Supplementary Information of

Control of crystalline J-dimer emission in interwoven metal-organic frameworks

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Contents

S1.	General Materials and Methods	S3
S2.	Synthetic Procedures	S6
S3.	Powder X-ray Diffraction	S11
S4.	Input/Output Composition	S12
S5.	Photophysical Data	S17
S6.	Lifetime Measurements	S27
S7.	SEM Images	S38
S8.	References	S42

Section S1. General Materials and Methods.

All starting materials and solvents, unless otherwise specified, were obtained from commercial sources (Aldrich, Fisher) and used without further purification. All reactions were performed at ambient laboratory conditions, and no precautions were taken to exclude oxygen or atmospheric moisture unless otherwise specified. Anhydrous *N*,*N*-dimethylformamide (DMF), Dichloromethane (CH₂Cl₂), and Tetrahydrofuran (THF) were purified using a custom-built alumina-column based solvent purification system (Inovative Technology). Anhydrous MeOH and dioxane were obtained from Aldrich (Sureseal). Et₃N and ⁱPr₂NH were degassed by placing in a septum sealed RBF and bubbled with N₂ gas for 30 min before use. Deuterated solvents (CDCl₃ and DMSO-*d*₆) were obtained from Cambridge Isotope Lab. K₂CO₃ was dried in a 120 °C oven for 24 h prior to use.

High-resolution ¹H, and ¹³C nuclear magnetic resonance (NMR) spectra were recorded using Bruker AVANCE-III 400 MHz spectrometer. The ¹H chemical shifts are given relative to tetramethylsilane as zero ppm, calibrated using the residual solvent signal. Data processing was performed using MNova version 9.0.1.

Powder X-ray diffraction measurements were performed using a Rigaku Miniflex 600 diffractometer, with θ -2 θ Bragg-Brentano geometry, and a 600 W (40 kV, 15 mA) Cu X-ray tube source using K α (λ = 1.5418 Å) radiation. Samples were measures with spinning from 2.5 to 50 2 θ -degrees with a step size of 0.02° and a scan rate of 1.5 s per step. Samples were prepared by dropping the powder sample in a Si zero background plate and pressing the powder with a razor blade spatula.

Crystals simulations and calculated patterns were made with the Reflex module in Materials Studio (v8.0, Biovia) starting with the CIF of **PIZOF-2** (803459) and **NNU-28** (1412713).

 N_2 gas adsorption isotherm analysis was performed using a Micromertics ASAP 2020 porosimetry analyzer. The measurements was performed at 77 K. Mass spectra were recorded on an Agilent 6230 TOF LC-MS instrument with an Agilent Zorbax SB-C18 analytical column.

The diffuse absorption spectra of TCPP and PCN-223(fb) were obtained using an Agilent Technologies 8453 UV-vis diode array spectrophotometer (1 nm resolution) where the sample compartment was replaced with an integration sphere. The powder samples were diluted by mixing with BaSO₄.

The steady-state emission spectra were obtained using a QuantaMaster Model QM-200-4E emission spectrophotometer from Photon Technology, Inc. (PTI). The excitation light source was a 75 W Xe arc lamp (Newport). The detector was a thermoelectrically cooled Hamamatsu 1527 photomultiplier tube (PMT). Samples were measured by sandwiching between two glass slides coated with grease. As a control experiment, a blank sample (with just a glass slide coated with grease) was always run (while measuring emission lifetime). Emission traces were analyzed using Origin 9.0. Time-

resolved fluorescence lifetimes were obtained via the time-correlated single photon counting technique (TCSPC) with the same QuantaMaster Model QM-200-4E emission spectrophotometer from Photon Technology, Inc. (PTI) equipped with a 415 nm LED and a Becker & Hickl GmbH PMH-100 PMT detector with time resolution of <220 ps FWHM. Florescence lifetime decays were analyzed with the help of Origin 9.0.

