Supporting Information

FRET-Enhanced Photoluminescence of Perylene Diimides by Combining Molecular Aggregation and Insulation

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1 General experimental detail

All reagents were used in reactions as received from the suppliers. Dried toluene was obtained from a glass contour solvent purification system. Flash chromatography purification was performed using standard methods on silica gel (Merck Silica Gel 60, 0.040-0.063 mm, 230-400 mesh ASTM). All reactions were monitored by thin-layer

chromatography using silica gel (Merck, Silica Gel 60 F254) coated glass sheets, examined under UV lamps (254 nm and 365 nm) in a black box. The ¹H and ¹³C NMR spectra were collected using Agilent MR400 (400 MHz), Oxford 500 (500 MHz) or Varian Inova 600 (600 MHz) instruments. All NMR spectra, if not otherwise specified, were measured at 25 °C and calibrated using the residual solvent signals. All FT-IR spectra were provided by a Perkin Elmer Spectrum One FT-IR spectrometer while UV-Vis spectra were recorded using a Cary UV-Vis spectrometer. All high-resolution mass spectrometry (HRMS) experiments were conducted with a commercially available hybrid orbital-trap and Fourier-transform ion cyclotron resonance mass spectrometer, equipped with electrospray ionization (ESI).

2 Synthesis detail

The synthesis of bPDI-1 to 4 are reported in literature.^[1]

2.1 *obPDI-1*

bPDI-1 (302.0 mg, 0.461 mmol) and $[RuH_2(CO)(PPh_3)_3]$ (92 mg, 0.10 mmol) were added to a microwave vial with dried and degassed 3,3-dimethyl-1-butene (1.2 mL, 9.3 mmol) and mesitylene (6.0 mL). The reaction was heated at 180°C for 2 days. Flash chromatography (dichloromethane: petroleum spirits 1:1) yielded the target product (orange powder, 178 mg, 39% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.38 (s, 2H), 7.39 (d, J = 8.1 Hz, 2H), 7.24 (d, J = 8.1 Hz, 2H), 3.53 (dd, J = 10.1, 6.4 Hz, 4H), 2.76 – 2.68 (m, 2H), 1.71 (dd, J = 18.9, 10.4 Hz, 6H), 1.51 – 1.40 (m, 2H), 1.06 (s, 18H), 0.98 (t, J = 7.3 Hz, 3H). ¹³C NMR (151 MHz, CDCl₃) δ 163.69, 152.22, 142.97, 133.73, 133.24, 132.32, 129.41, 128.45, 126.78, 124.16, 120.20, 45.16, 35.47, 33.27, 32.27, 30.98, 29.38, 22.56, 13.97. FT-IR (ATR, cm⁻¹, neat): 2955, 2929, 2861, 1697, 1657, 1547, 1334, 1223, 880, 824, 764, 750

HRMS ESI+ (m/z): calcd. for [M+H⁺] $C_{68}H_{83}N_2O_4$, 991.63528; found [M+H⁺], 991.63354.

2. 2 obPDI-4

bPDI-4 (10.1 mg, 5.24 μ mol) and [RuH₂(CO)(PPh₃)₃] (4 mg, 4.3 μ mol) were added to a microwave vial with dried and degassed 3,3-dimethyl-1-butene (70 μ L, 0.54 mmol) and mesitylene (0.5 mL). The reaction was heated at 180°C for 2 days. Flash chromatography (toluene: petroleum spirits 4:1) yielded the target product (orange powder, 2.8 mg, 24% yield).

¹H NMR (600 MHz, CDCl₃) δ 8.21 (d, J = 20.2 Hz, 2H), 7.35 (d, J = 6.0 Hz, 2H), 7.25 (s, 2H), 7.06 – 6.95 (m, 38H), 3.07 – 2.99 (m, 4H), 2.80 – 2.73 (m, 2H), 1.76 (dt, J = 15.5, 7.7 Hz, 2H), 1.51 – 1.40 (m, 6H), 0.99 (t, J = 7.4 Hz, 3H), 0.96 (d, J = 9.8 Hz, 18H).

