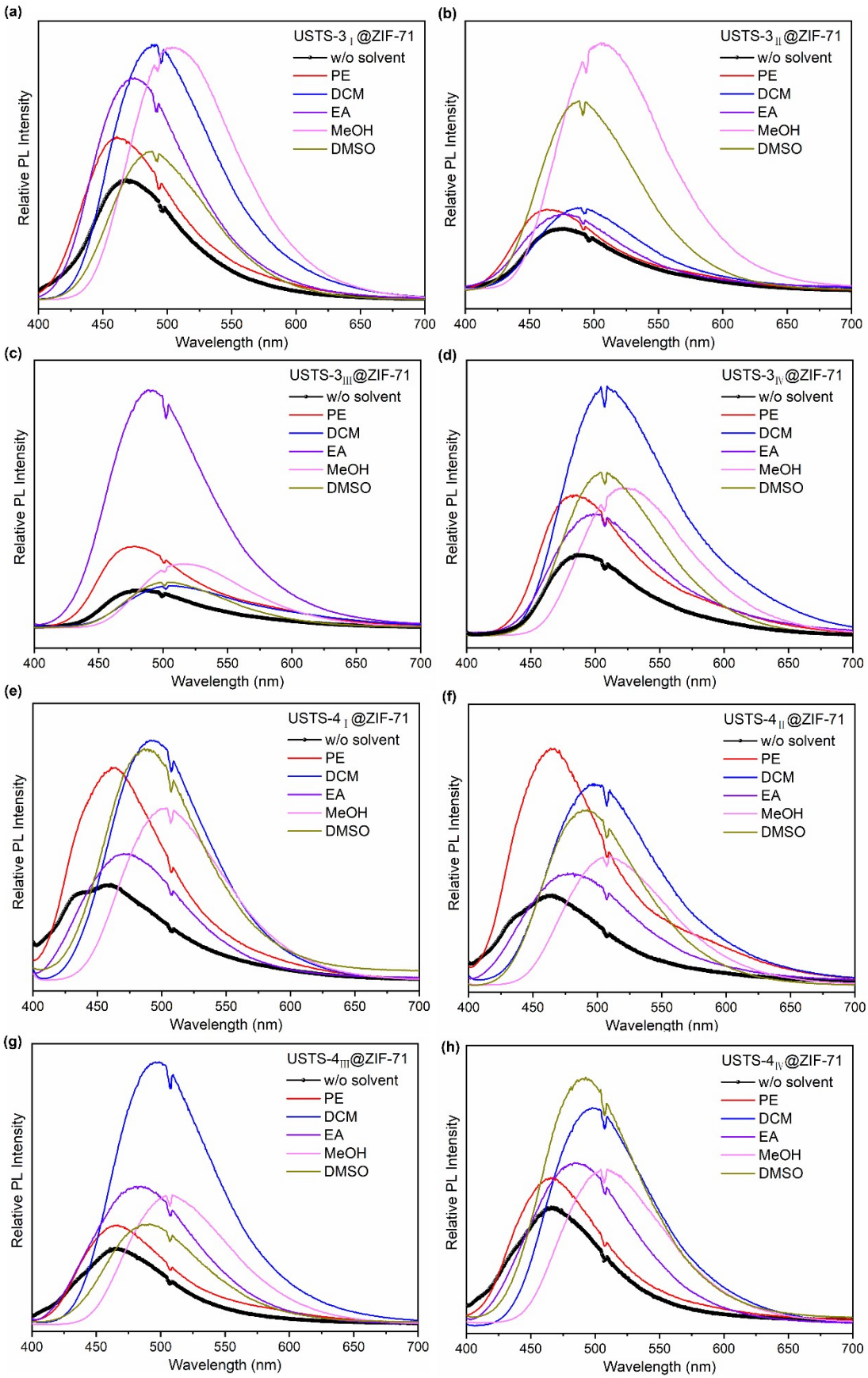

Fig. S18 Normalized PL spectra of USTS-3/4$_n$@ZIF-71 upon solvent treatment, where the PL intensity of the sample without solvent is defined as 1 for each case.

