SUPPORTING INFORMATION

Rational Design of a High-Efficiency, Multivariate Metal-Organic Framework Yellow Phosphor for White LED Bulbs

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S1. LMOF-305 single crystal data

Several crystals were tried, and the best crystal was used. The diffraction pattern showed twinning. Using Cell_now, two orientation matrices were determined. The data were integrated using the two matrices in SAINT. SAINT determined the transformation between the two cells to be -1 0 -1 0 -1 0 0 0 1. TWINABS was used to produce a merged HKLF4 file, for structure solution and initial refinement, and HKLF5 file for final structure refinement. The HKLF5 file contained the merged reflections first component and those that overlapped with this component, which were split into 2 reflections. TWINABS indicated the twin faction to be 50:50. The structure was solved using the HKLF4 file, however the best refinement was given by the HKLF4 file. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed geometrically, then constrained and refined using a riding model. One FLAT comment was used to keep F1' in the plane with is phenyl ring. Once the modelling of the framework was complete attempts were made to locate the solvent molecules (DMA) and water. However, no meaningful molecules could be found in the difference map, so SQUEEZE was used. SQUEEZE reported Solvent Accessible Volume of 6290 Å^3 and Electrons Found in S.A.V. to be 1245. As there is a mixture of solvents used, it was not possible to approximate the amount of solvent, and no solvent was included in the chemical formula.

Table S1. Single crystal data for LMOF-305 at 100 K

Compound	$Zn_2(tcbpe)_{0.8}(tcbpe\text{-}F)_{0.2}\cdot x$DMA (LMOF-305)
Formula	$C_{54}H_{31.02}O_8F_{0.8}Zn_2$
M	953.93
Crystal system	Monoclinic
Space group	C 2/c
a/Å	37.1066(17)
b/Å	31.733(15)
c/Å	11.8903(6)
α/°	90
β/°	99.208(2)
γ/°	90
V/Å^3	13533.1(11)
Z	8
Temperature (K)	100
λ(radiation wavelength) Å	0.7749
D, g/cm^3	0.936
Reflections collected	12941
R1[a] [I > 2σ(I)]	0.0807
wR2[b] [I > 2σ(I)]	0.2512
Goodness-of-fit	1.24
CCDC No.	1946919

