

Supporting Information

Green Fluorescent Organic Nanoparticles by Self-Assembly Induced Enhanced Emission of a Naphthalene Diimide Bolaamphiphile

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General Methods

Atomic Force Microscopy (AFM): AFM measurements were performed on a Veeco diInnova SPM operating in tapping mode regime. Micro-fabricated silicon cantilever tips doped with phosphorus and with a frequency between 235 and 278 kHz and a spring constant of 20-40 Nm^{-1} were used. The samples were prepared by drop casting 10^{-3} M solution of **1** in 90 % (v/v) water in methanol on glass substrate and dried in air followed by vacuum drying at room temperature.

Optical Measurements: Electronic absorption spectra were recorded on a Perkin Elmer Lambda 900 UV-Vis-NIR Spectrometer and emission spectra were recorded on Perkin Elmer Ls 55 Luminescence Spectrometer. UV-Vis and emission spectra were recorded in 1 mm path length cuvette. Fluorescence spectra of solutions were recorded with 350 nm excitation wavelength.

NMR Measurements: NMR spectra were obtained with a Bruker AVANCE 400 (400 MHz) Fourier transform NMR spectrometer with chemical shifts reported in parts per million (ppm) with respect to TMS. 10^{-2} M stock solution of **1** was prepared in D_2O which was injected to appropriate volume of D_2O to obtain the sample of required concentrations.

Matrix-assisted laser desorption ionization time-of-flight (MALDI-TOF): MALDI-TOF spectra were obtained on a Bruker ultraflex 2 MALDI-TOF mass spectrometer with α -cyano-4-hydroxycinnamic acid matrix.

Dynamic light scattering Experiments (DLS): The measurements were carried out using a NanoZS (Malvern UK) employing a 532 nm laser at a back scattering angle of 173° . 10^{-2} M

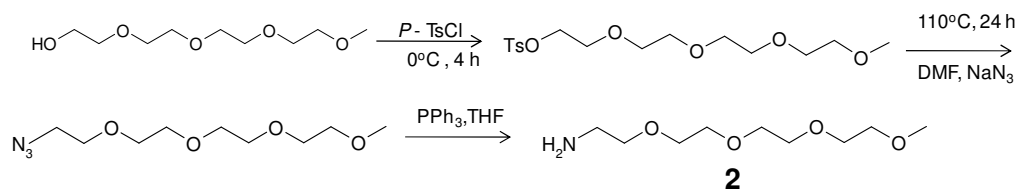
stock solution of **1** was prepared in methanol, calculated volume of which was injected into solvent mixtures to obtain the required solution.

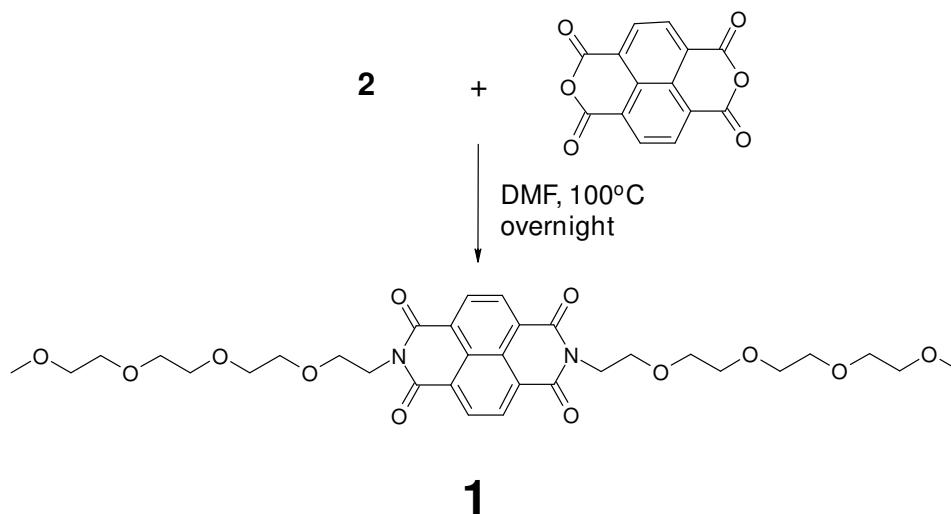
Confocal Microscopy Imaging: Confocal Microscopy imaging was done at room temperature using a Zeiss LSM 510 META laser scanning confocal microscope. The microscope objective of 63X (NA 1.4) and 20X (NA 0.5) were employed. Sample was prepared by sealing the solution between two glass plates.