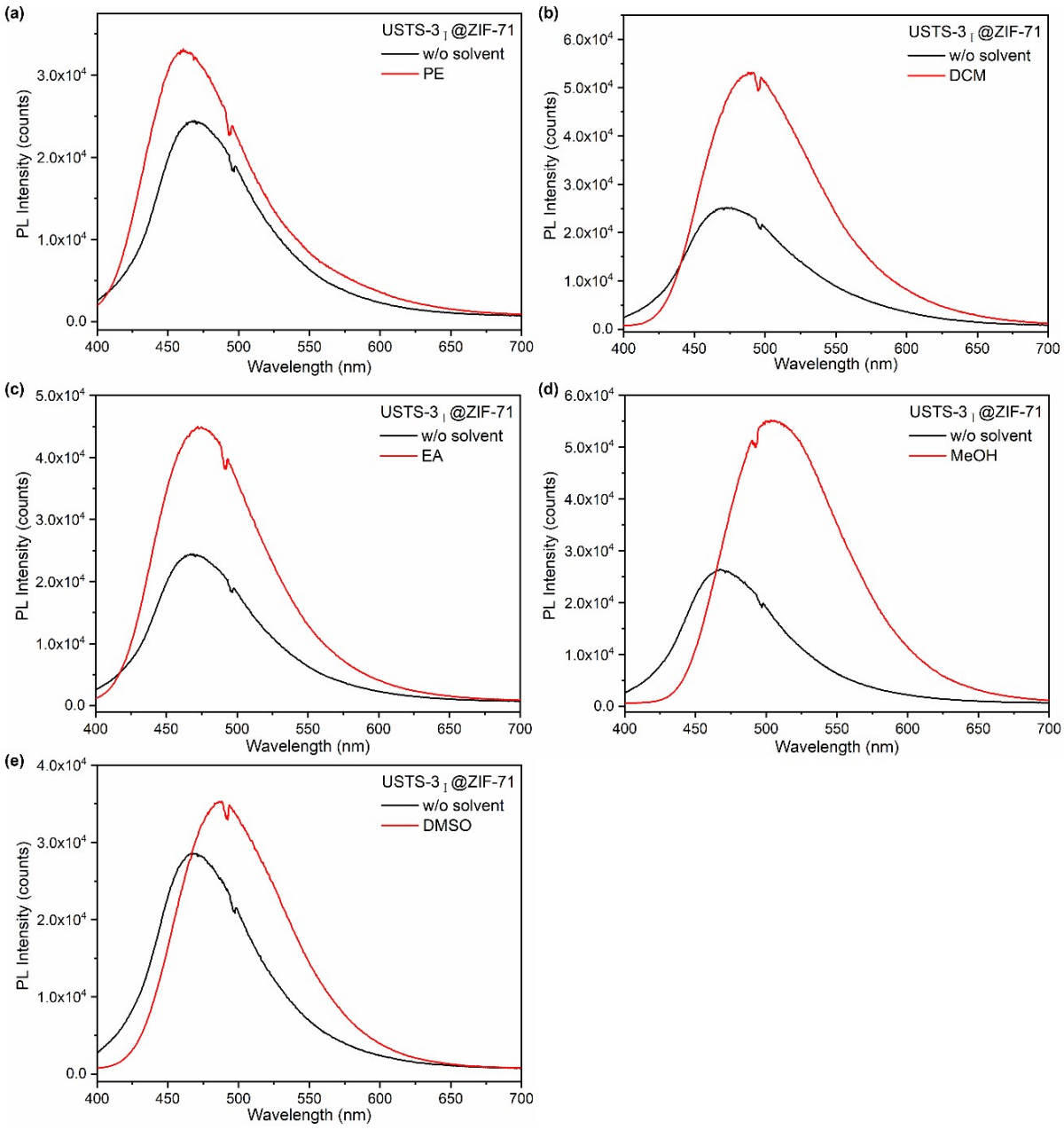

Fig. S19 PL spectra of USTS-3$_I$@ZIF-71 before and after exposure to different polar solvents: (a) PE, (b) DCM, (c) EA, (d) MeOH, and (e) DMSO.