[a] $R1 = \sum|F_o - F_c| / \sum|F_o|$

[b] $wR2 = \sum[w(F_o^2 - F_c^2)^2] / w(F_o^2)^2]^{1/2}$

S2. Steady state photoluminescence spectra

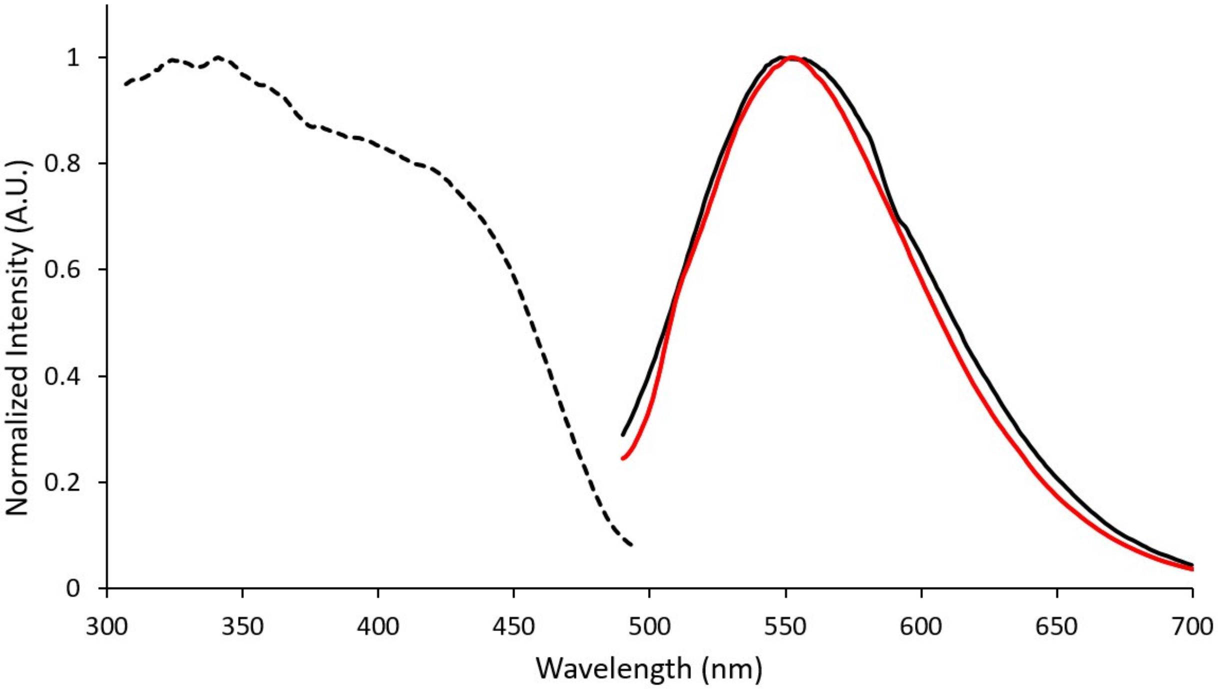

Figure S1. Excitation spectrum (dashed line) from LMOF-231 monitored at 550 nm, with emission spectra (solid line) from LMOF-231 under 365 nm (black) and 455 nm (red) emission.