Calculation of Dimerization Constant

To calculate the dimerization constant, K_D , in solution, a sufficiently high dilution is required to avoid the formation of trimers and larger aggregates. At these high dilutions an equilibrium exists between the monomeric and dimeric species:

$$M + M \rightleftharpoons D$$
 (S1)

If *C* represents to total fluorophore concentration and *M* and *D* represent the concentration of the monomer and dimer respectively, then:

$$C = 2D + M \tag{S2}$$

The dimerization equilibrium constant, can be written as:

$$K_D = \frac{D}{M^2}$$
(S3)

Rewriting (S2) in terms of *M* and then substituting into (S3) gives the following equation:

$$K_D = \frac{D}{\left(C - 2D\right)^2}$$
(S4)

(S4) can be rewritten as a quadratic function:

$$4D^2K_D - (4K_DC + 1)D + K_DC^2 = 0$$
(S5)

Using the quadratic formula *D* is found to equal the following:

$$D = \frac{4K_{D}C + 1 \pm \sqrt{8K_{D}C + 1}}{8K_{D}}$$
(S6)

The mole fraction of dimer (χ_D) is represented as follows, replacing *D* with equation (S6) results in an equation in terms of K_D and *C*:

$$\chi_{D} = \frac{2D}{C} = \frac{4K_{D}C + 1 \pm \sqrt{8K_{D}C + 1}}{4K_{D}C}$$
(S7)

Substituting (S4) into (S7) results in an equation with mole fraction of dimer in terms of only the dimeric concentration and total concentration of the fluorophore:

$$\frac{2D}{C} = \frac{4D^2 + C^2 \pm C^2 - 4D^2}{4DC}$$
(S8)

From here the positive and negative values of $C^2 - 4D^2$ must be considered. By solving both equations it is found that the positive term does not converge while the negative term does. This results in the final equation (S9), as only one term will result in a real answer.

$$\chi_D = \frac{2D}{C} = \frac{4K_DC + 1 - \sqrt{8K_DC + 1}}{4K_DC}$$
(S9)

The measurable quantity when studying fluorescence is the λ_{max} , and the change in spectral shift, $\Delta\lambda_{max}$, is proportional to the mole fraction of dimer [1] using a scaling factor, A, the following equation can be obtained and an experimental dimerization constant can be solved using a non-linear least squares regression.

$$\Delta\lambda_{max} = A\chi_D[C, K_D] \tag{S10}$$





Anthracene PEPEP ester (S1): Adapted from literature procedure.[2] A 150 mL round bottom flask was charged with 9,10-dibromoanthracene (2.00 g, 5.95 mmol, 1.0 eq), hexyl 4-ethynyl-benzoate (3.02 g, 13.1 mmol, 2.2 eq), $PdCl_2(PPh_3)_2$ (125 mg, 0.179 mmol, 0.03 eq), and Cul (68 mg, 0.36 mmol, 0.06 eq). The flask was evacuated and backfilled with nitrogen thrice and charged with 15 mL of anhydrous THF and 45 mL of degassed Et₃N. Under nitrogen atmosphere, the reaction was heated to reflux, 90 °C, for 48 h and then cooled to room temperature. The reaction was quenched with 1 M HCl (50 mL) and diluted with 200 mL of water. The reaction mixture was extracted three times with CH_2Cl_2 , the combined organic layers were washed with 1 M HCl, water, and

brine. The organic layer was then dried over Na₂SO₄ and filtered. The crude mixture was purified via column chromatography (SiO₂, 40% v/v CH₂Cl₂/hexanes) affording **S1** as a red powder (2.67 g, 71% yield). ¹H NMR (400 MHz, CDCl₃, 25 °C) δ (ppm) 8.73 – 8.64 (m, 4H), 8.17 – 8.09 (m, 4H), 7.87 – 7.79 (m, 4H), 7.73 – 7.63 (m, 4H), 4.37 (t, *J* = 6.7 Hz, 4H), 1.85 – 1.75 (m, 4H), 1.47 (q, *J* = 7.1, 6.4 Hz, 4H), 1.43 – 1.32 (m, 8H), 0.97 – 0.90 (m, 6H). ¹³C NMR (101 MHz, CDCl₃, 25 °C) δ 166.22, 132.28, 131.66, 130.40, 129.81, 127.92, 127.27, 127.24, 118.53, 101.97, 89.38, 65.58, 31.63, 28.84, 25.87, 22.72, 14.17.