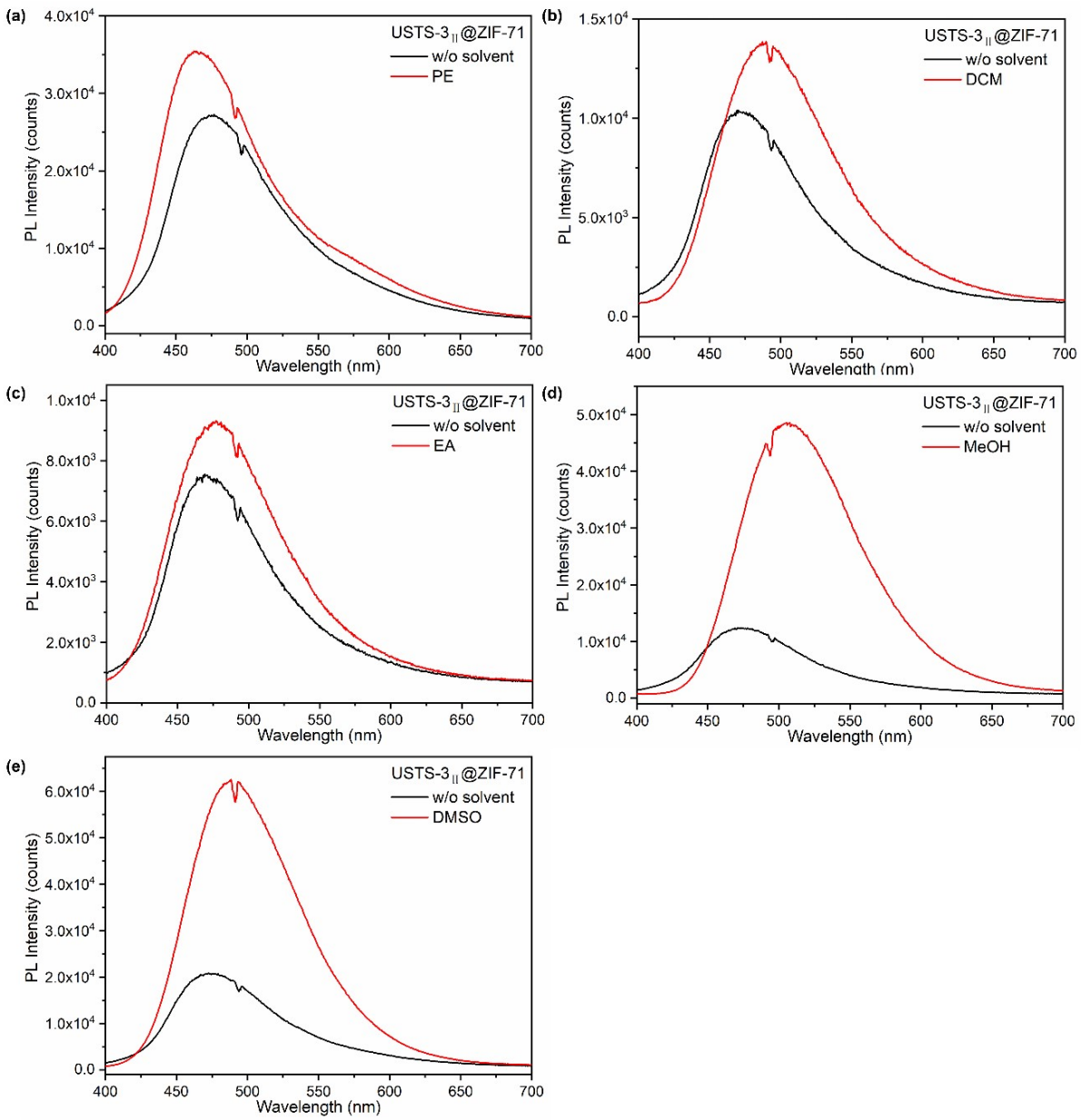

Fig. S20 PL spectra of USTS-3_{II}@ZIF-71 before and after exposure to different polar solvents: (a) PE, (b) DCM, (c) EA, (d) MeOH, and (e) DMSO.