S3. Stability under ambient conditions

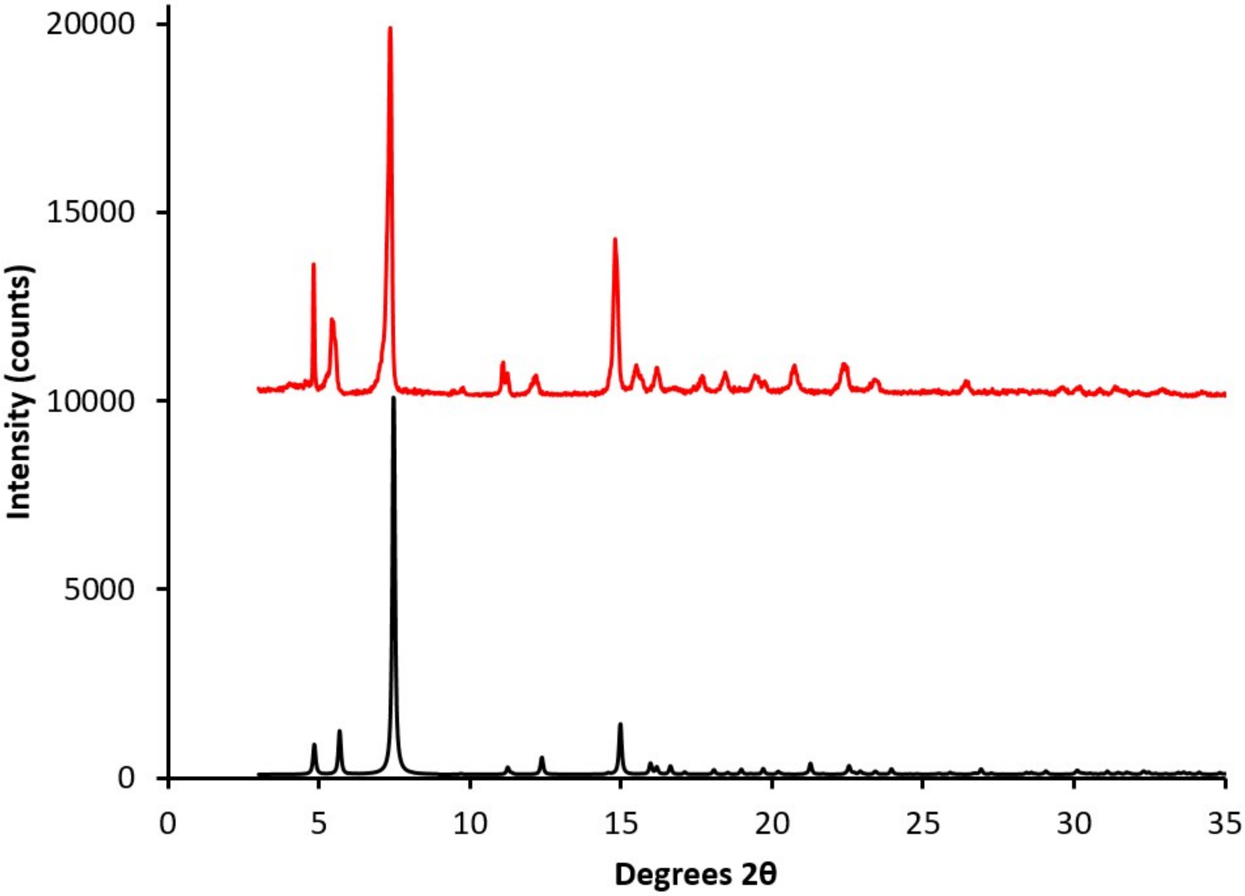

Figure S2. PXRD patterns of the simulated (black) LMOF-305 and experimental (red) sample sitting in air for two months under ambient conditions.

Table S2. Quantum yield of freshly prepared LMOF-305 and LMOF-305 after exposed to air for two months (under ambient conditions)

Sample	**Quantum Yield (455 nm ex.)**
LMOF-305, fresh	88%
LMOF-305, 2 month storage	83%

S4. Variable tcbpe-F LMOF qualification

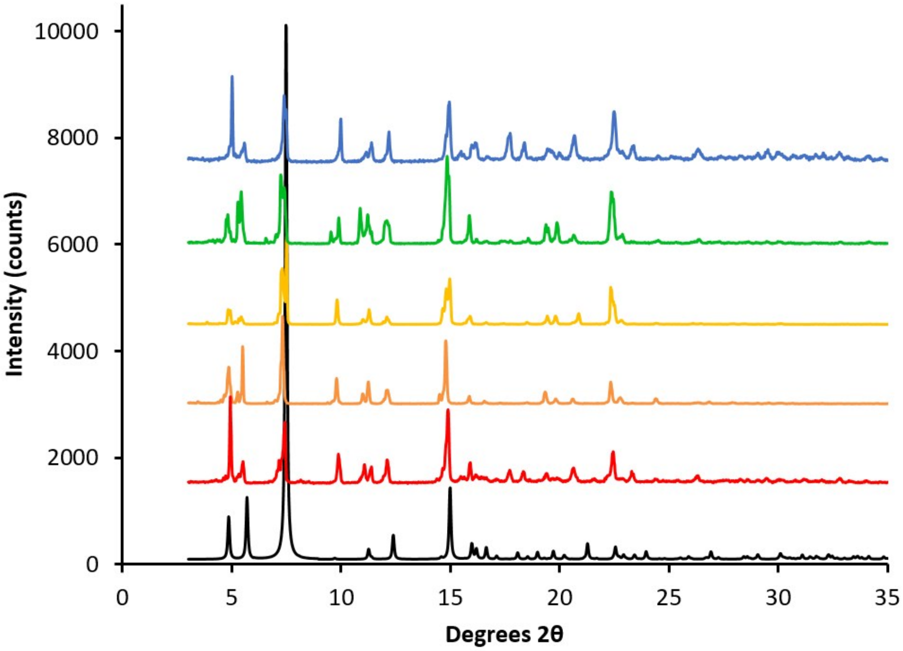

Figure S3. PXRD patterns of the LMOF samples with varying amounts of tcbpe-F overlaid on the simulated PXRD pattern of LMOF-305 (black). Samples are LMOF-231 (100:0 tcbpe:tcbpe-F), red; LMOF-305’ (95:5 tcbpe:tcbpe-F), orange; LMOF-305’’ (90:10 tcbpe:tcbpe-F), yellow; LMOF-305’’’ (85:15 tcbpe:tcbpe-F), green; LMOF-305 (80:20 tcbpe:tcbpe-F), blue.

