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Incorporation of narcissistic self-sorting supramolecular interactions for the spontaneous fabrication of multiple-color solid-state materials for OLED applications†

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† Dedicated to Prof. J.-M. Lehn on the occasion of his 80th birthday.

Supplementary Information

Contents

1. Optical image measurements.

Measurements were performed on a Picoquant Microtime 200 inverted confocal fluorescence microscope (CFM), using a PicoHarp 300 multichannel single-photon counter and two MPD SPADs. The excitation originated from a diode laser at 375nm (PicoQuant LDH-D-C-375) operated in pulsed mode (40–300ps at 5MHz repetition rate) or in continuous mode. The laser beam was coupled into a polarization maintaining single-mode fiber optic, collimated and finally injected by 90° reflection on a 80%T/20%R spectrally flat beam splitter into the microscope oil immersion objective (100 X UPLSAPO, N.A. 1.4). Emitted light was collected by the same objective and backscattered excitation light was rejectied by a 405 nm long-pass filter. After the tube-lens and the pinhole, the fluorescence was diverted either into an intensity-corrected spectrometer (Andor SR300i) equipped with a Newton EMCCD for emission micro-spectroscopy measurements, eitherto a MPD SPAD for Fluorescence Lifetime Imaging Microscopy (FLIM).. In FLIM images, a fast-FLIM algorithm was used to calculate the average lifetime of each pixel, defined as the mean time of photon arrival (or first moment of photon arrival times) minus the time of steepest increase in the onset of the decay. For the hyperspectral images, the spectra were intensity corrected with a correction function obtained using a calibration source (Ocean Optics DH-2000). Kinetic series of spectra were acquired so that the integration time per spectrum matched the integration time of a pixel in the CFM (typically 6 ms), and a dedicated custom-made software calculated for each pixel its spectrum, CIE coordinates and corresponding RGB values. The same software allowed upon selection of an arbitrary Region of Interest (ROI), to calculate a 3D distribution of the CIE coordinates, represented in a 3D surface plot.

2. Characterization of emission from m1, m2, and m3

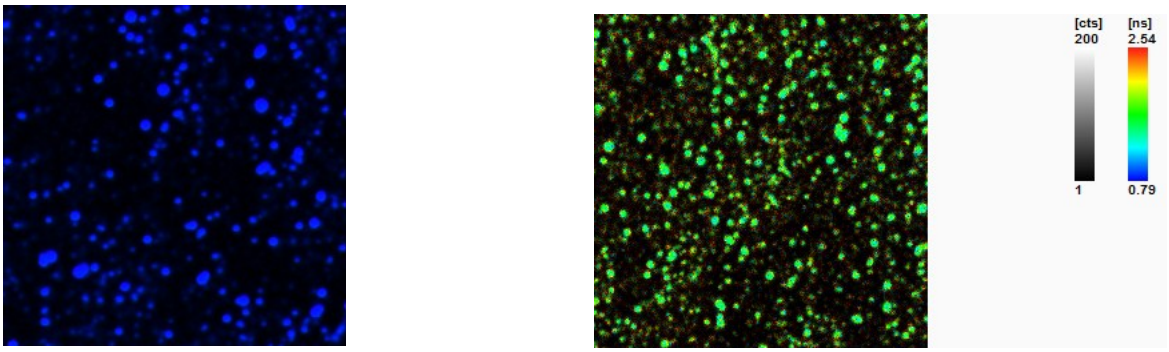

Fig. S1 Color-corrected confocal fluorescence image (left) and FLIM image of **m1** aggregates (λ_{ex} = 375 nm).