Anthracene PEPEP link (An): Adapted from literature procedure.² A 50 mL round bottom flask was charged with S1 (1.3 g, 2.5 mmol, 1.0 eq), Bu₄NOH (5.13 mL, 7.5 mmol, 3.0 eq), and 28 mL of THF (0.09 M). The solution was stirred at room temperature for 18 h. The solvent was then reduced using a rotary evaporator, the residue was suspended in water and quenched with 7.7 mL of 1 M HCI. The red precipitate was collected via vacuum filtration, rinsed with water and a small portion of cold methanol. (1.1 g, 96% yield). ¹H NMR (400 MHz, DMSO-*d*₆, 25 °C) δ (ppm) 8.74 – 8.70 (m, 4H), 8.11 – 8.07 (m, 4H), 8.05 – 8.00 (m, 4H), 7.84 (dd, *J* = 6.7, 3.2 Hz, 4H). ¹³C NMR (101 MHz, DMSO-*d*₆, 25 °C) δ (ppm) 166.73, 131.80, 131.38, 131.10, 129.67, 127.97, 126.74, 126.35, 117.53, 102.13, 88.26.



Xylene PEPEP ester (S2): Followed literature procedure.³ A 250 mL schlenk flask was charged with 2,5-diiodoxylene (3.6 g, 10.1 mmol, 1.0 eq), hexyl 4-ethynyl-benzoate (4.86 g, 21.1 mmol, 2.1 eg), PdCl₂(PPh₃)₂ (212 mg, 0.302 mmol, 0.03 eg), and Cul (115 mg, 0.60 mmol, 0.06 eq). The flask was evacuated and backfilled with nitrogen thrice and charged with 53 mL of degassed toluene and 27 mL of degassed diisopropylamine. Under the nitrogen atmosphere the reaction was then heated to 50 °C for 18 h and then cooled to room temperature. The reaction was guenched with 1 M HCI (60 mL) and diluted with 200 mL of DI-water. The reaction mixture was extracted three times with CH₂Cl₂, the combined organic layers were washed with 1 M HCl, water, and brine. The organic layer was then dried over Na₂SO₄ and filtered. The crude mixture was purified via column chromatography (SiO₂, 40% v/v CH₂Cl₂/hexanes) affording S2 as a white powder (4.34 g, 77% yield). ¹H NMR (400 MHz, CDCl₃, 25 °C) δ (ppm) 8.05 – 8.01 (m, 4H), 7.61 – 7.56 (m, 4H), 7.40 (s, 2H), 4.33 (t, J = 6.7 Hz, 4H), 2.48 (s, 6H), 1.77 (dg, J = 8.0, 6.7 Hz, 4H), 1.50 - 1.41 (m, 4H), 1.35 (tdd, J = 7.1, 4.4, 3.2 Hz, 8H), 0.97 - 0.86(m, 6H). ¹³C NMR (101 MHz, CDCl₃, 25 °C) δ (ppm) 171.14, 166.22, 137.70, 132.99, 131.51, 130.08, 129.65, 127.99, 123.04, 94.16, 91.20, 77.48, 76.84, 65.49, 31.61, 28.81, 25.85, 22.70, 20.17, 14.16.



Xylene PEPEP link (Xy): Adapted from literature procedure.³ A 50 mL round bottom flask was charged with **S2** (4.3 g, 7.7 mmol, 1.0 eq), Bu₄NOH (15.7 mL, 23 mmol, 3.0 eq), and 85 mL of THF (0.09 M). The solution was stirred at room temperature for 18 h. The solvent was then reduced using a rotary evaporator, and the residue was suspended in water and quenched with 24 mL of 1 M HCI. The white precipitate was collected via vacuum filtration, rinsed with water and a small portion of cold methanol. (2.65 g, 88% yield). ¹H NMR (400 MHz, DMSO-*d*₆, 25 °C) $\overline{0}$ (ppm) 8.04 (d, J = 8.6 Hz, 4H), 7.73 (d, J = 8.6 Hz, 4H), 7.57 (s, 2H), 2.50 (s, 6H). ¹³C NMR (101 MHz, DMSO-*d*₆, 25 °C) $\overline{0}$ (ppm) 166.67, 137.47, 132.66, 131.48, 130.65, 129.61, 126.55, 122.34, 94.11. 90.49, 19.53