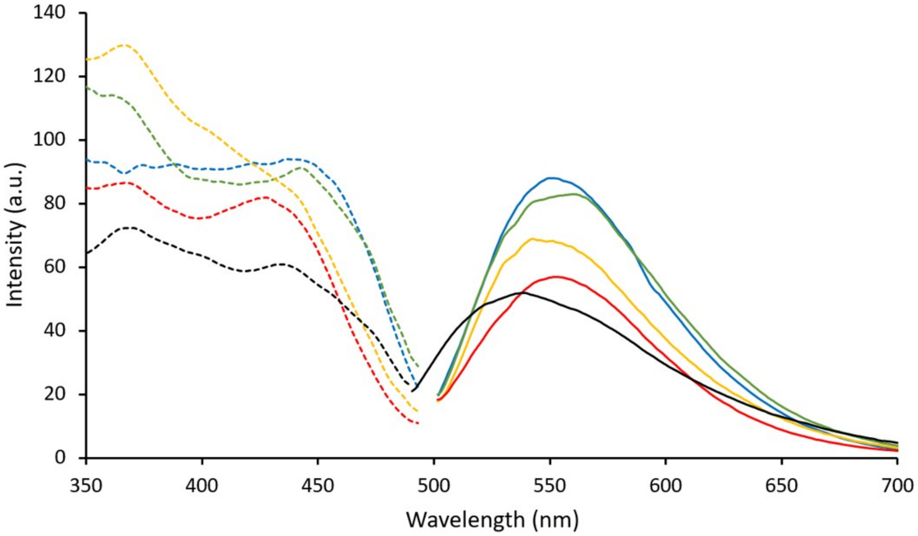

Figure S4. Excitation (dotted) and emission (solid) spectra for LMOF and ligand samples with varying amounts of tcbpe-F. Samples are LMOF-305’ (95:5 tcbpe:tcbpe-F), red; LMOF-305’’ (90:10 tcbpe:tcbpe-F), yellow; LMOF-305’’’ (85:15 tcbpe:tcbpe-F), green; LMOF-305 (80:20 tcbpe:tcbpe-F), blue; physical mixture of ligands (80:20 tcbpe:tcbpe-F), black. The intensities of excitation and emission spectra are scaled to the quantum yield of each sample.

S5. Excited state lifetime data

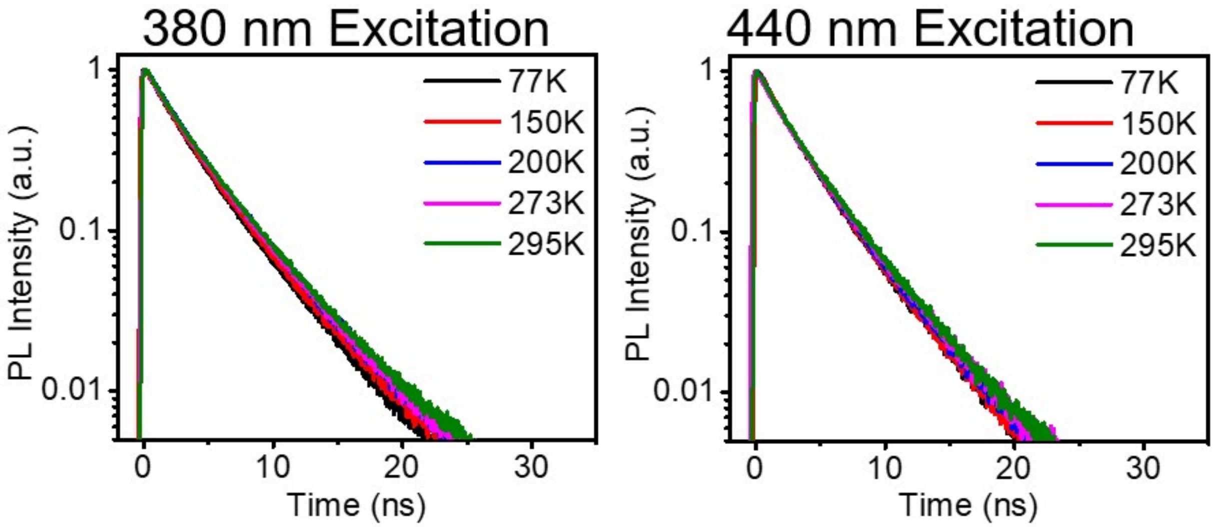

Figure S5. Luminescence decay profiles for H_4tcbpe at various temperatures under 380 (left) and 440 nm (right) excitation.