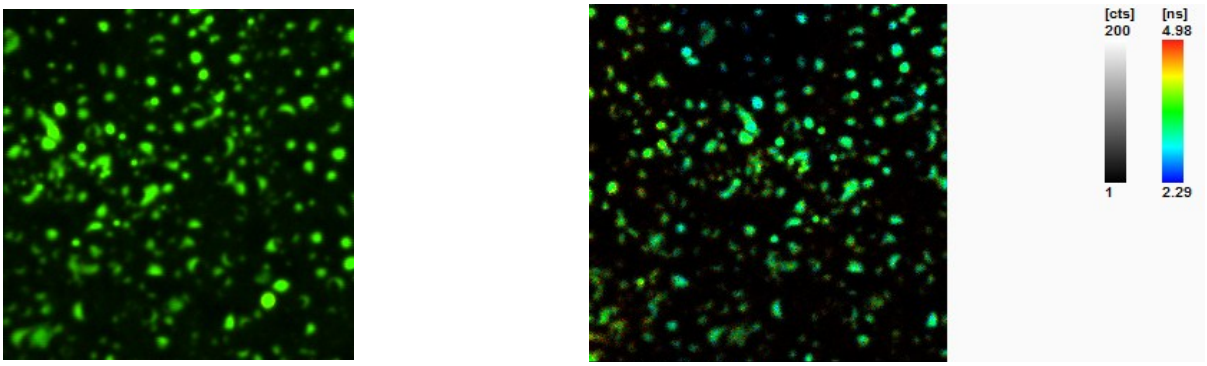

Fig. S2 Color-corrected confocal fluorescence image (left) and FLIM image of **m2** aggregates (λ_{ex} = 375 nm).

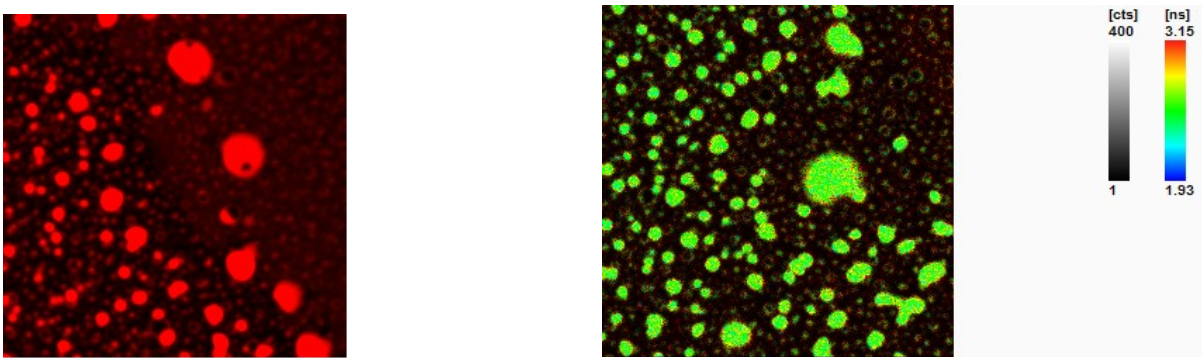

Fig. S3 Color-corrected confocal fluorescence image (left) and FLIM image of **m3** aggregates (λ_{ex} = 375 nm).

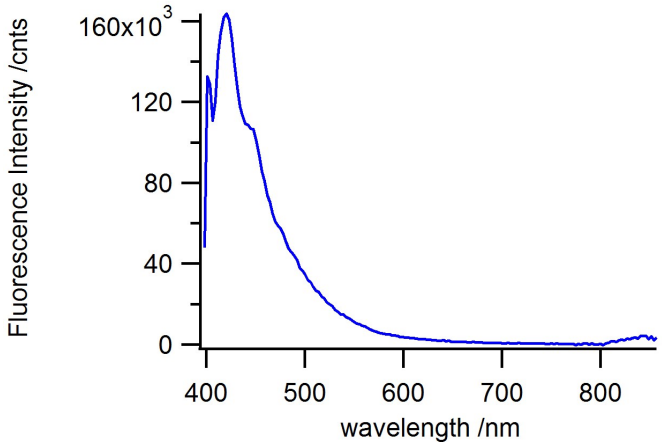

Fig. S4 Emission spectrum collected from a single aggregate of **m1** (λ_{ex} = 375 nm)

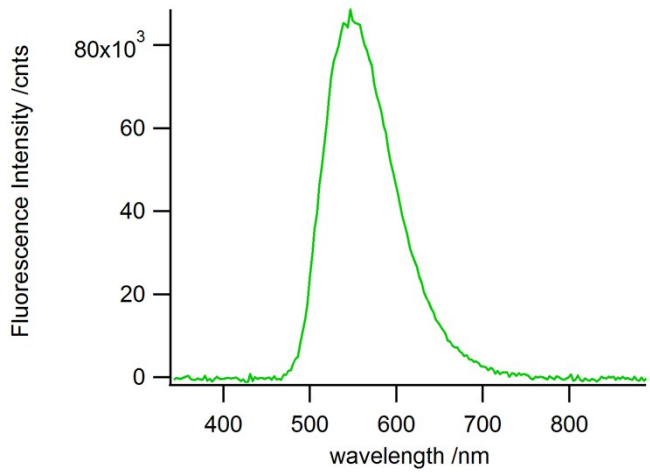

Fig. S5 Emission spectrum collected from a single aggregate of **m2** (λ_{ex} = 375 nm)