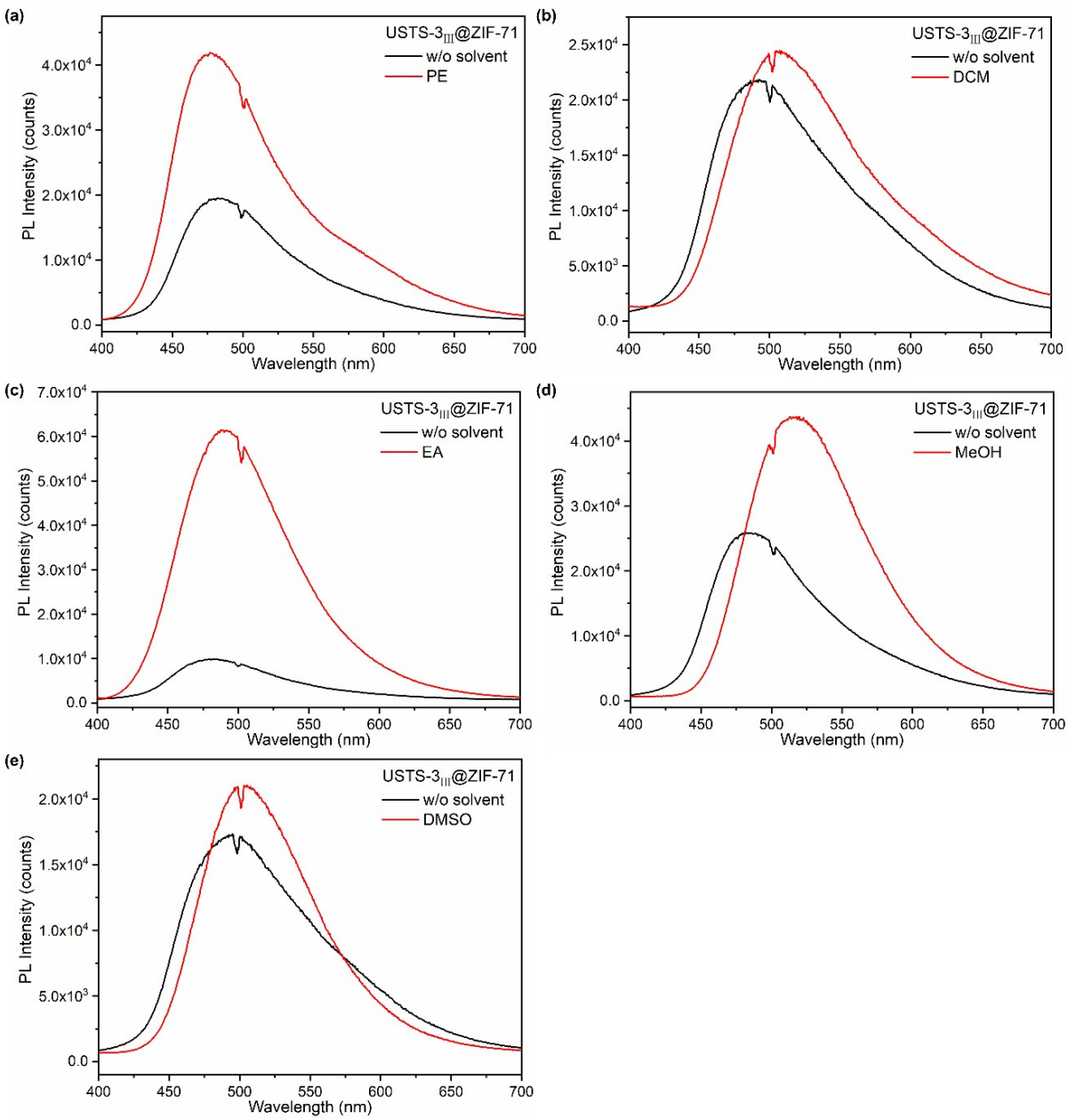

Fig. S21 PL spectra of USTS-3_{III}@ZIF-71 before and after exposure to different polar solvents: (a) PE, (b) DCM, (c) EA, (d) MeOH, and (e) DMSO.

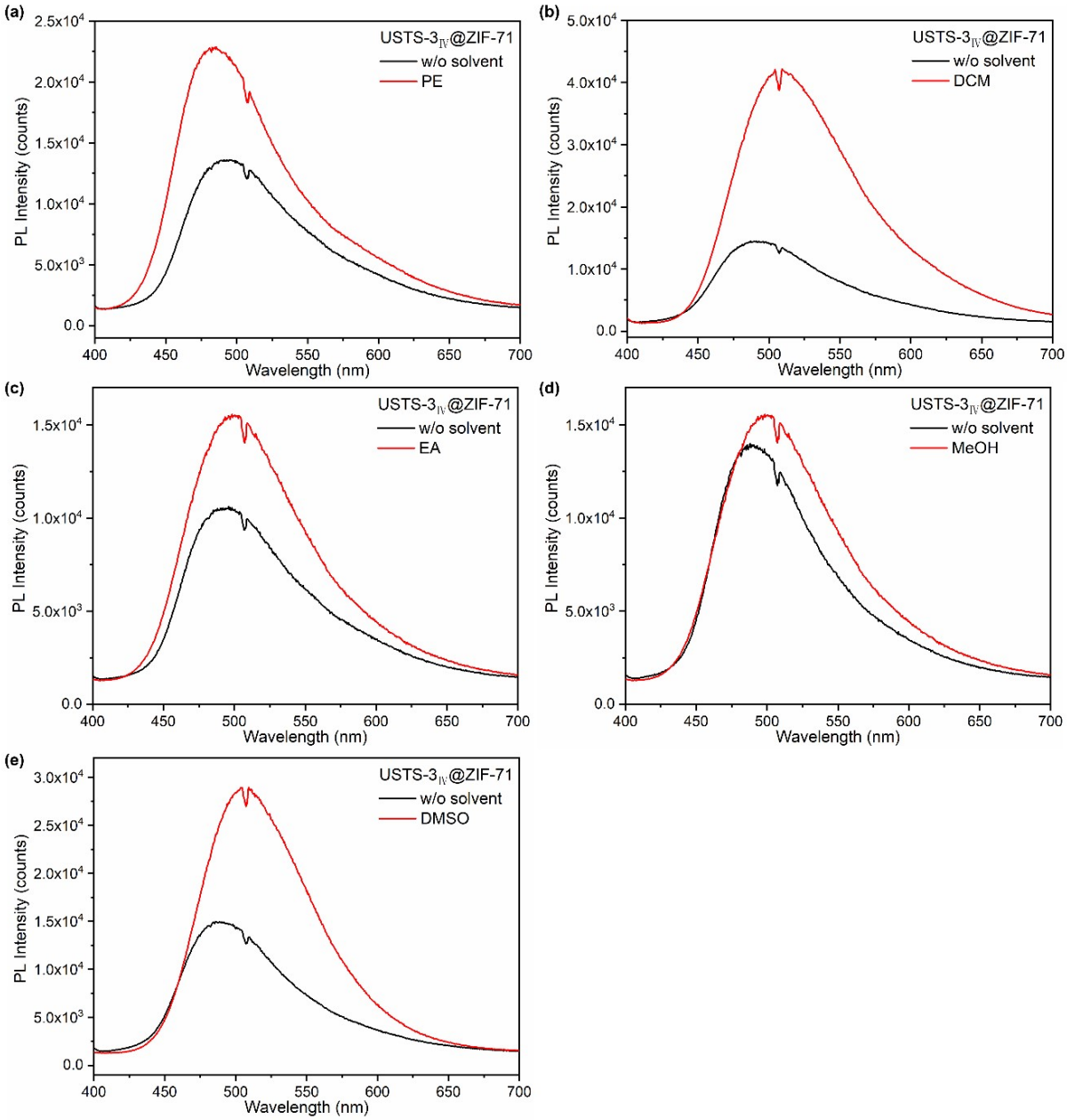

Fig. S22 PL spectra of USTS-3_{IV}@ZIF-71 before and after exposure to different polar solvents: (a) PE, (b) DCM, (c) EA, (d) MeOH, and (e) DMSO.

