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Enhanced Luminescence in Multivariate Metal-Organic Frameworks through Isolated-Ligand Strategy

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1. Figure.

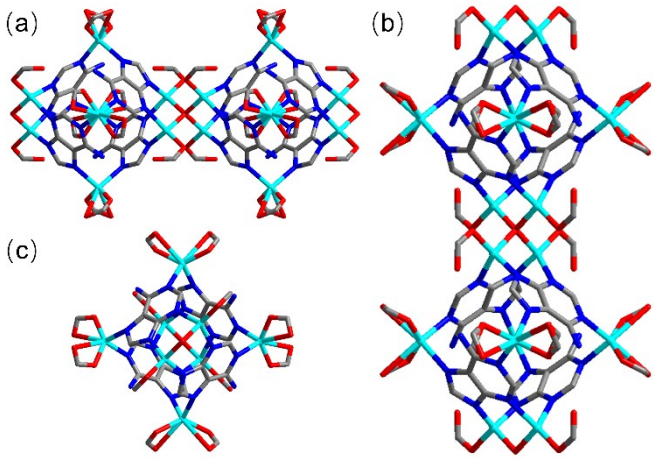

Figure S1. The SBUs of ZJU-235 viewed along the (a) *a* direction, (b) *b* direction and (c) *c* direction. Light blue, dark blue, red, and gray represent Zn, N, O and C atoms, respectively.

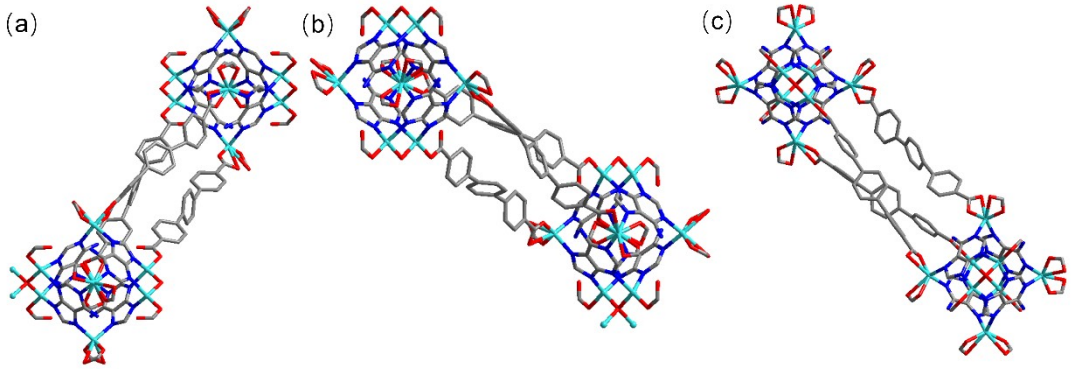

Figure S2. The connection characteristics of organic ligands and the SBUs in ZJU-235 viewed along the (a) a direction, (b) b direction and (c) c direction. Light blue, dark blue, red, and gray represent Zn, N, O and C atoms, respectively.

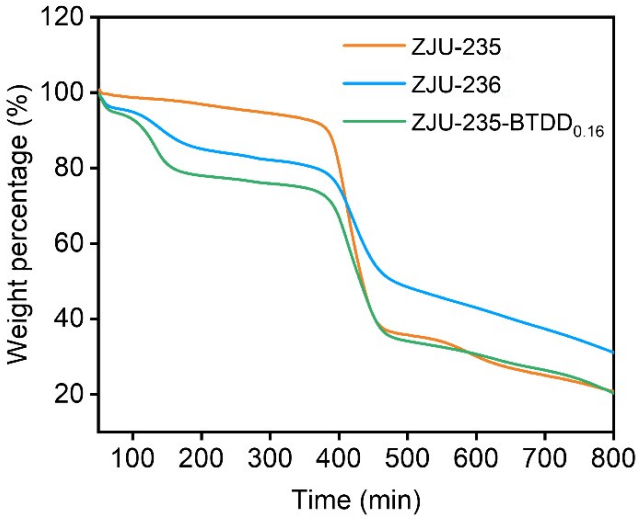

Figure S3. TGA of ZJU-235, ZJU-236 and ZJU-235-$BTDD_{0.16}$.