Transmission Electron Microscopy (TEM): TEM measurements were performed on a JEOL, JEM 3010 operated at 300 kV. Samples were prepared by placing a drop of the solution on carbon coated copper grids followed by drying at room temperature. The images were recorded with an operating voltage 300 kV. In order to get a better contrast sample was stained with uranyl acetate (1 wt % in water) before the measurements.

Single Photon Counting Spectrometer: Fluorescence decay was recorded in a time-correlated single-photoncounting spectrometer of Horiba-Jobin Yvon with 350-450 nm picosecond Ti-sapphire laser.

Synthetic Scheme





Scheme S1. Synthesis of naphthalene diimide bolaamphiphile **1**.
Supporting Figures

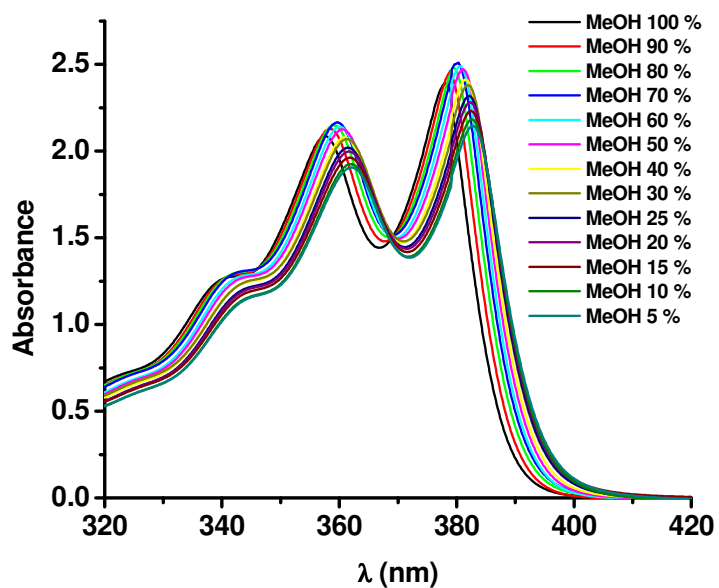


Fig. S1 Steady state absorption spectra of **1** in water-methanol mixtures at 10^{-3} M concentration, 1 mm path length.

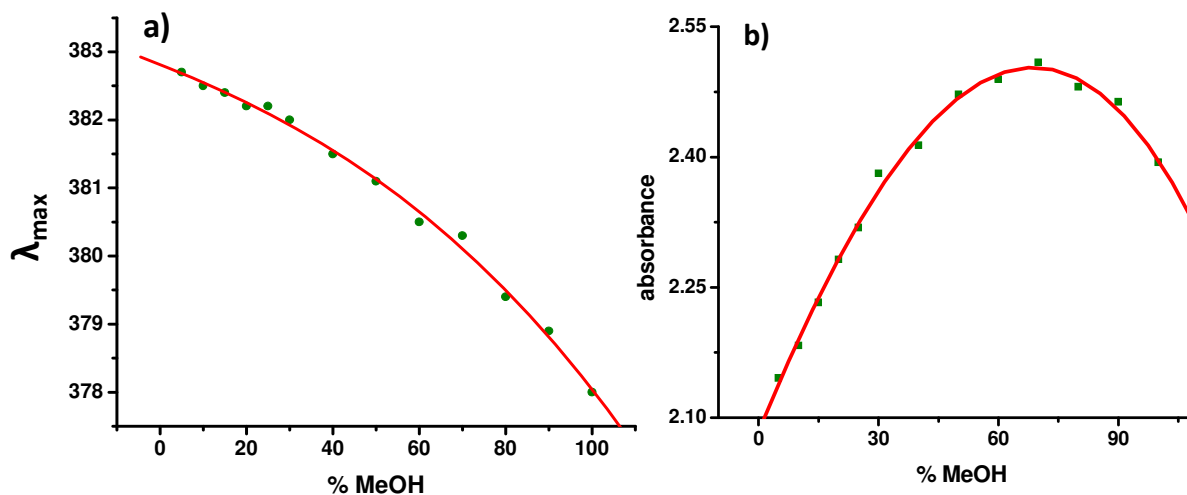


Fig. S2 Plots of MeOH composition against a) λ_{max} and b) absorbance of **1** (green dots). corresponding polynomial fits (red line) shows the non – linear nature of the plot thereby ruling out the possibility of solvatochromic effect.