¹³ NMR (151 MHz, CDCl₃) δ 163.69, 152.22, 142.97, 133.73, 133.23, 132.32, 129.41,
128.45, 126.78, 124.16, 120.20, 45.16, 35.47, 33.27, 32.27, 30.98, 29.38, 22.56, 3.97.
FT-IR (ATR, cm⁻¹, neat): 3085, 3055, 3028, 2955, 2931, 2864, 1697, 1662, 1549, 1332,
1229, 832, 747, 701

HRMS ESI+ (m/z): calcd. for $[M+H^+]$ C₁₆₈H₁₅₅N₂O₄, 2265.20204; found $[M+H^+]$, 2265.20459.

Characterisation spectra for obPDI-1



Figure S1. The ¹H and ¹³C NMR spectra of obPDI-1.



Figure S2. The HRMS of obPDI-1.

Characterisation spectra for obPDI-4



Figure S3. The 1H and 13C NMR spectra of obPDI-4.



Figure S4. The HRMS of obPDI-4.

3 X-ray crystallography

Intensity data for obDPA-1 was collected at 100 K on the MX1 beamline at the Australian Synchrotron,^[2] while obPDI-4 and pBDI-1 were collected at 100 K on a Rigaku Synergy diffractometer. The structures were solved by direct methods and difference Fourier synthesis.^[3] Thermal ellipsoid plots were generated using the program ORTEP-3 integrated within the WINGX suite of programs.^[4]

3.1 Crystal data of obDPI-1

jmwbz750 syn	
1949530	
$C_{68} H_{82} N_2 O_4$	
991.35	
100.0(1) K	
0.710918 Å	
Monoclinic	
P 21/c	
a = 5.5770(11) Å	<i>α</i> = 90°.
b = 27.722(6) Å	$\beta = 95.05(3)^{\circ}$.
c = 18.567(4) Å	$\gamma = 90^{\circ}$.
2859.4(10) Å ³	
2	
1.151 Mg/m ³	
0.070 mm ⁻¹	
1072	
0.15 x 0.10 x 0.01 mm ³	
1.469 to 32.334°.	
-8<=h<=8, -40<=k<=40, -	26<=l<=26
51069	
8608 [R(int) = 0.0699]	
99.7 %	
Semi-empirical from equit	valents
Full-matrix least-squares of	on F ²
8608 / 0 / 341	
1.049	
R1 = 0.0633, WR2 = 0.178	36
R1 = 0.0802, wR2 = 0.198	30
n/a	
0.383 and -0.349 e.Å ⁻³	
	jmwbz750_syn 1949530 C_{68} H ₈₂ N ₂ O ₄ 991.35 100.0(1) K 0.710918 Å Monoclinic P 21/c a = 5.5770(11) Å b = 27.722(6) Å c = 18.567(4) Å 2859.4(10) Å ³ 2 1.151 Mg/m ³ 0.070 mm ⁻¹ 1072 0.15 x 0.10 x 0.01 mm ³ 1.469 to 32.334°. -8<=h<=8, -40<=k<=40, -51069 8608 [R(int) = 0.0699] 99.7 % Semi-empirical from equi Full-matrix least-squares of 8608 / 0 / 341 1.049 R1 = 0.0633, wR2 = 0.178 R1 = 0.0802, wR2 = 0.198 n/a 0.383 and -0.349 e.Å ⁻³