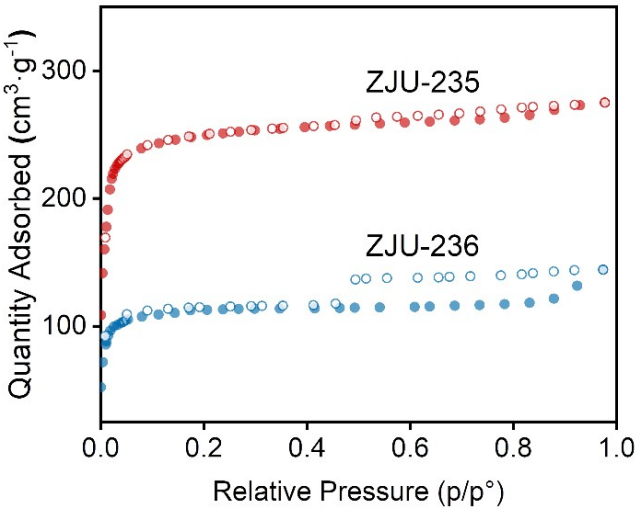

Figure S4. N_2 adsorption (filled) and desorption (empty) isotherms (77 K) for ZJU-235 and ZJU-236.

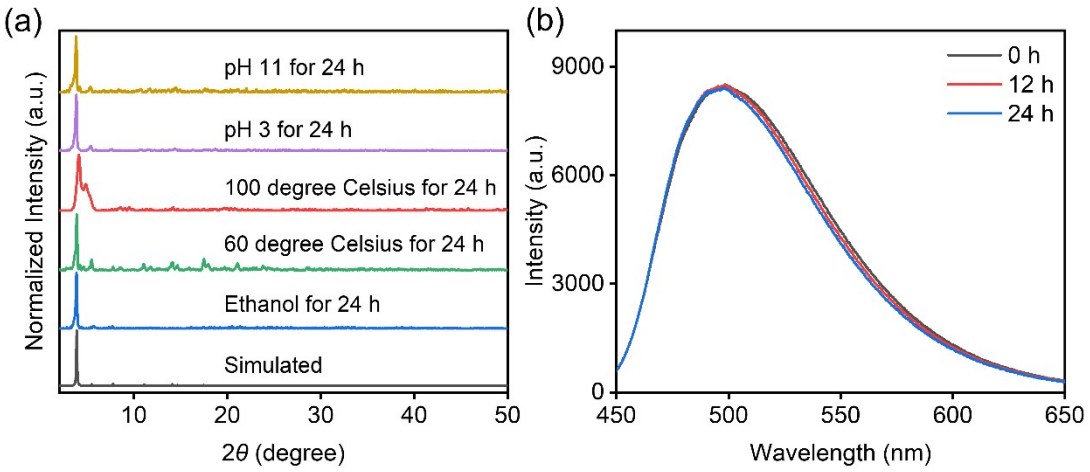

Figure S5. (a) PXRD patterns of ZJU-235 after different treatment conditions. (b) PL spectra of ZJU-235-BTDD$_{0.02}$ after being placed in the air for 0, 12 or 24 hours at room temperature.