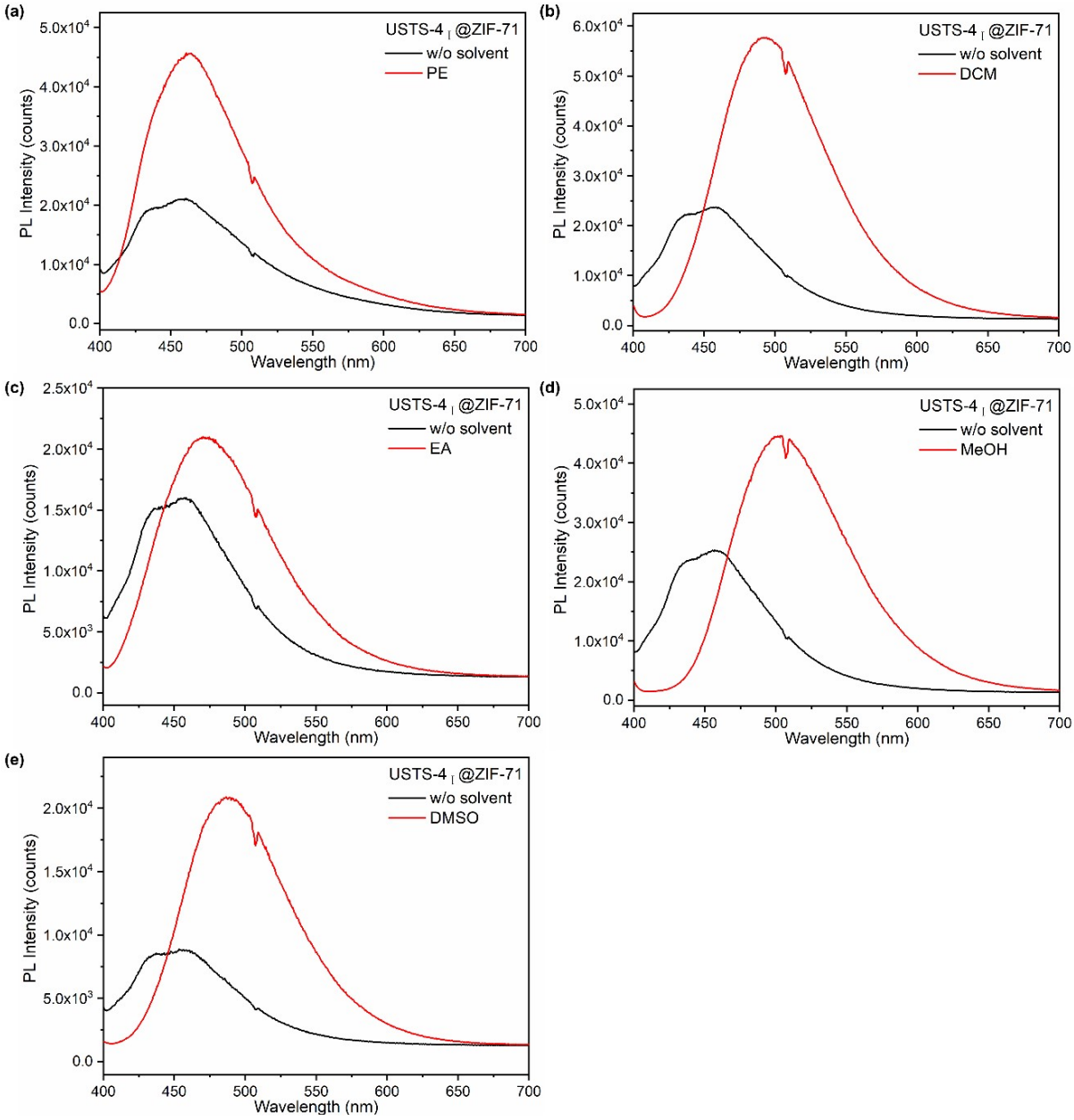

Fig. S23 PL spectra of USTS-4$_I$@ZIF-71 before and after exposure to different polar solvents: (a) PE, (b) DCM, (c) EA, (d) MeOH, and (e) DMSO.