3.2 Crystal data of obPDI-4

Identification code	jmwbz75	
CCDC Code	1949529	
Empirical formula	C ₂₀₄ H ₂₀₂ N ₂ O ₄	
Formula weight	2745.66	
Temperature	130.0(1) K	
Wavelength	1.54184 Å	
Crystal system	triclinic	
Space group	P-1	
Unit cell dimensions	a = 14.994(2) Å	$\alpha = 69.703(16)^{\circ}$.
	b = 17.388(3) Å	$\beta = 83.772(13)^{\circ}$.
	c = 17.985(3) Å	$\gamma = 64.782(16)^{\circ}$.
Volume	3974.6(13) Å ³	
Z	1	
Density (calculated)	1.147 Mg/m ³	
Absorption coefficient	0.504 mm ⁻¹	
F(000)	1472	
Crystal size	0.16 x 0.096 x 0.03 i	mm ³
Theta range for data collection	4.05 to 73.685°	
Index ranges	-18<=h<=16, -18<=	k<=21, -22<=l<=21
Reflections collected	25004	
Independent reflections	15497 [R(int) = 0.16]	603]
Completeness to theta = 25.242°	98.6 %	-
Absorption correction	Semi-empirical from	n equivalents
Refinement method	Full-matrix least-squ	ares on F ²
Data / restraints / parameters	4566 / 0 / 959	
Goodness-of-fit on F ²	0.948	
Final R indices [I>2sigma(I)]	R1 = 0.1035, WR2 =	0.1908
R indices (all data)	R1 = 0.2464, WR2 =	0.2911
Extinction coefficient	n/a	
Largest diff. peak and hole	0.383 and -0.349 e.Å	X-3

3.3 Crystal data of bPDI-1.

Identification code	jmwbz202		
CCDC Code Empirical formula Formula weight Temperature Wavelength Crystal system Space group Unit cell dimensions	1949528 $C_{44} H_{34} N_2 O_4$ 654.73 100.00(10) K 1.54184 Å Monoclinic P 21/c a = 22.1082(14) Å b = 6.9749(5) Å c = 21.5434(11) Å	$\alpha = 90^{\circ}.$ $\beta = 102.839(5)^{\circ}.$ $\gamma = 90^{\circ}.$	
Volume	3239.0(4) Å ³		
L Density (calculated) Absorption coefficient F(000)	4 1.343 Mg/m ³ 0.684 mm ⁻¹ 1376		
Crystal size Theta range for data collection Index ranges Reflections collected Independent reflections Completeness to theta = 67.684° Absorption correction Max. and min. transmission Refinement method Data / restraints / parameters Goodness-of-fit on F ² Final R indices [I>2sigma(I)] R indices (all data) Extinction coefficient	ystal size $0.331 \times 0.042 \times 0.012$ himneta range for data collection 4.102 to 70.343° .dex ranges $-26 <=h <= 26, -8 <=k <= 4, -100$ eflections collected 15482 dependent reflections $5603 [R(int) = 0.0684]$ pompleteness to theta = 67.684° 94.3% bsorption correction $8emi$ -empirical from equiax. and min. transmission 1.00000 and 0.67872 efinement method 1.00000 and 0.67872 ata / restraints / parameters $5603 / 9 / 482$ oodness-of-fit on F ² 1.024 nal R indices [I>2sigma(I)] $R1 = 0.0808$, wR2 = 0.18 indices (all data) $R1 = 0.1446$, wR2 = 0.21 xtinction coefficient n/a		
Largest diff. peak and hole	0.331 and -0.291 e.Å ⁻³		

4 Thin-film sample quantum yield measurement

4.1 Thin-film sample preparation

All the glass (MENZEL-<u>GLÄSER</u> Microscope Slides, 76 × 26 mm) slides were cut to 1.25 cm × 1.25 cm × 0.1 cm, cleaned by sonicating sequentially in CHCl₃, acetone, NaOH (a.q.), distilled water, isopropanol and acetone, then dried using a strong flow of N₂. The samples were prepared by spin coating 20 μ L casting solution on top of the above-mentioned glass slides. The spin-coating conditions were 2000 rpm (2000 rpm/s) for 1 minute to deposit the PMMA thin-film matrix. The casting solutions were prepared by dissolving the required quantity of fluorophores in either PMMA solution (8% w/w in toluene). The correct quantity of added fluorophores was determined by measuring aliquots from stock solutions (5 mM in toluene) using an automatic pipette, the solvent was removed using a vacuum drying oven (60°, 35 mbar), before adding to the matrix solution.