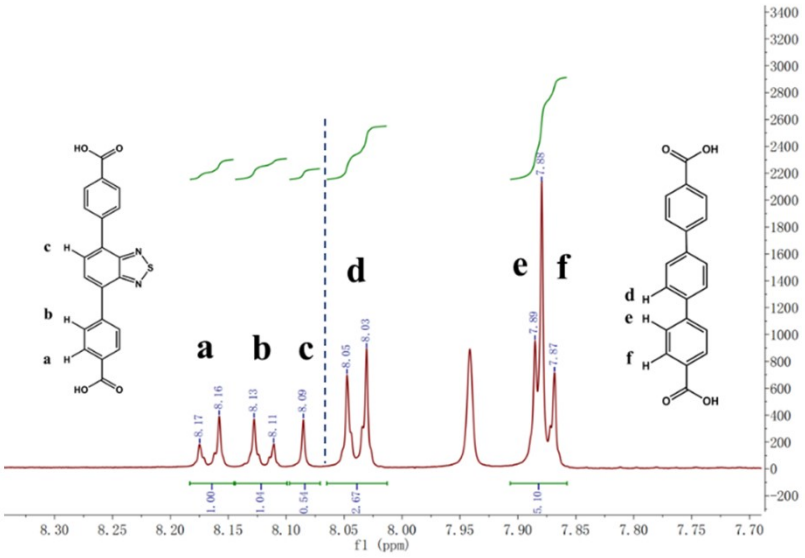

Figure S6. ^{1}H NMR of digested ZJU-235-BTDD with HNO_3 in DMSO-d_6.

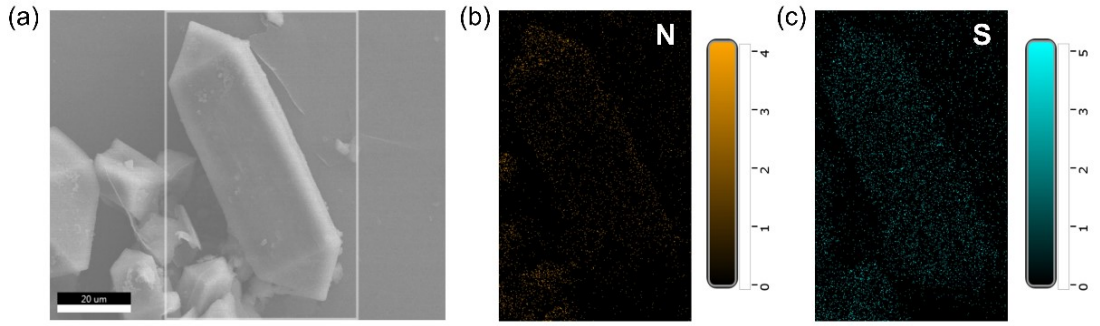

Figure S7. (a) SEM image and (b) N, (c) S element EDS mapping of ZJU-235-$BTDD_{0.16}$.

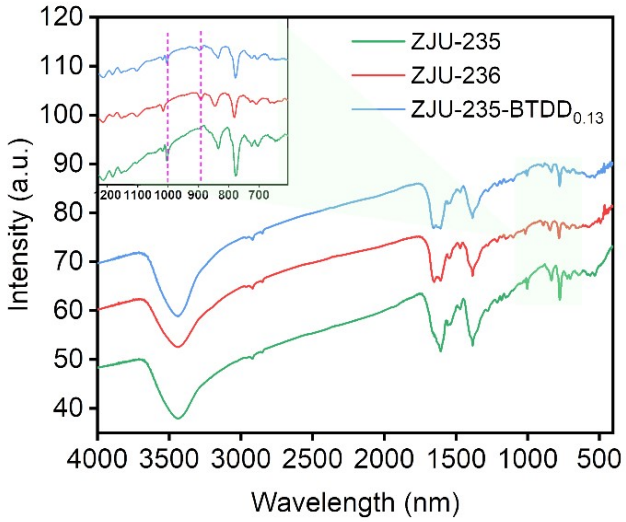

Figure S8. FT-IR spectra of ZJU-235, ZJU-236 and ZJU-235-$BTDD_{0.13}$.