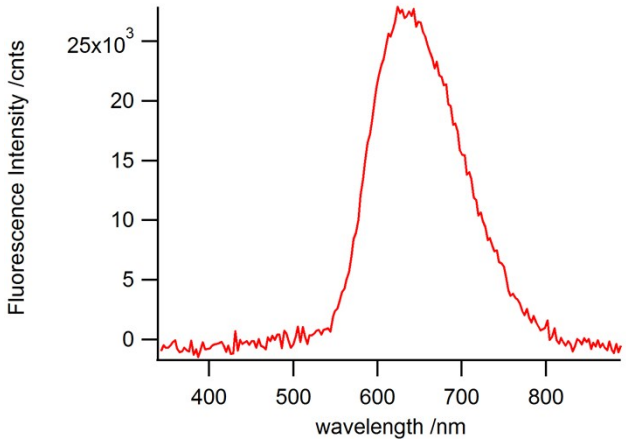

Fig. S6 Emission spectrum collected from a single aggregate of **m3** (λ_{ex} = 375 nm)

3. Calculation of FRET

The probability of FRET between the **m1** and **m2** donor and **p3** acceptor molecules was calculating the Förster radius (R_0) for each system. The latter depends on the overlap integral between the emission spectrum of the donor and the absorption spectrum of the acceptor (Fig. S7). The results are tabulated below.

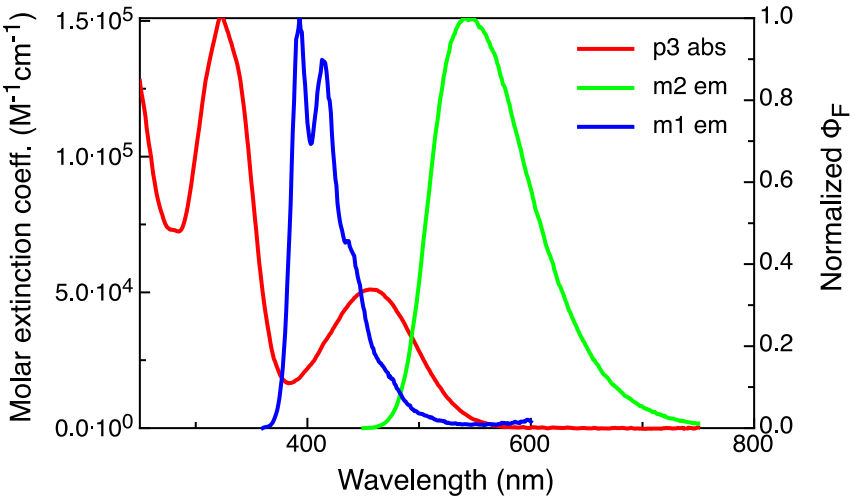

Fig. S7. Overlap between the normalized emission of the donor (**m1**, blue line or **m2**, green line) and the absorption spectrum of the **p3** acceptor (red line).

Table S1. Calculated FRET radius for various donors and **p3** acceptor.[a]

Donor	Φ_D	R_0 (Å)
m1	0.85	45
m2	0.98	39

[a]A value of $\kappa = 2/3$ and n = 1.42 was used for the calculations.