MOF Synthesis

PIZOF-2 MOF (0 mol% **An): Xy** (20 mg, 0.051 mmol, 0.8 eq) was placed in a 4 mL glass vial followed by L-proline (29.2 mg, 0.254 mmol, 5 eq) and $ZrCI_4$ (13.0 mg, 0.056 mmol, 1.1 eq). Then 0.75 mL of 72.6 mM HCl in DMF was added followed by 1.46 mL of DMF (total concentration of 0.023 M with respect to **Xy**). The vial was tightly capped and immersed in an ultra-sonication bath until a fine suspension was obtained. The vial was then placed in a 120 °C isothermal oven for 24 h. The precipitate formed was collected by vacuum filtration and rinsed with DMF and CH_2CI_2 . The powder was immersed in DMF for 72 h, replacing the DMF every 24 h through the solvent exchange process and then the DMF was replaced with DCM for 48 h. The MOF was then dried under ultrahigh vacuum, 25 mTorr. Yield = 23.4 mg.

Low Anthracene Concentration MOFs ($0 \le x \le 50$): **Xy** (See table S1) was placed in a 4 mL glass vial followed by L-proline (See table S1) and ZrCl₄ (See table S1). A 13.0 mM solution of **An** in DMF was prepared and the required amount was added to the reaction vial followed by 72.6 mM HCl in DMF solution, fresh DMF (total concentration of 0.017 M with respect to total moles of links), and *o*-DCB (10% v/v). The vial was tightly capped and immersed in an ultra-sonication bath until a fine suspension was obtained. The vial was then placed in a 120 °C isothermal oven for 24 h. The precipitate formed was collected by vacuum filtration and rinsed with DMF and CH₂Cl₂. The powder was immersed in DMF for 72 h, replacing the DMF every 24 h through the solvent exchange process and then the DMF was replaced with DCM for 48 h. The MOF was then dried under ultrahigh vacuum, 25 mTorr. Yield = 23.8 mg. A similar procedure was followed for the 1, 5, 10, 30, 40, and 50% input MOFs with 40 and 50% not requiring DCB for a homogeneous output.

Mid Anthracene Concertation MOFs($50 \le x \le 70$): **An** (See table S1), **Xy** (See table S1) was placed in a 4 mL glass vial followed by benzoic acid (See table S1, 30 eq w/r to **An**), L-proline (See table S1, 5 eq w/r to **Xy**) and ZrCl₄ (See table S1) followed by 72.6 mM HCl in DMF solution and fresh DMF (total concentration of 0.017 M with respect to total moles of links) The vial was tightly capped and immersed in an ultrasonication bath until a fine suspension was obtained. The vial was then placed in a 120 °C isothermal oven for 72 h. The precipitate formed was collected by vacuum filtration and rinsed with DMF and CH₂Cl₂. The powder was immersed in DMF for 72 h, replacing the DMF every 24 h through the solvent exchange process and then the DMF was replaced with DCM for 48 h. The MOF was then dried under ultrahigh vacuum, 25 mTorr. Yield = 27.5 mg. A similar procedure was also followed for both 60% and 70% input MOF.

High Anthracene Concertation MOFs: An (See table S1) was placed in a 4 mL dramglassvialfollowedbybenzoic

acid (See table S1) and ZrCl₄ (See table S1). **Xy** (See table S1) was added to the vial followed by fresh DMF (0.017 M with respect to total moles of links). The vial was tightly capped and immersed in an ultra-sonication bath until a fine suspension was obtained. The vial was then placed in a 120 °C isothermal oven for 72 h. The precipitate formed was collected by vacuum filtration and rinsed with DMF and CH_2Cl_2 . The powder was immersed in DMF for 72 h, replacing the DMF every 24 h through the solvent exchange process and then the DMF was replaced with DCM for 48 h. The MOF was then dried under ultrahigh vacuum, 25 mTorr. Yield = 5.1 mg. A similar procedure was followed for the 80%, 90%, and 100% input MOFs.