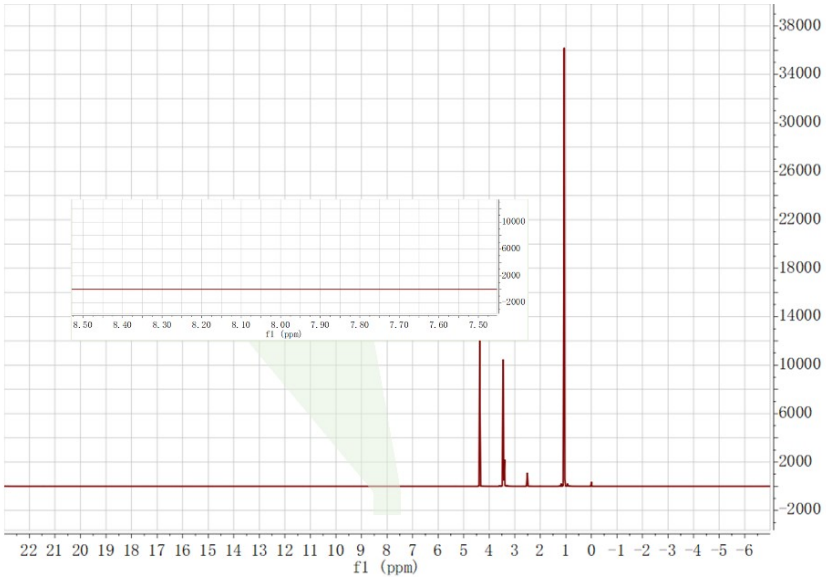

Figure S9. ^{1}H NMR spectra of the eluate for ZJU-235-BTDD$_{0.16}$ after washing with ethanol and deionized water three times.

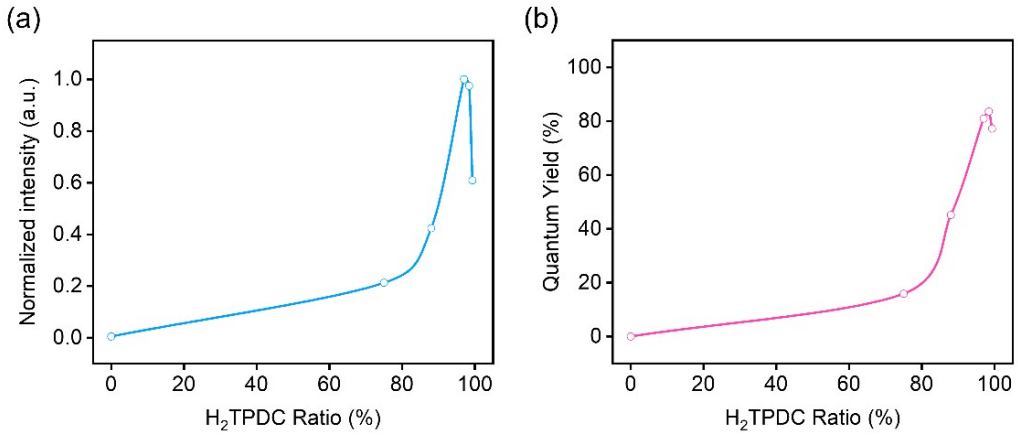

Figure S10. (a) Fluorescence intensity (excited at the optimum excitation wavelength, respectively) and (b) QY as a function of feeding ratio H_2BTDD.

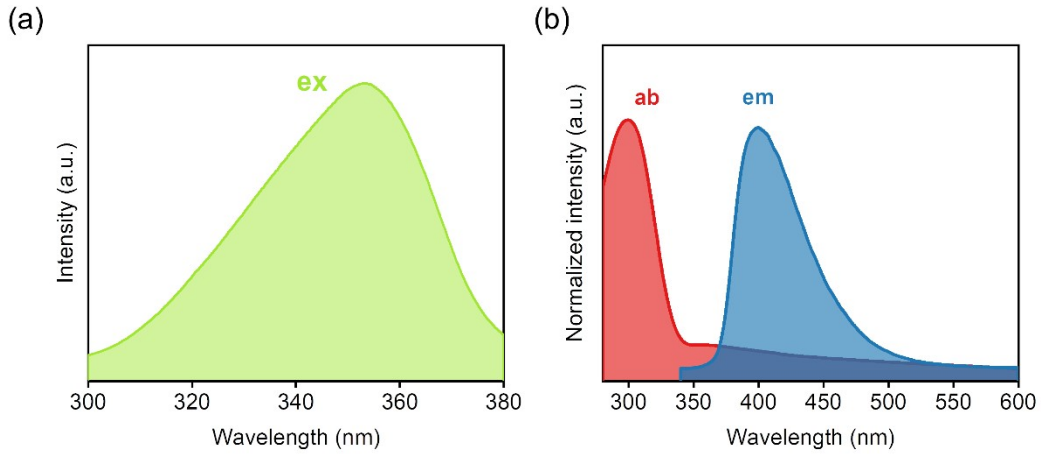

Figure S11. (a) Excitation spectra, (b) absorption spectra (1 mg in 1 mL DMF) and emission spectra of ZJU-235.