4. Partial self-sorting of m2 / m3 system

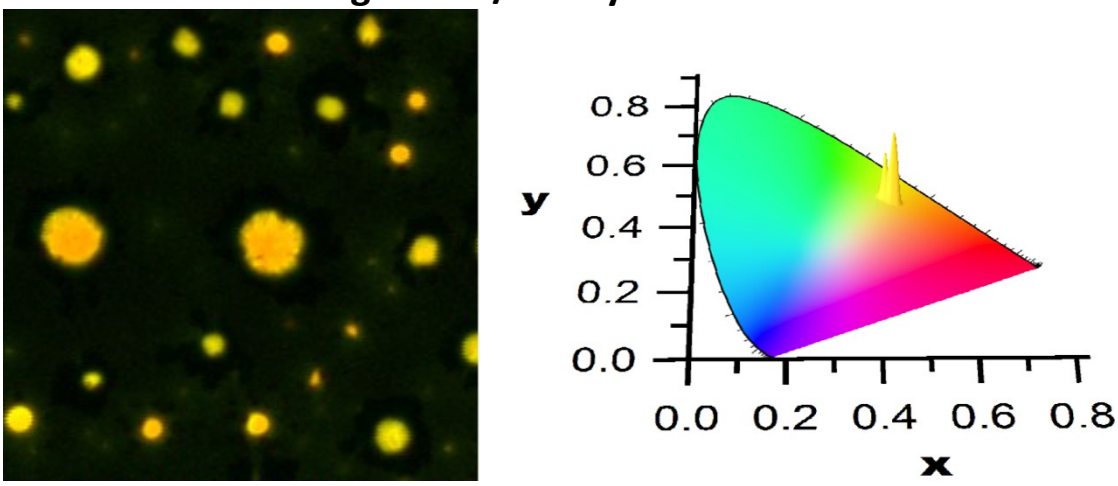

Fig. S8 Bimodal chromatic dispersion observed in aggregates deposited from a solution of **m2** and **m3** (100 : 10, 10^{-4} M in THF).

5. Estimation of the composition of the constituents of the self-sorted vesicles formed from m1 / p3 and m2 / p3 systems.

To estimate the relative proportion of the constituents in the self-sorted vesicles, a series of solutions containing varying proportions of **m1** and **m3** or **m2** and **m3** were prepared and deposited onto glass substrates. The, the CIE color coordinated of the vesicles were determined and plotted on a chromatic CIE chart (Fig. S9). For each point in each system, the length of a vector whose origin is located at the CIE coordinates of the pure **m1** or **m2** aggregates was calculated and plotted as a function of the relative composition of the solution. The results are shown in Fig. S10.

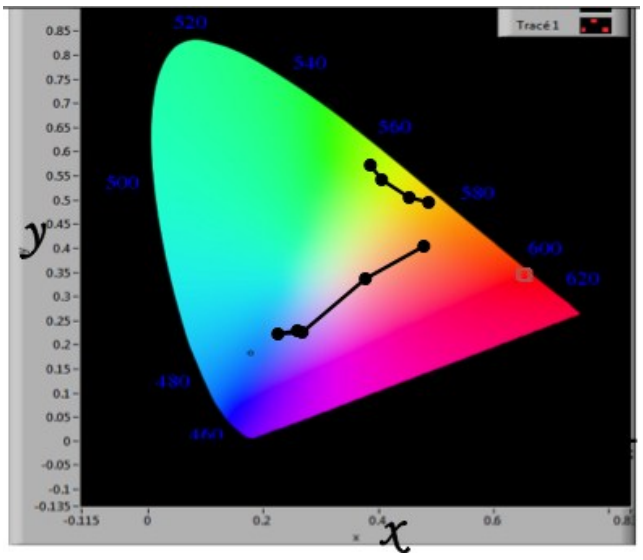

Fig. S9 Color of aggregates obtained by mixing varying proportions of **m1** and **m3** or **m2** and **m3**.

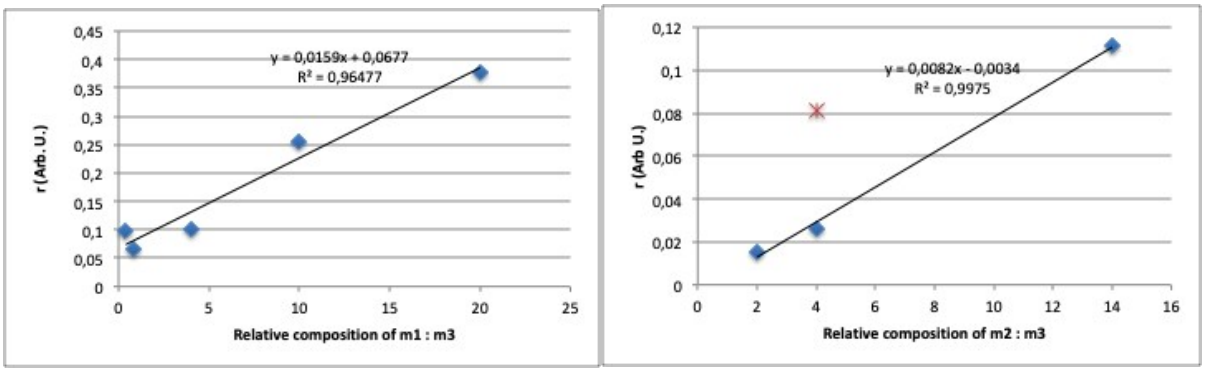

Fig. S10 Chart showing the relationship between the length of a vector connecting each experimental point in Fig S8 and an origin defined by the location of the color of **m1** (left) or **m2** (right). Straight line is best fit through points. Orange X indicates location of an outlying point not used for the linear regression.