Table S3. Excited state lifetime data for H_4tcbpe under 380 nm and 440 nm excitation at various temperatures.

	380 nm excitation			440 nm excitation		
Temp	**Avg. amp. weighted τ**	**τ1 (ns)**	**τ2 (ns)**	**Avg. amp. weighted τ**	**τ1 (ns)**	**τ2 (ns)**
77 K	3.40	2.38 (57.3%)	4.76 (42.7%)	3.29 ns	2.56 (69.0%)	4.91 (31.0%)
150 K	3.54	2.51 (58.0%)	4.97 (42.0%)	3.21 ns	2.23 (55.9%)	4.47 (44.1%)
200 K	3.65	2.45 (51.8%)	4.95 (48.2%)	3.30 ns	2.25 (54.1%)	4.54 (45.9%)
273 K	3.63	2.31 (48.8%)	4.90 (51.2%)	3.43 ns	2.08 (42.7%)	4.43 (57.3%)
295 K	3.67	2.30 (48.7%)	4.98 (51.3%)	3.44 ns	2.11 (44.2%)	4.49 (55.8%)

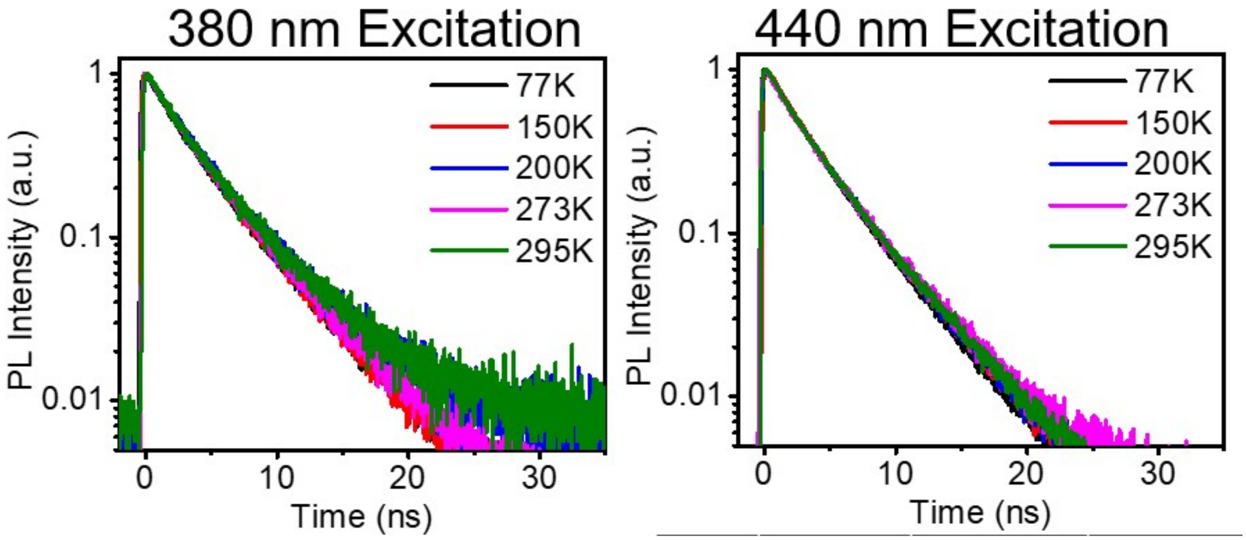

Figure S6. Luminescence decay profiles for H_4tcbpe-F at various temperatures under 380 (left) and 440 nm (right) excitation.