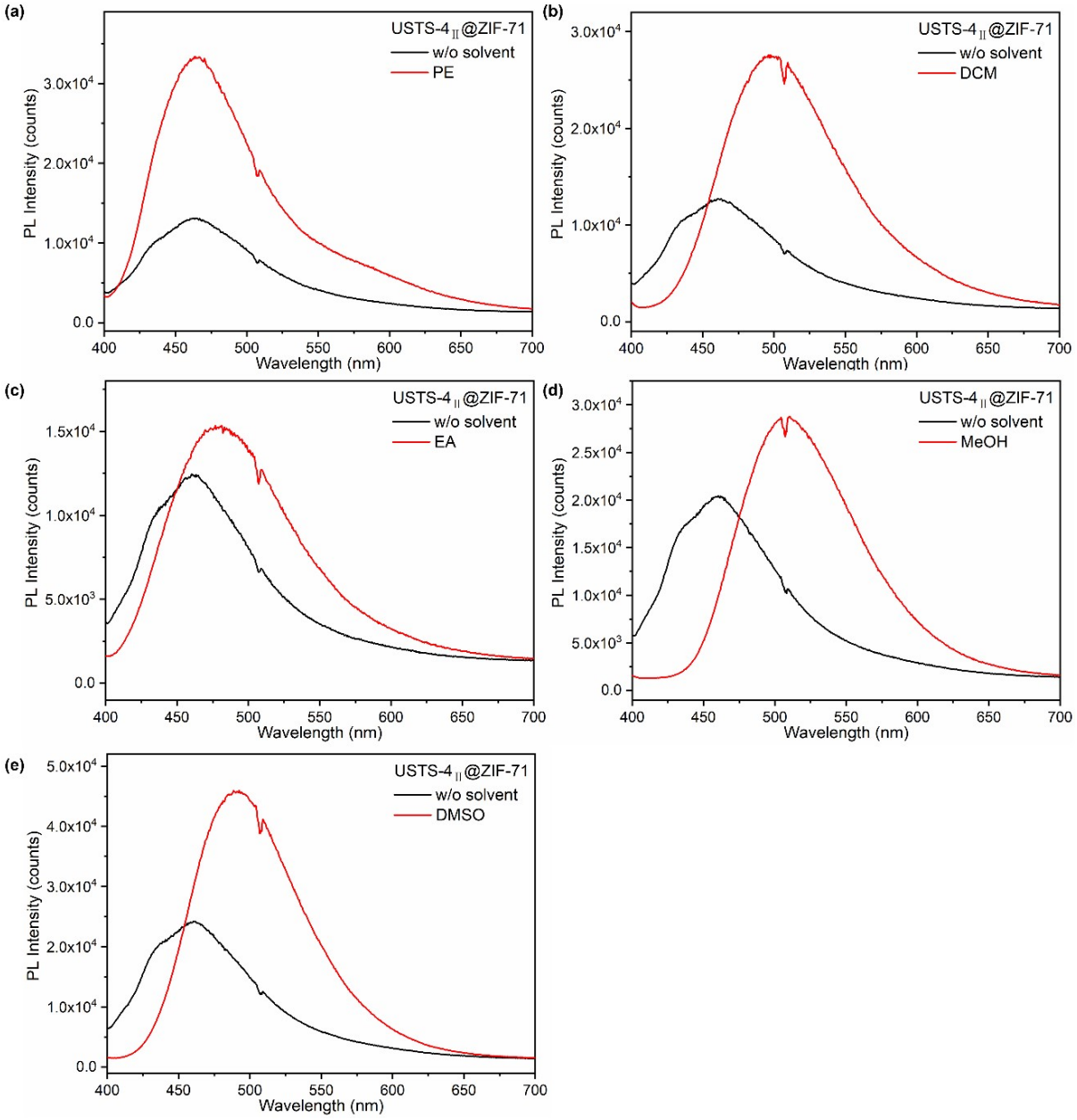

Fig. S24 PL spectra of USTS-4_{II}@ZIF-71 before and after exposure to different polar solvents: (a) PE, (b) DCM, (c) EA, (d) MeOH, and (e) DMSO.