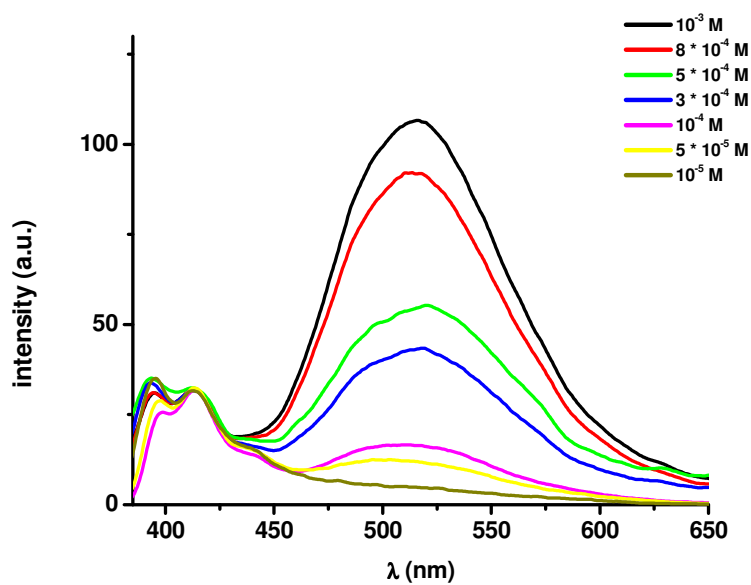


Fig. S3 Concentration dependent (normalized) emission spectra ($\lambda_{\text{exc}} = 350$ nm) (normalized) of **1** in water.

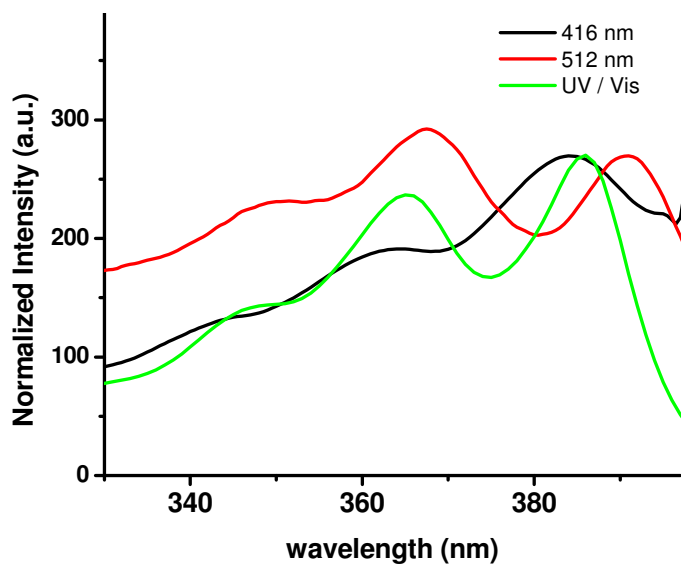


Fig. S4 Normalized excitation spectra monitored for the monomer emission at 416 nm, excimer emission at 512 nm and absorption spectra of **1** in water at 10^{-3} M concentration.

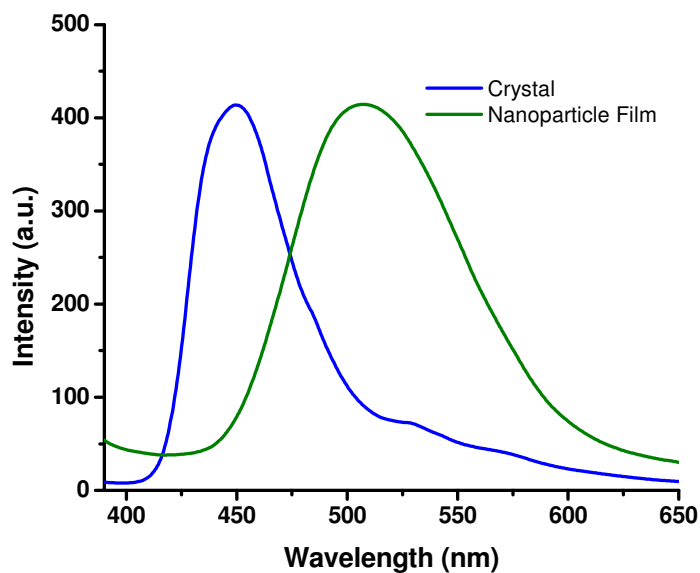


Fig. S5 Normalized emission spectra of **1** ($\lambda_{\text{exc}} = 350$ nm) in crystalline and nanoparticle film state.