Table S4. Excited state lifetime data for H_4tcbpe-F under 380 nm and 440 nm excitation at various temperatures.

	380 nm excitation			440 nm excitation		
Temp	**Avg. amp. weighted τ**	**τ1 (ns)**	**τ2 (ns)**	**Avg. amp. weighted τ**	**τ1 (ns)**	**τ2 (ns)**
77 K	3.61	2.30 (47.0%)	4.78 (53.0%)	3.52 ns	2.73 (66.5%)	5.08 (33.5%)
150 K	3.63	2.65 (60.3%)	5.12 (39.7%)	3.55 ns	2.38 (49.0%)	4.68 (51.0%)
200 K	3.86	2.97 (69.6%)	5.89 (30.4%)	3.60 ns	2.38 (47.7%)	4.71 (52.3%)
273 K	3.67	2.49 (55.2%)	5.16 (44.8%)	3.58 ns	2.10 (41.7%)	4.63 (58.3%)
295 K	3.80	2.58 (58.0%)	5.48 (42.0%)	3.57 ns	2.34 (50.5%)	4.83 (49.5%)

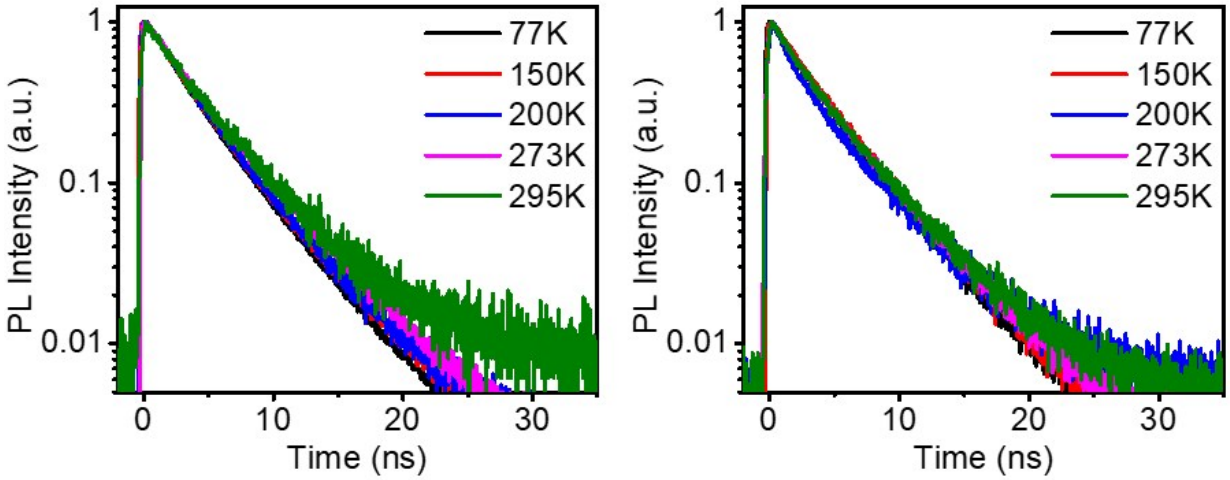

Figure S7. Luminescence decay profiles for LMOF-231 at various temperatures under 380 nm (left) and 440 nm (right) excitation.

Table S5. Excited state lifetime data for LMOF-231 under 380 and 440 nm excitation at various temperatures.

	380 nm excitation			**440 nm excitation**		
Temp	**Avg. amp. weighted τ**	**τ1 (ns)**	**τ2 (ns)**	**Avg. amp. weighted τ**	**τ1 (ns)**	**τ2 (ns)**
77 K	3.64 ns	3.07 (82.0%)	6.23 (18.0%)	3.85 ns	3.13 (69.1%)	5.47 (30.9%)
150 K	3.73 ns	3.04 (76.7%)	6.00 (23.3%)	3.90 ns	2.82 (47.0%)	4.87 (53.0%)
200 K	3.82 ns	3.36 (89.2%)	7.63 (10.8%)	3.24 ns	1.38 (43.5%)	4.67 (56.5%)
273 K	4.07 ns	3.22(69.2%)	6.00 (30.8%)	3.81 ns	2.10 (36.3%)	4.79 (63.7%)
295 K	4.14 ns	3.02 (56.3%)	5.59 (43.7%)	3.80 ns	1.98 (35.6%)	4.80 (64.4%)