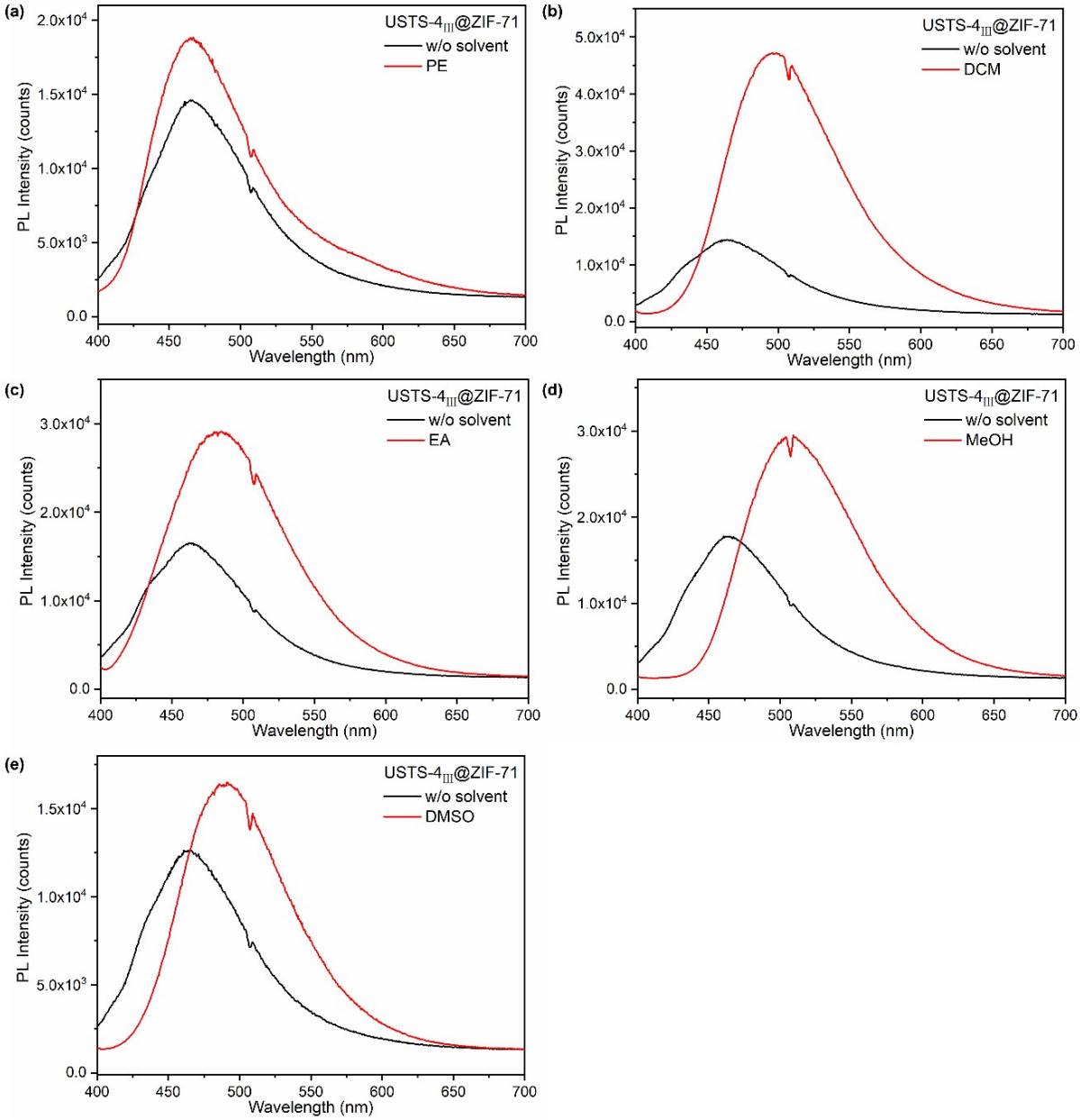

Fig. S25 PL spectra of USTS-4_{III}@ZIF-71 before and after exposure to different polar solvents: (a) PE, (b) DCM, (c) EA, (d) MeOH, and (e) DMSO.

