

Electronic Supplementary Information (ESI)

Energy Transfer Mediated White Light Emission from Nile Red Doped 9,10-diphenylanthracene Nanoaggregate upon Excitation with Near UV-Light

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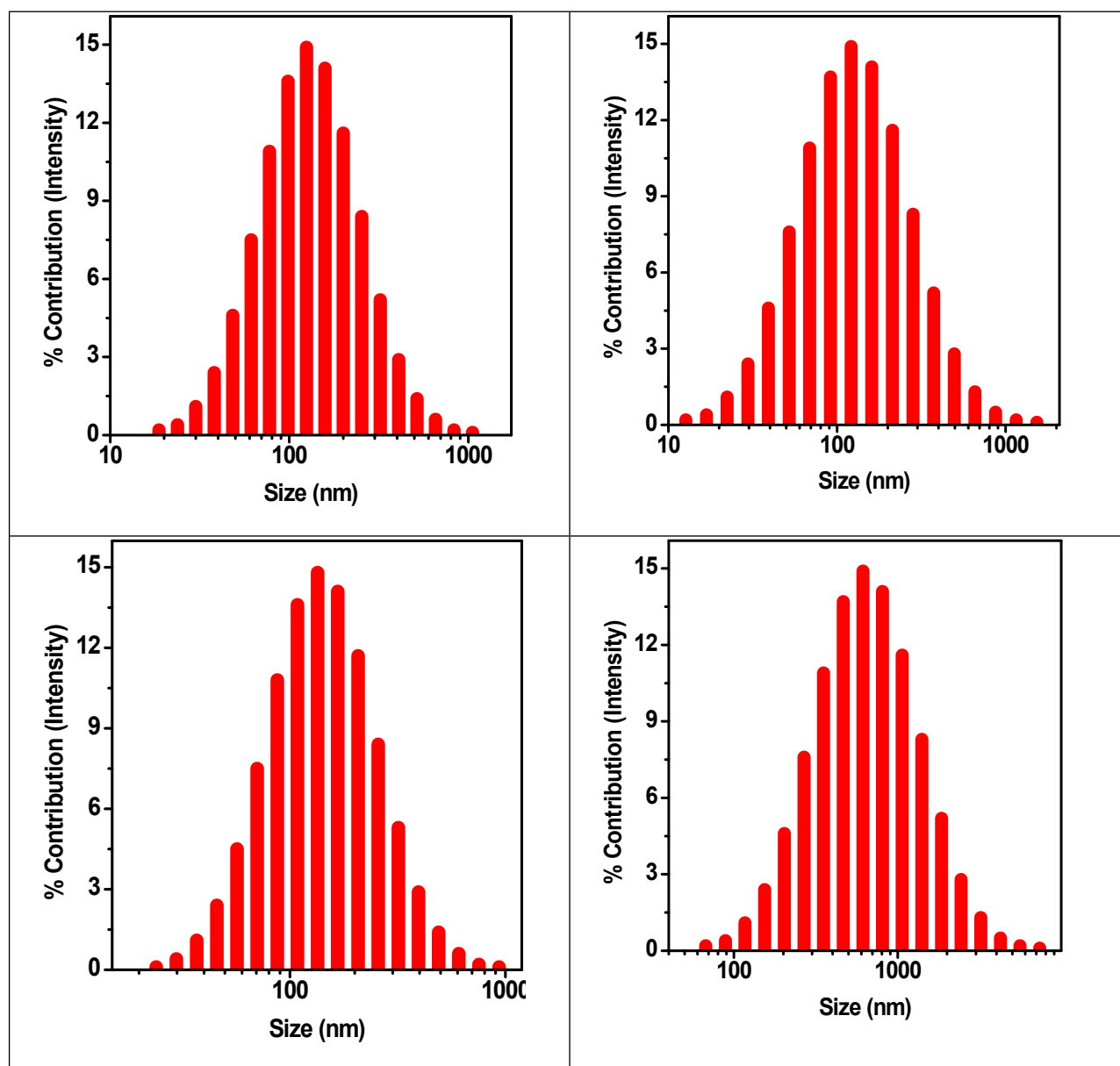


Figure S1: Size distribution obtained from DLS measurements (A) DPA NA, (B) 0.032 % NR doping, (C) 0.4% NR doping and (D) NR NA