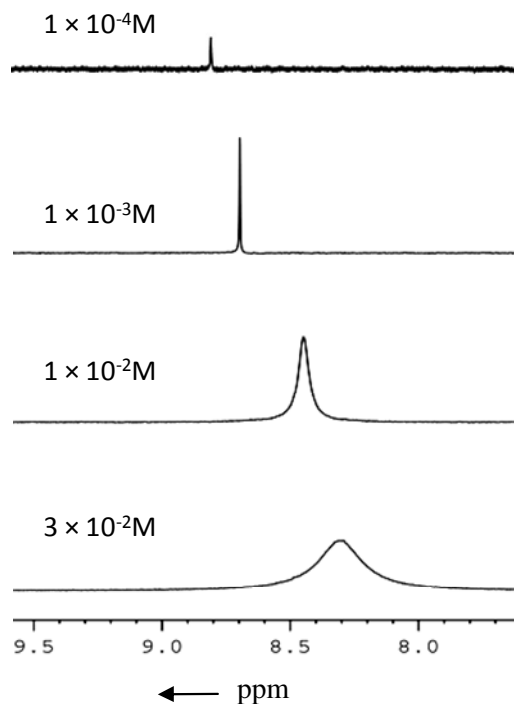


Fig. S6 Concentration dependent ^1H NMR spectra (aromatic proton) of **1** in D_2O showing an upfield chemical shift with broadening of the peak on increasing sample concentration.

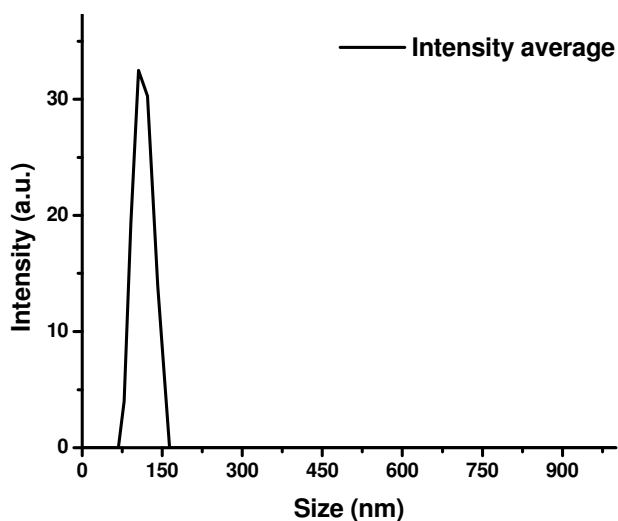


Fig. S7 Hydrodynamic size distribution of **1** in 90 % (v/v) water in methanol (self-assembled nanoparticles) as measured by DLS (10^{-3}M). This is a repeated measurement to confirm the nanoparticles in solution.

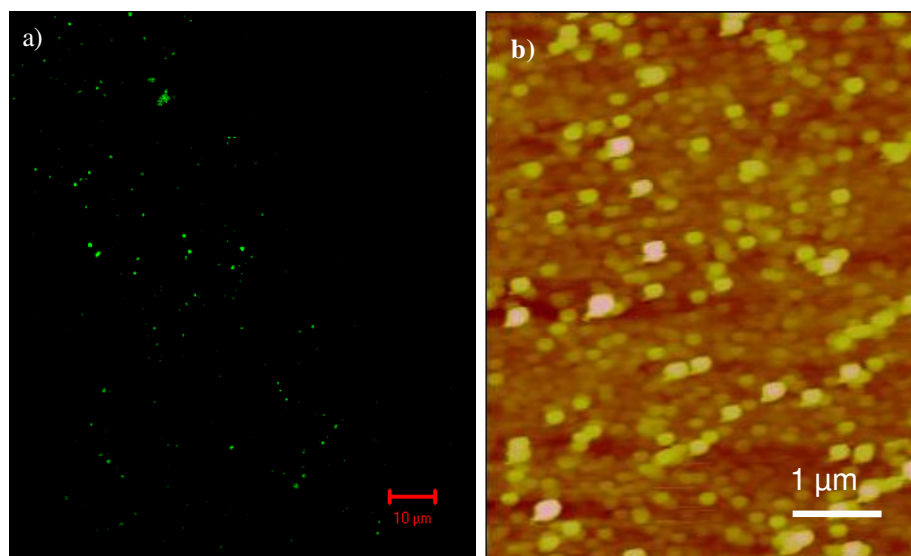


Fig. S8 Large-area images of NDI nanoparticles. a) Confocal fluorescent microscopy and b) tapping mode AFM images of the NDI nanoparticles of **1** at 1×10^{-3} M.