4.2 *Absolute quantum yield measurement*

Absolute photoluminescence quantum yield measurements of all samples were performed according to the experimental approach described elsewhere^[5] using the integrating sphere accessory (F3018, Horiba Jobin Yvon) for a Fluorolog[®]-3 fluorimeter. The angle of the excitation beam to the normal of the sample surface can be modified using the variable sample holder. All spectra for the absolute quantum yield measurements were corrected for the light source noise, wavelength sensitivity and the transmittance of the filters. The photon counts of all the measurements on the Fluorolog[®]-3 fluorimeter were within the linear response range of the detector (2×10^6 cps).

5 Spectroscopy Summary

5.1 *Time-correlated single photon counting (TCSPC) measurement*

As described previously^[1a], the excitation source was a mode-locked and cavity dumped Ti:Sapphire laser (Coherent Mira 900F/APE PulseSwitch) pumped by a Coherent Verdi-10 DPSS Nd:YVO₄ laser. The laser output (880 nm wavelength, 5.4 MHz repetition rate) was frequency doubled to provide an excitation wavelength of 440 nm. The individual fluorescence decay curves were collected using the time-correlated single photon counting technique. Synchronization of the laser pulses was achieved using a fast photodiode (Becker & Hickl, PHD-400-N) fed through a nanosecond delay box and constant fraction discriminator (Tennelec TC455) as the stop signal for the time-to-amplitude converter (Ortec model 457). The fluorescence decay profiles of the bPDI samples were collected at the magic angle relative to the (vertical) excitation polarization. The fluorescence decay profiles were analyzed by the FAST software (Edinburgh Instruments Ltd) using exponential components analysis.

Table S1.	. Summary of photophysical prope	rties for obPDI-1 and ob	PDI-4 at different
concentrat	tion conditions.		

Compound	Concentration ^a	Absorption	Emission	Average	$\phi_{PL^{\mathrm{b}}}$
		maximum	maximum	fluorescence	(%)
		(nm)	(nm)	lifetime, τ (ns)	
obPDI-1	solution	521	535	3.64	91
	10 mM PMMA film	487	617	10.35	82.6 ± 0.1
	120 mM PMMA film	487	621	8.85	56.4 ± 0.3
	amorphous neat film	487	628	0.96	10.5 ± 0.2
obPDI-4	solution	520	536	3.89	98
	10 mM PMMA film	521	536	4.35	89.0 ± 0.3
	120 mM PMMA film	521	536	1.58	40.3 ± 0.1
	amorphous neat film	522	583	0.53	14.2 ± 0.2

^a the concentration of solutions was 10⁻⁵ M in chloroform.

^b the ϕ_{PL} and standard deviation of the film samples were the average values over 3 measurements. The uncertainty of the relative and absolute ϕ_{PL} measurement are ~6.0% and 5.5% respectively.^[6]

5.2 Time-resolved fluorescence spectra

The excitation pulses were generated by coupling a συπερχοντινουμ white light laser source (NKT Extreme, 2.69 MHz rep rate after pulse picker) with a tunable single line filter (NKT Varia, 480 nm, 10 nm bandwidth). The film samples were excited within a TCSPC Lifetime Fluorometer (Horiba DeltraFlex), and the resulting emission was passed through a 500 nm long-pass filter (Thorlabs) before being diffracted by a time domain monochromator (Horiba TDM_1600) onto a photon counting detector (Horiba PPD-850). The instrument response was generated by collecting the scattered excitation light from a glass slide, after removing the long-pass filter. The intensities for each wavelength were calibrated by comparing a steady-state emission spectrum from this setup with the emission spectrum from a mini spectrometer (Ocean Optics Flame).