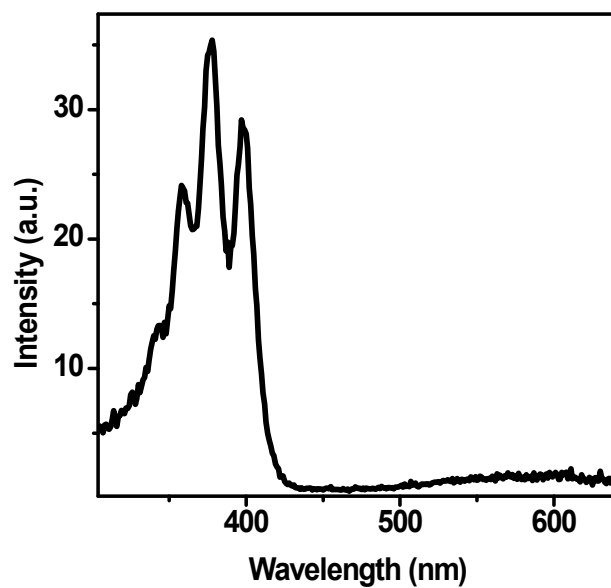


Figure S2: The excitation spectra recorded for 650 nm emission with 0.06% NR doped 9,10-DPA NA sample

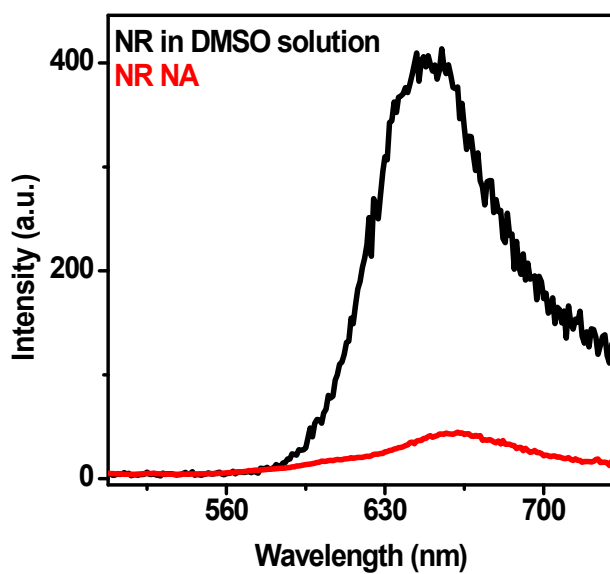


Figure S3: photoluminescence spectra recorded with 350 nm light excitation for NR in DMSO solution and NR NA synthesized using reprecipitation method. It shows almost on order decrease in emission quantum yield for nanoaggregate sample.

Table S1: Fluorescence quantum yield and CIE 1931 (X,Y) coordinate values for different Nile red doped 9,10-DPA NA samples.

Dopant %	Φ_f	CIE 1931 Coordinate	
		X	Y
0	0.4	0.221	0.324
0.008	0.39	0.25	0.333
0.016	0.423	0.26	0.33
0.032	0.442	0.281	0.334
0.04	0.451	0.3	0.342
0.05	0.438	0.315	0.342
0.06	0.443	0.325	0.343
0.076	0.432	0.335	0.346
0.1	0.398	0.356	0.35
0.2	0.32	0.393	0.349
0.4	0.221	0.425	0.359
1	0.136	0.442	0.366
2	0.107	0.446	0.363