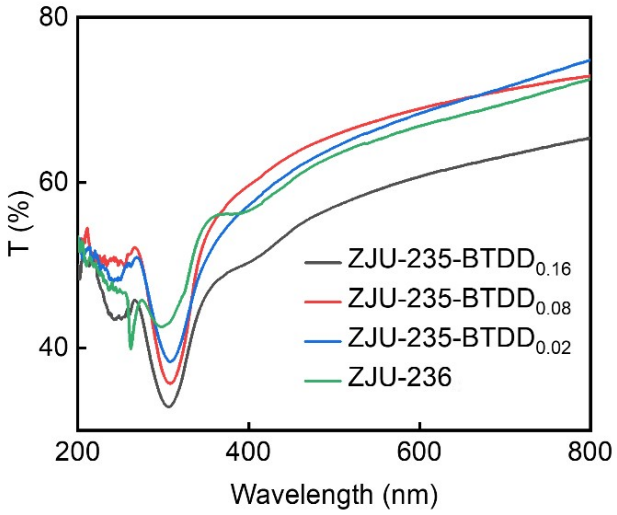

Figure S12. Absorption spectra (0.1 mg in 1 mL DMF) of ZJU-236 and ZJU-235-BTDD$_x$ (x = 0.02, 0.08, 0.16).

2. Table

Table S1. Crystallographic Data collection and Refinement result for ZJU-235.

	ZJU-235
CCDC No.	2089981
Chemical formula	$C_{100}H_{56}N_{20}O_{17}Zn_8$
Formula weight	2332.60
Temperature (K)	298(2)
Wavelength (Å)	1.54178
Crystal system	Tetragonal
Space group	*P*4/*nbm*
a (Å)	32.1500(6)
b (Å)	32.1500(6)
c (Å)	11.1411(3)
α (º)	90
β (º)	90
γ (º)	90
V (Å^3)	11515.7(5)
Z	2
Density (calculated g·cm^{-3})	0.673
Absorbance coefficient (mm^{-1})	1.181
F(000)	2344
R_{int}	0.1302
Goodness of fit on F^2	1.043
*R*1, *wR*2 (I>2σ(I))[a]	0.1275, 0.3184
*R*1, *wR*2 (all data)[a]	0.1609, 0.3351
Largest difference peak and hole (e/Å^3)	0.772, -0.635

a. $R1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}$; $wR2 = \sqrt{\frac{\sum w(|F_o|^2 - |F_c|^2)^2}{\sum w(F_o^2)^2}}$

Table S2. Element analysis results of ZJU-235.

Element	C	N	H
Mass fraction (%)	46.18	9.02	3.98

Table S3. QY results of H_2BTDD ligand.

State of matter	QY (%)	Scatter Range (nm)	Emission Range (nm)
Solid	2.00	392.5~407.5	447.0~650.0
Solution (5 μM in DMF)	7.46	374.5~386.0	386.5~650.0

Table S4. The original molar ratio and the actual molar ratio of H_2BTDD/H_2TPDC in ZJU-235-BTDD$_x$ confirmed by ^{1}H NMR.

Sample	The feeding ratio	The real molar ratio
ZJU-235-BTDD$_{0.02}$	0.03:0.97	0.02:0.98
ZJU-235-BTDD$_{0.08}$	0.12:0.88	0.08:0.92
ZJU-235-BTDD$_{0.16}$	0.25:0.75	0.16:0.84

Table S5. QY of ZJU-235 and ZJU-236.

Sample	QY
ZJU-235	32.17%
ZJU-236	~0.00%