x	Xy mg (mmol)	An mg (mmol)	ZrCl₄ 1.1 eq mg	Proline(HCl) mg	Benzoic Acid mg	72.6 mM HCI in DMF	DMF mL (0.017 M)	o-DCB mL
0	15 (0.038)	-	9.75	21.8	-	0.56	1.68	-
1	15 (0.038)	0.18* (0.0004)	9.85	22.1	-	0.57	1.46	0.226
5	15 (0.038)	0.93* (0.002)	10.3	23.0	-	0.59	1.50	0.235
10	15 (0.038)	1.97* (0.004)	10.8	24.3	-	0.62	1.56	0.249
20	20 (0.05)	5.91* (0.013)	16.3	36.5	-	0.935	2.26	0.373
30	20 (0.05)	10.1* (0.022)	18.6	41.7	-	1.07	2.50	0.426
40	15 (0.038)	11.8 (0.025)	16.3	36.5	-	0.935	2.79	-
50	12 (0.030)	14.2 (0.030)	15.6	35.0	-	0.897	2.68	-
60	10 (0.025)	17.7 (0.038)	16.3	14.6	139.3	0.374	3.35	-
70	7 (0.018)	19.3 (0.041)	15.2	10.2	151.7	0.262	3.22	-
80	5** (0.013)	23.7 (0.051)	16.3	-	232	-	2.51	-
90	2.5** (0.006)	26.6 (0.057)	16.3	-	232	-	3.14	-
100	-	27 (0.058)	15.0	-	212	-	3.40	-

Table S1: Reaction conditions for $Zr_6O_4(OH)_4[An_xXy_{1-x}]_6$.

* An added to the reaction mixture via an 80.3 mM stock solution in DMF

** Xy added to the reaction mixture via a 10.7 mM stock solution in DMF

Section S3: Powder X-ray Diffraction





Figure S2: Change in linker overlap from the $Fd^{3}m$ (**Xy**, top) to $R^{3}m$ (**An**, bottom) space group.



Section S4: Input/Output Composition

Procedure: 2.5 mg of MOF was placed in a 4 mL vial with 2 mL of 0.25 M Bu₄NOH in DMF and 0.5 mL of H₂O. The suspension was sonicated for 20 min then mixed in a vortex fixture until a homogeneous suspension was formed. The mixture was then filtered through a 45 μ m pipette filter (Aura Industries). The filtrate was then diluted (x10,000) in DMF, the emission profile was collected from 470-600 nm with an excitation wavelength of 453 nm. Peak emission was used to calculate solution based concentration based on a calibration curve and back calculation and conversion to solid state molality were completed based on the mass of MOF that was decomposed. Average molality values were converted to mol% utilizing the crystallographic density of each MOF and the max molar concentration in each phase pure MOF (*i.e.* for the 0 mol% **An** MOF the total number of links per cell is 48 with a unit cell volume of 63113 Å³, resulting in a max concentration [links]_{max} = 1.263 M).





MOF Trial	Anthracene Input (% mol)	Anthracene Output (m <i>m</i>)	Average Output	Standard Deviation	
1	1	0.293			
2	1	0.368	0.314	0.048	
3	1	0.280			
4	5	1.01			
5	5	1.02	1.00	0.015	
6	5	0.986			
7	10	2.25		0.27	
8	10	2.04	2.00		
9	10	1.71			
10	20	2.77			
11	20	3.28	3.19	0.39	
12	20	3.54			
13	30	4.00			
14	30	5.20	4.43	0.66	
15	30	4.10			

 Table S2: Input vs output concentration of An MOFs without o-DCB addition

Anthracene Standard Average Output Anthracene MOF Trial Output Deviation Input (% mol) (molality) (molality) (molality) 1 1 0.00760 2 1 0.00626 0.00665 8.24*10-4 3 1 0.00609 5 4 0.0440 5 5 0.0428 0.0447 2.3*10⁻³ 5 6 0.0473 7 10 0.131 8 10 0.133 0.131 0.002 9 10 0.129 10 20 0.285 11 20 0.297 0.292 0.006 12 20 0.293 13 30 0.422 14 30 0.494 0.433 0.056 15 30 0.384 40 16 0.398 17 40 0.483 0.488 0.093 18 40 0.583 19 50 0.622 20 50 0.556 0.571 0.046 21 50 0.534 22 60 1.19 23 60 0.917 1.02 0.14 24 60 0.969 25 70 1.11 70 1.08 0.14 26 1.18 27 70 1.34 28 80 1.84 29 80 1.75 1.82 0.058 30 80 1.86 31 90 1.79 32 1.79 90 1.59 0.35 33 90 1.18