Nile red in DMSO : X=0.65, 0.3

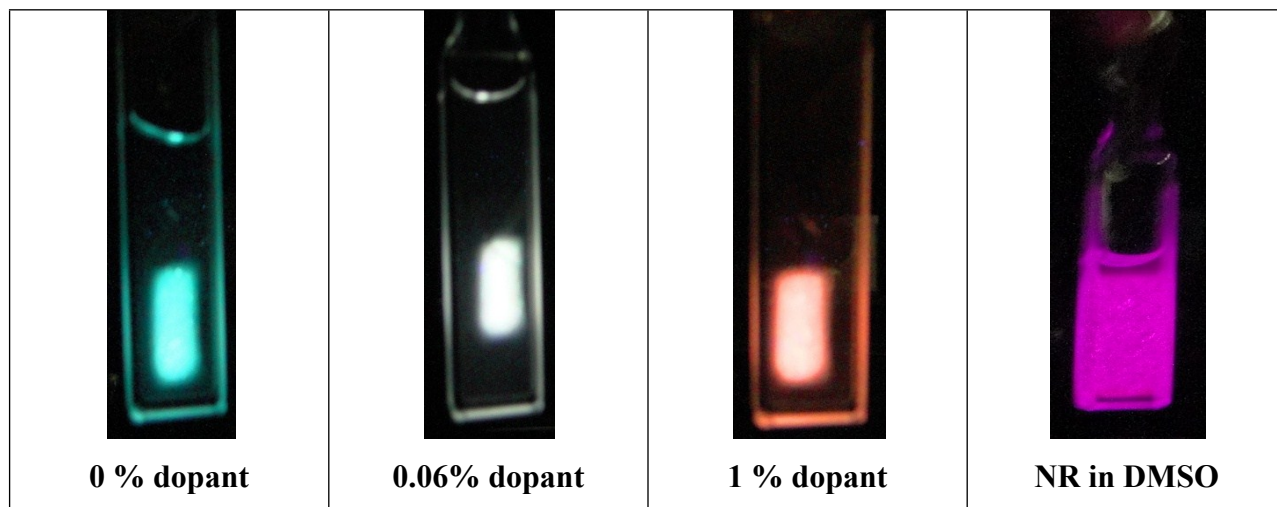


Figure S4: Photograph of the different NR doped 9,10-DPA sample under 355 nm light illumination.

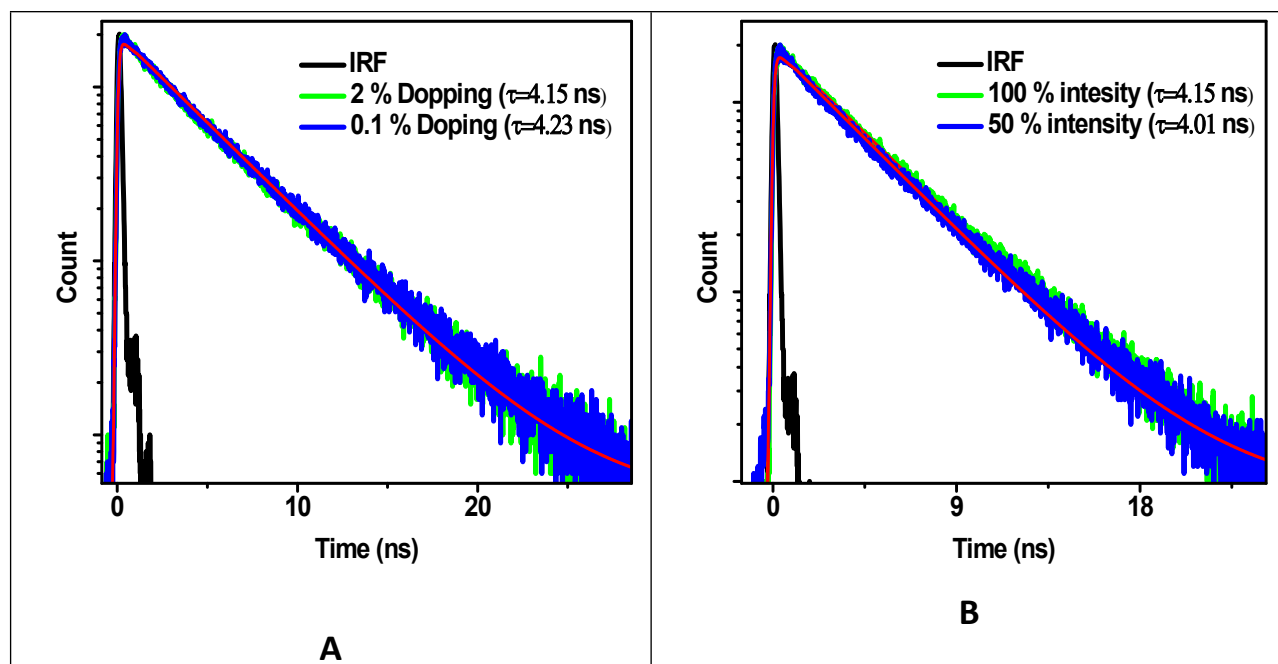
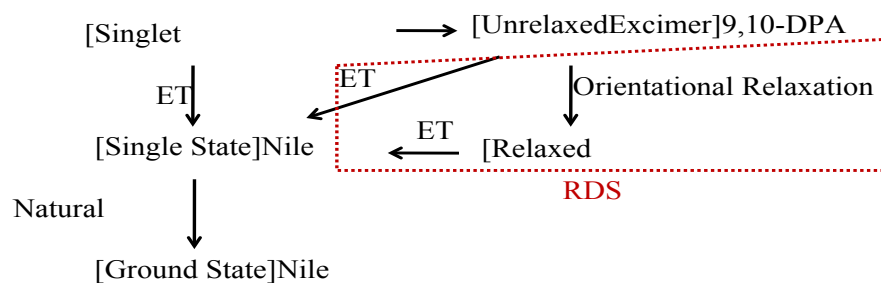


Figure S5: (A) Temporal profiles recorded at 640 nm after exciting the doped nanoaggregates samples with 510 nm light. (B) The temporal profiles recorded with 2 % NR doped DPA nanoaggregates after exciting with full intensity of 510 nm light and half intensity of the initial.