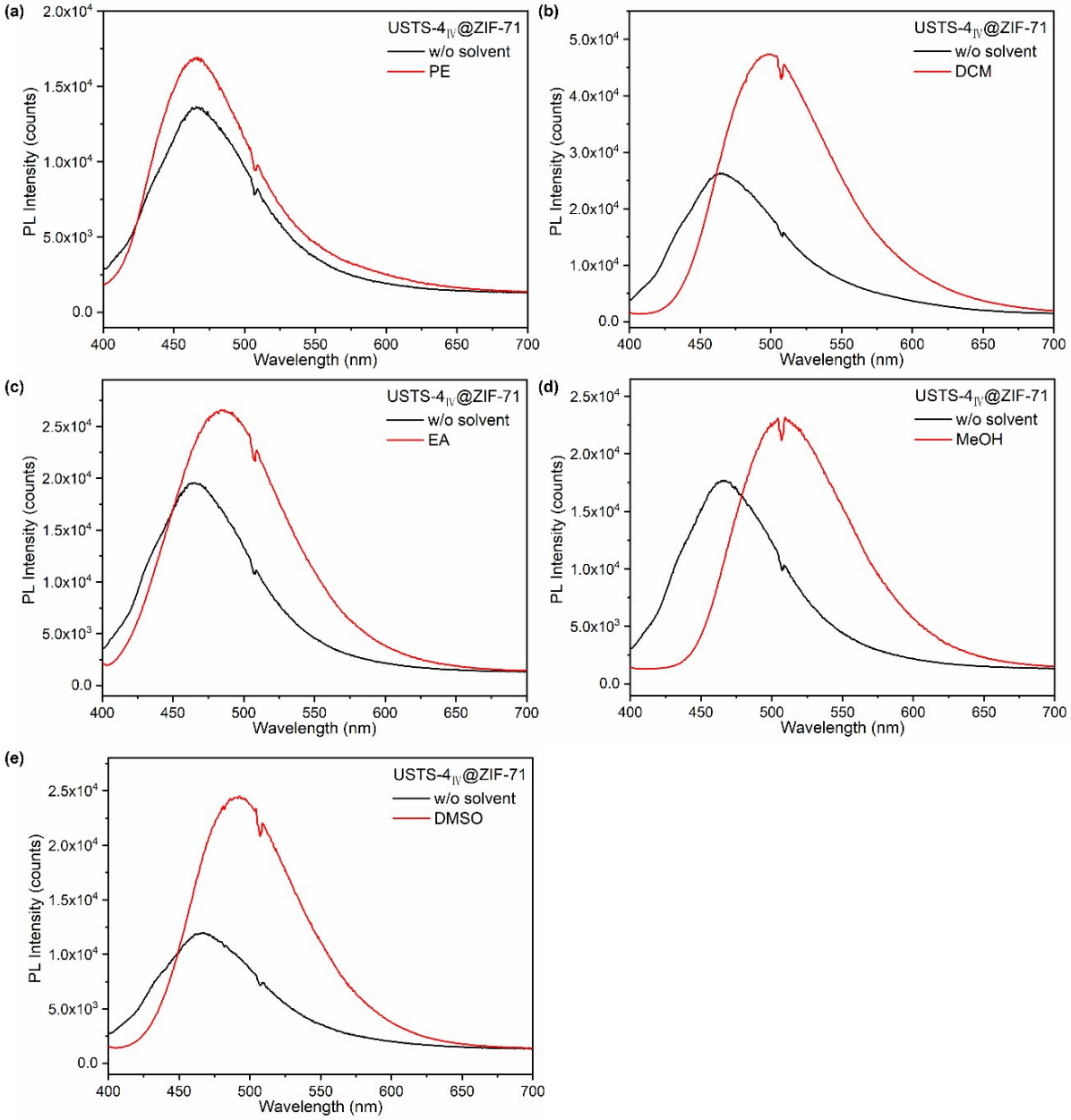

Fig. S26 PL spectra of USTS-4_{IV}@ZIF-71 before and after exposure to different polar solvents: (a) PE, (b) DCM, (c) EA, (d) MeOH, and (e) DMSO.

Table S1 Solid-state PLE, PL lifetime and PLQY of USTS-3/4@ZIF-71 with different USTS-3/4 concentrations**.**

	USTS-3				USTS-4			
	λ_{ex} [a] nm	λ_{em} nm	Φ_{PL} [b] %	τ ns	λ_{ex} [a] nm	λ_{em} nm	Φ_{PL} [b] %	τ ns
I	377	472	59.85	1.42	371	452	51.71	1.01
II	378	475	62.10	1.52	373	454	30.49	1.07
III	380	482	62.54	1.60	375	461	42.52	1.13
IV	381	486	60.52	1.63	380	464	33.70	1.17
solid	380	505	12.50	0.15	380	477	35.61	0.75

[a] Solid-state PLE of USTS-3/4@ZIF-71 with different USTS-3/4 concentrations.

[b] PLQY of USTS-3_n/4_n@ZIF-71.

Table S2 PL lifetime of USTS-3 and USTS-4 in different solvents with concentrations of 10 μM, 100 μM and 1/0.5 mM measured under 365 nm wavelength excitaion.

	USTS-3			USTS-4		
	10 μM	100 μM	1 mM	10 μM	100 μM	0.5 mM
	τ ns	τ ns	τ ns	τ ns	τ ns	τ ns
PE	1.81	2.02	2.43	1.73	1.77	2.35
DCM	3.06	3.12	4.08	2.86	2.88	3.68
EA	2.84	2.87	3.65	2.75	2.78	3.42
MeOH	2.94	2.95	3.17	3.51	3.51	3.72
DMSO	2.93	2.96	3.53	3.27	3.29	3.62

Table S3 Photophysical data of solid-state USTS-3/4 and USTS-3_{I-IV}/USTS-4_{I-IV}@ZIF-71 with adding various solvents (30 μL).

	USTS-3/4		**USTS-3_n/USTS-4_n@ZIF-71**							
	in solvents		n = I		n = II		n = III		n = IV	
	λ_{ex} nm	λ_{em} nm	λ_{ex} nm	λ_{em} nm	λ_{ex} nm	λ_{em} nm	λ_{ex} nm	λ_{em} nm	λ_{ex} nm	λ_{em} nm
PE	381/377	455/446	380/374	466/452	378/363	476/452	381/369	473/449	380/371	485/456
DCM	383/381	520/506	383/380	493/482	381/381	478/488	380/382	481/487	380/382	489/487
EA	381/377	507/500	380/374	482/464	382/374	486/465	380/372	489/468	380/377	489/484
Me_2CO	381/378	527/520	380/380	491/481	375/377	479/475	377/340	493/473	380/347	498/479
CH_3CN	381/378	540/529	380/380	497/495	380/377	494/481	380/375	501/480	377/378	506/482
MeOH	383/381	560/550	380/383	517/501	381/381	518/500	381/381	524/502	380/380	518/502
DMSO	383/381	553/544	383/377	506/488	380/380	497/491	377/377	509/496	380/377	512/488
Δλ (nm)	105/104 nm		51/49 nm		42/48 nm		51/53 nm		33/46 nm	

Table S4 Photophysical data of solid-state PL of Prodan@ZIF-71 and USTS-3_I@NKU-110 with adding various solvents (30 μL).

	Prodan@ZIF-71		USTS-3_I@NKU-110	
	λ_{ex} nm	λ_{em} nm	λ_{ex} nm	λ_{em} nm
w/o solvent	383	440	385	476
PE	377	443	383	475
CH_3CN	377	447	385	475
MeOH	377	465	385	475