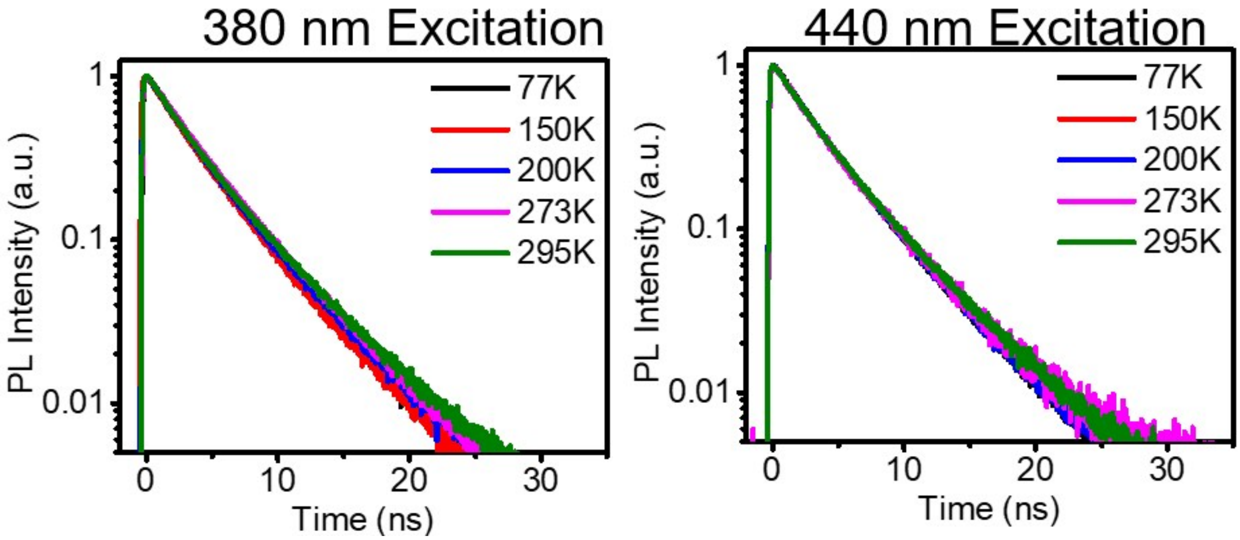

Figure S8. Luminescence decay profiles for LMOF-305 at various temperatures under 380 (left) and 440 nm (right) excitation.

Table S6. Excited state lifetime data for LMOF-305 under 380 nm and 440 nm excitation at various temperatures.

	380 nm excitation			**440 nm excitation**		
Temp	**Avg. amp. weighted τ**	**τ1 (ns)**	**τ2 (ns)**	**Avg. amp. weighted τ**	**τ1 (ns)**	**τ2 (ns)**
77 K	3.92	3.39 (84.2%)	6.74 (15.8%)	3.96 ns	3.44 (85.5%)	7.05 (14.5%)
150 K	3.78	2.92 (65.2%)	5.38 (34.8%)	3.97 ns	2.66 (47.8%)	5.16 (52.2%)
200 K	3.92	3.12 (74.3%)	6.23 (25.7%)	3.97 ns	3.15 (69.9%)	5.86 (30.1%)
273 K	4.09	3.41(78.6%)	6.61 (21.4%)	3.98 ns	3.00 (66.2%)	5.91 (33.8%)
295 K	3.99	2.87 (64.6%)	6.04 (35.4%)	4.05 ns	3.05 (66.2%)	6.00 (33.8%)