Table S2. Summary of the analysis of the decay profiles from the time-resoluved

 fluorescence spectra determined from the MCR-ALS analysis.

obPDI-1 120 mM	A ₁ ^a	A ₂	A ₃	$\tau_1(ns)$	$\tau_2(ns)$	$\tau_3(ns)$	τ (ns) ^b
component 1	0.37	0.42	0.21	0.20	1.01	4.01	1.36
component 2	0.47	0.53		2.62	11.51		7.30
••mpononi 2	0.17	0.00		2:02	11.01		7.00

obPDI-4 120 mM	Ag	A ₁	A ₂	$\tau_{g}(ns)^{c}$	$\tau_1(ns)$	$\tau_2(ns)$	τ (ns)
component 1		0.19	0.81		0.25	1.03	0.88
component 2	1.00	0.94	0.06	0.35	2.92	10.58	3.37

obPDI-4 120 mM / bPDI-2 20 mM	Ag	A ₁	A ₂	$\tau_g(ns)$	$\tau_1(ns)$	$\tau_2(ns)$	τ (ns)
component 1		0.98	0.02		0.21	1.50	0.24
component 2		0.57	0.43		0.76	3.54	1.94
component 3	1.00	1.00		0.36	9.93		9.93

^a The fraction of each decay exponential is normalized to 1.

^b The amplitude average fluorescence lifetimes for the decay profile of each component. The component corresponding to the emission growth is excluded.

^c The subscript 'g' refers to growth of the fluorescence decay profiles.



Figure S5. The absorption and emission spectra (λ_{ex} = 490 nm) of a) bPDI-1, b) bPDI-2, c) bPDI-3 and d) bPDI-4. These spectra have been reported in our previous literature.^[1b]



Figure S6. The emission spectra of bPDI-2 alone at 10 mM and 20 mM in PMMA matrix.

6 Calculations

We employed the multi-configurational DFT/MRCI^[7] method for computing the excited state properties of bPDI aggregates. It is used in conjunction with the tight set of empirical parameters allowing faster energy convergence with respect to the truncation of the configuration space. The Kohn-Sham one-particle basis for the electron configurations was computed with the BHLYP^[8] exchange-correlation functional using TURBOMOLE^[9] software. The split valence Gaussian-type orbital basis set def-SV(P)^[10] was utilized for all atomic centers in our calculations.

We analyzed the singlet excited-state wave function of the aggregated bPDI using one particle transition density matrix.^[11] Here, a supramolecular electronically excited wave-function is characterized by the percentage of the underlying local and charge-transfer components, which are effectively reflected by the elements of Ω -matrix. In the following, indices a and b designate the monomer label, such that:

$$\Omega = \begin{bmatrix} \omega_{aa} & \omega_{ab} \\ \omega_{ba} & \omega_{bb} \end{bmatrix}$$

The diagonal elements represent the weight of local excitations at the respective monomer, and the o-diagonal elements refer to the percentage of charge density transferred from one subsystem to another. The result of this analysis is summarized in Table 1.

The spin-orbit (SO) matrix elements between singlet and triplet DFT/MRCI wave functions were computed using the SPOCK module.^[12] The two-electron part in the Breit-Pauli SO operator was treated with help of effective mean-field approximation. We compactly define the magnitude of the SO interaction as follows:

$$\langle S_i | \hat{H}_{SO} | T_j \rangle = \sqrt{\sum_{m=0, \pm 1} |\langle S_i | \hat{H}_{SO} | T_{j,m} \rangle|^2}$$

where index m runs over triplet sublevels. where index m runs over spin sublevels of a triplet state, see Table S2. Here, we consider only the T_3 and T_4 states as they are in energetic proximity to the singlet states.