Table S3: Input vs output concentration of **An** MOFs with the addition of *o*-DCB in low concentration samples

Table S4: Input vs output concentration of **An** MOFs with the addition of *o*-DCB in low concentration samples (1-30%) and without in higher concentration (40-100%) given in mol%.

Anthracene Input (mol%)	Average Output (<i>mol %</i>)	Standard Deviation (<i>mol%</i>)
1	0.331	0.041
5	2.24	0.12
10	6.41	0.39
20	14.9	0.30
30	22.5	2.9
40	25.7	4.9
50	30.4	2.4
60	55.9	7.8
70	65.1	7.8
80	102.0	3.2
90	90.1	19.9

Figure S4: Input vs. output in mol% for cubic An MOFs





Figure S5: Input vs. output in mol% for rhombohedral An MOFs

Section S5: Photophysical Data

Figure S6: Fluorescence spectra, emphasizing differences between MOFs crystalized without *o*-DCB (left) and with 10% v/v *o*-DCB (Right)







Figure S8: Excitation/emission profiles of S1 25 μ M in DCE 298 K







Figure S10: Excitation/emission profiles of S1 85 μ M in DCE 298 K







Figure S12: Excitation/emission profiles of S1 300 μ M in DCE 298 K



Figure S13: Normalized emission profiles of S1 in DCE 298 K, top normalized to peak at 480 nm, bottom normalized to peak at 520 nm.







Figure S15: Excitation/emission profiles of S1 25 μ M in DCE 77 K

Figure S17: Excitation/emission profiles of S1 85 μ M in DCE 77 K

Figure S19: Excitation/emission profiles of S1 300 μ M in DCE 77 K

Figure S20: Normalized emission profiles of S1 in DCE 77 K

Figure S21: Emission Profiles of An in DMF 298 K

Figure S22: Excitation/emission profiles of 1 mol% **An** without the addition of DCB at 298 K indicating the overlap in excitation and emission.

Section S6 Lifetime Measurements

Figure S23: Lifetime measurement of Blank (Grease and slide) at 298 K with 415 nm excitation

Figure S24: Lifetime measurement of 1 mol% An at 298 K with 415 nm excitation

Figure S25: Lifetime measurement of 5 mol% An at 298 K with 415 nm excitation

Figure S26: Lifetime measurement of 10 mol% An at 298 K with 415 nm excitation

Figure S27: Lifetime measurement of 20 mol% An at 298 K with 415 nm excitation

Figure S28: Lifetime measurement of 30 mol% An at 298 K with 415 nm excitation

Figure S29: Lifetime measurement of 40 mol% An at 298 K with 415 nm excitation

Figure S30: Lifetime measurement of 50 mol% An at 298 K with 415 nm excitation

Figure S31: Lifetime measurement of 60 mol% An at 298 K with 415 nm excitation

Figure S32: Lifetime measurement of 70 mol% An at 298 K with 415 nm excitation

Figure S33: Lifetime measurement of 80 mol% An at 298 K with 415 nm excitation

Figure S34: Lifetime measurement of 90 mol% An at 298 K with 415 nm excitation

Figure S35: Lifetime measurement of 100 mol% An at 298 K with 415 nm excitation

Section S7 SEM images

Figure S36: SEM of phase impure **60%-An MOF** where cubic crystals are of the rhombohedral phase and octahedral crystals are of the cubic phase.

Figure S37: SEM of phase impure **70%-An MOF** where cubic crystals are of the rhombohedral phase and octahedral crystals are of the cubic phase.

Figure S39: SEM of 60%-An MOF

Figure S41: SEM of 90%-An MOF

Figure S42: SEM of 100%-An MOF

Section S8 NMR data

Figure S43: ¹HNMR of S1 at 298 K

Figure S49: ¹HNMR of Xy at 298 K

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