Scheme S1: Sequential photoexcited processes of nile red in nile red doped 9,10-DPA nanoaggregates



CalculationS1: Estimation of nile red concentration (for 2 % doping) inside nanoaggregates

$$\text{Volume of the nanoaggregate} = \pi \times (125/2)^2 \times 50 \text{ nm}^3 = 6.13 \times 10^5 \text{ nm}^3$$

Volume of one 9,10-DPA is $\sim 0.31 \text{ nm}^3$ (Estimated from molecular volume calculation following reference: J. Chem. Educ. 1970, 47, 261-270)

$$\text{Number of 9,10-DPA in one aggregate} = 6.13 \times 10^5 / 0.31 = 2 \times 10^6$$

2% doping of NR: Number of NR in one NA = 4×10^4

Molecular concentration of NR in NA = $4 \times 10^4 \times 10^{24} / 6.13 \times 10^5 \times 6.023 \times 10^{23} = 0.108 \text{ M}$ or 108 mM

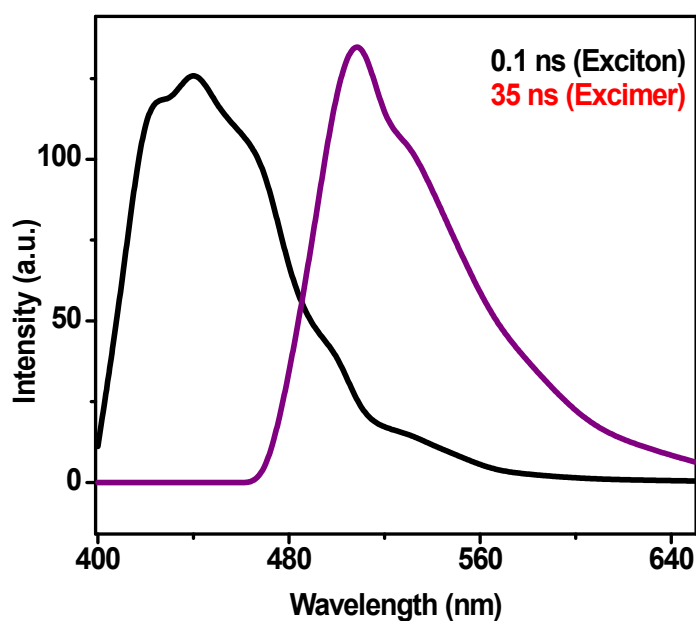


Figure S6: *TRANES spectra obtained at 0.1 ns and 35 ns delay with pure DPA nanoaggregates*

Text S1: Simulation procedure through Matlab software module (For excimer donor and NR acceptor)

Our simulation follows these steps,

- 1) Estimation of the average number of acceptor molecules present per nanoaggregate for different concentration of the acceptor.
- 2) The minimum distance between the acceptor and donor species = molecular radius of donor + molecular radius of acceptor = 1.07 nm
- 3) We have generated random position of the donor or DPA exciton inside one nanoaggregate (say j^{th} nanoaggregate). Then the acceptor positions are generated randomly inside this nanoaggregate. The distance between the donor and acceptor has been calculated. This distance

must be greater than 1.07 nm. To impose this condition, we have rejected all such conditions where the evaluated distance between any donor and acceptor species is less than 1.07 nm. The condition where all the donor – acceptor distances are more than 1.07 nm are only considered for the next step of the simulation. Among these distances the minimum intermolecular distance between donor and acceptor species has been shorted and taken for k'_{ET} calculation.

Although the dipole-dipole interaction between donor and acceptor molecule can occur for all the donor-acceptor pairs inside a nanoaggregates, we expect energy transfer to a single acceptor molecule only. Because of the resonance energy transfer condition one donor should not donate its energy to multiple acceptors, simultaneously. The ET rate constant follows R^{-6} relationship. Therefore, we expect in most of the cases the energy transfer will take place to the nearest acceptor molecule. Thus we estimate the ET rate constant considering the minimum intermolecular distance (R_j) between the donor-acceptor pair. We have taken 9.5 ns lifetime for excimer donor for this calculation. R_0 value is estimated for excimer - Nile red pair having value of 3.9 nm.

4) Thousands of nanoaggregates remain present in the excitation region, during steady state and TCSPC study. The observed ET rate is actually the average feature for all those nanoaggregates. Therefore, to evaluate the similar condition, we have estimated the ET rate for 5000 cases (equivalent to N_p) and finally take the average value.