Table S3. Results of DFT/MRCI calculations and transition density matrix analysis. S and T refer to excited singlet and triplet states. %S and %D represent relative contribution of one- and two-electron excitation configurations. ω_{AA} , ω_{BB} , ω_{AB} and ω_{BA} are the Frenkel and CT components of the transition density matrix. E gives the Vertical excitation energies (above the ground state) in eV and f gives the oscillator strength of the electronic transition. N designates the excited-state character: L — local excitation, CT — charge-transfer excitation, TT — doubly excited state composed of two local triplets.

	%S	%D	ω_{AA}	ω_{BB}	ω_{AB}	ω_{BA}	Ν	E (eV)	f (L)
obPDI-1									
\mathbf{S}_1	87.5	5.6	0.49	0.49	0.01	0.01	\mathbf{L}	2.26	0.00
S_2	86.8	5.9	0.40	0.40	0.10	0.10	\mathbf{L}	2.32	1.15
S_3	61.3	31.4	0.02	0.02	0.48	0.48	CT	2.60	0.00
$\mathbf{S_4}$	85.1	8.7	0.11	0.11	0.39	0.39	CT	2.68	0.31
\mathbf{S}_5	8.3	78.9					TT	2.72	0.00
T_1	87.5	4.9					\mathbf{L}	1.32	0.00
T_2	87.3	5.0					\mathbf{L}	1.34	0.00
T_3	80.9	12.4					CT	2.56	0.00
T_4	85.9	8.2					CT	2.60	0.00
bPDI-2									
S_1	87.6	5.5	0.08	0.90	0.01	0.01	\mathbf{L}	2.32	0.60
$\mathbf{S_2}$	87.6	5.5	0.88	0.07	0.02	0.03	\mathbf{L}	2.33	0.66
S_3	81.3	13.0	0.04	0.02	0.85	0.09	CT	2.43	0.02
S_4	85.1	9.4	0.04	0.03	0.09	0.84	CT	2.49	0.03
\mathbf{S}_5	5.9	82.7					TT	2.84	0.00
T_{1}	88.1	4.8					\mathbf{L}	1.37	0.00
T_2	88.3	4.8					\mathbf{L}	1.40	0.00
T_3	85.3	9.0					CT	2.39	0.00
T_4	84.7	9.5					CT	2.42	0.00
bPDI-1									
S_1	87.8	6.0	0.70	0.18	0.02	0.11	\mathbf{L}	2.10	0.19
\mathbf{S}_2	86.3	8.5	0.08	0.07	0.03	0.82	CT	2.24	0.01
S_3	86.3	8.3	0.09	0.09	0.80	0.03	CT	2.32	0.14
${ m S}_4$	86.7	5.9	0.17	0.70	0.12	0.02	\mathbf{L}	2.40	0.98
\mathbf{S}_5	0.2	88.3					TT	2.65	0.00
T_1	88.7	5.0					\mathbf{L}	1.22	0.00
T_2	88.5	4.7					\mathbf{L}	1.43	0.00
T_3	87.0	7.7					CT	2.15	0.00
T_4	86.7	8.0					CT	2.26	0.00

	S_1	S_2	S_3	S_4
bPDI-1				
${f T_3} {f T_4}$	$0.251 \\ 0.405$	$0.051 \\ 0.175$	$0.037 \\ 0.030$	$0.049 \\ 0.170$
bPDI-2				
$\begin{array}{c} T_3 \\ T_4 \end{array}$	$0.200 \\ 0.268$	$0.086 \\ 0.177$	$0.011 \\ 0.019$	$0.013 \\ 0.019$
obPDI-1				
${f T_3}\ {f T_4}$	1×10^{-4} 0.047	$0.056 \ 3 \times 10^{-4}$	1×10^{-4} 0.045	$0.012 \\ 4 \times 10^{-4}$

Table S4. Spin-orbit matrix elements (cm⁻¹) between singlets and triplets.

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