S6. Polarized photoluminescence spectra

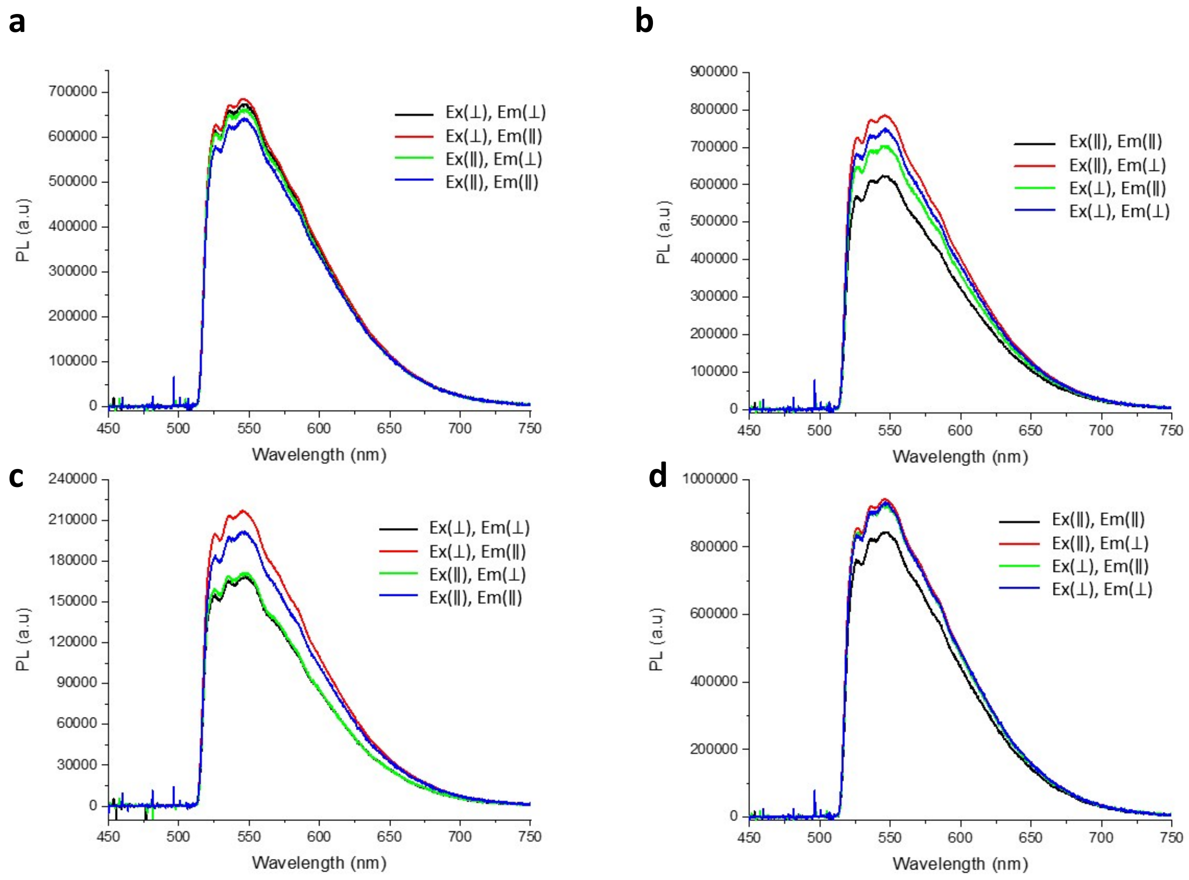

Figure S9. a) Polarized PL spectra from sample A of LMOF-305, with the crystal oriented such that the *b* crystallographic axis was parallel with 90° on the polarization stage. b) Polarized PL spectra from sample A of LMOF-305, with the crystal oriented such that the *b* crystallographic axis was parallel with 0° on the polarization stage. c) Polarized PL spectra from sample B of LMOF-305, with the crystal oriented such that the *b* crystallographic axis was parallel with 90° on the polarization stage. d) Polarized PL spectra from sample B of LMOF-305, with the crystal oriented such that the *b* crystallographic axis was parallel with 0° on the polarization stage. In all cases, the parallel/perpendicular notations given in the spectra key correspond to the orientation of the relevant polarization filter with respect to the crystallographic *c* axis.