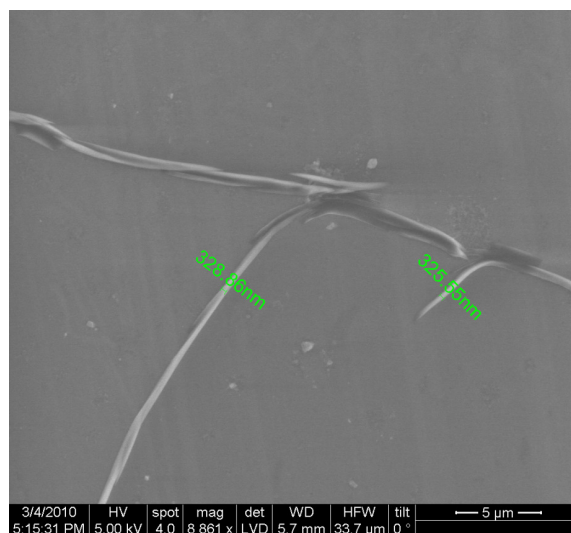


Fig. S9 FE-SEM image of the crystals of **1** on a glass substrate.

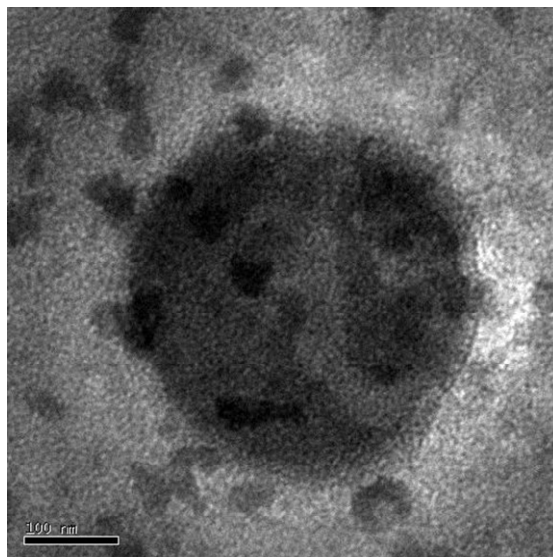


Fig. S10 TEM image of **1** recorded by drop casting an aggregated sample of **1** on a copper grid with uranyl acetate as the staining agent.

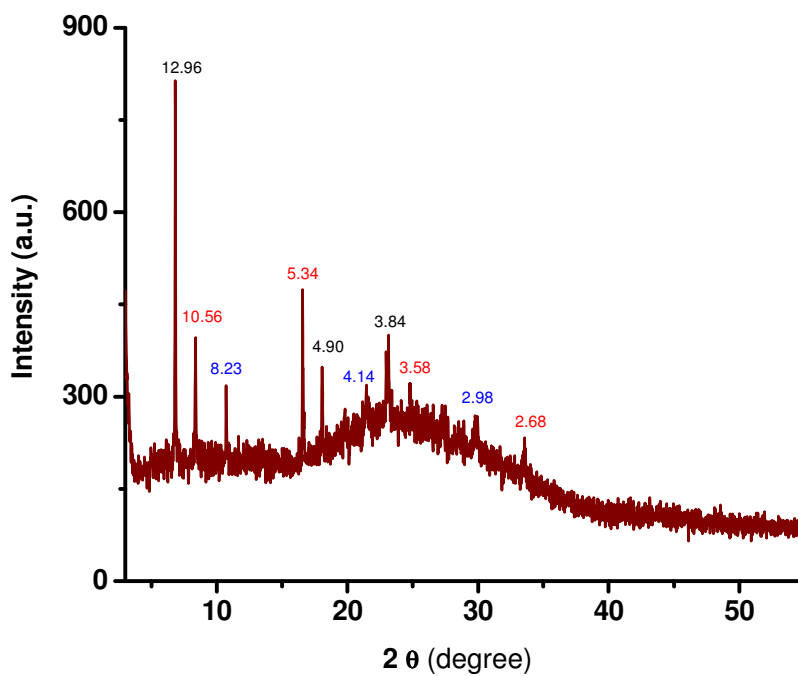


Fig. S11 PXRD pattern of **1** in the crystal state.