Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Fluorescence Resonance Energy Transfer in Multifunctional Nanofibers Designed *via* Block Copolymer Self-Assembly

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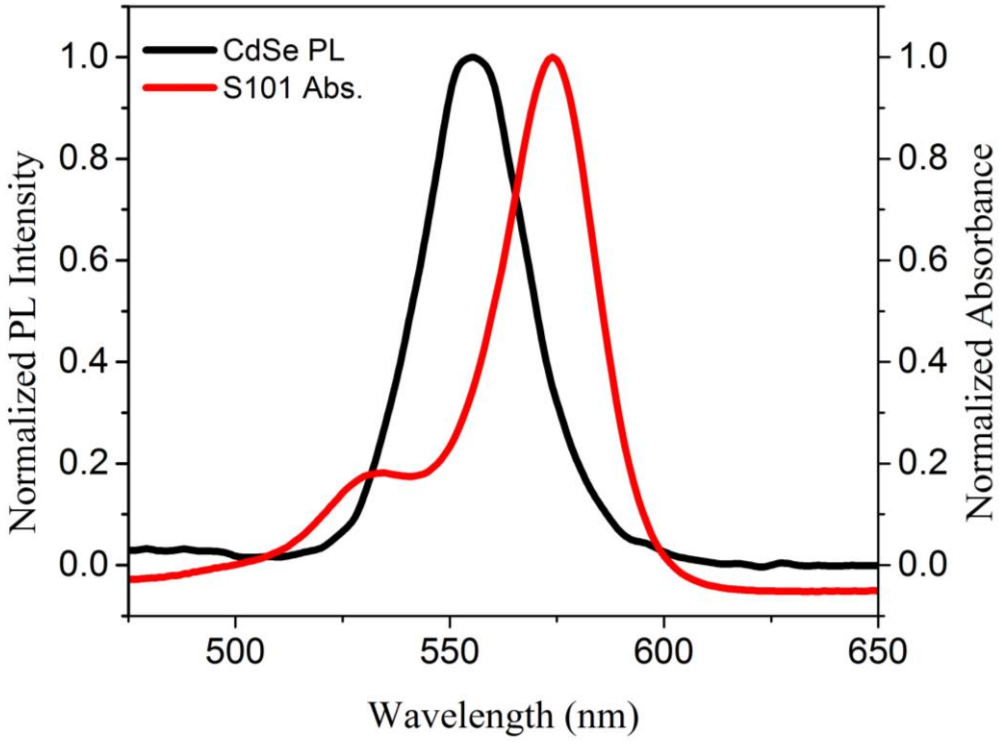

Figure S1: Overlapping of emission spectrum of CdSe QDs in black line and absorption spectrum of S101 dye in red line.

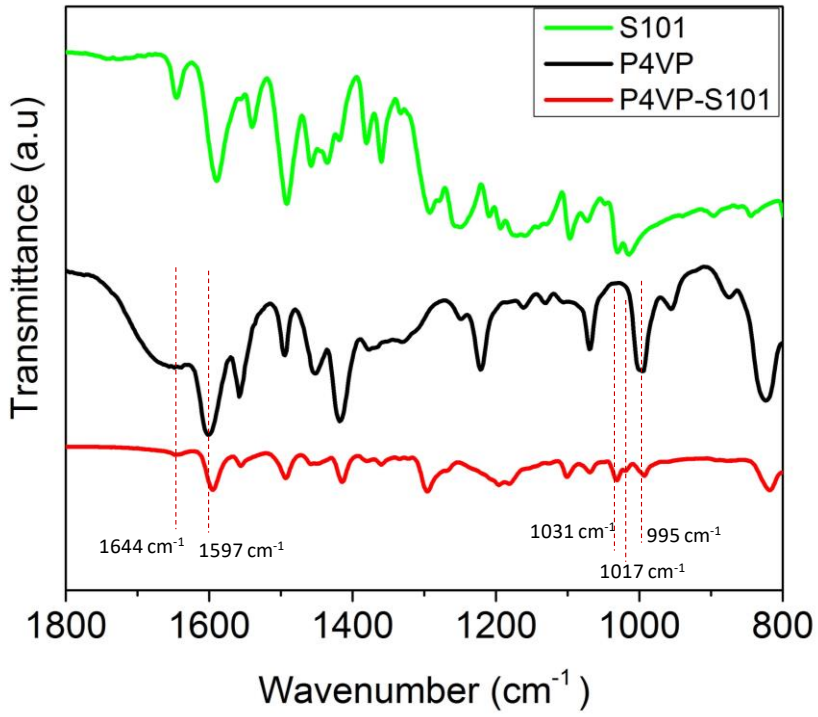

Figure S2: FTIR spectra for the ionic complexation between the P4VP and S101 dye at the ratio of 1:0.05, respectively.

The chemical association of S101 molecules to P4VP was ascertained by FTIR, as shown in Figure S2. As per the past studies on similar complexes, the most affected bands of P4VP are the stretching bands at 1597, 1570, and 995 cm^{-1}. Figure S2 depicts that the intensity of pure P4VP absorption band at 995 cm^{-1} diminished on complete protonation and gets replaced by two new bands of almost similar strength at 1017 and 1031 cm^{-1}. The characteristic bands of pure P4VP at 1570 and 1597 cm^{-1} were observed due to the pyridine ring stretching. On complete protonation, the bands are replaced by an extra band at 1644 cm^{-1}, which can be attributed to the hydrogen-bonded pyridinium ring.

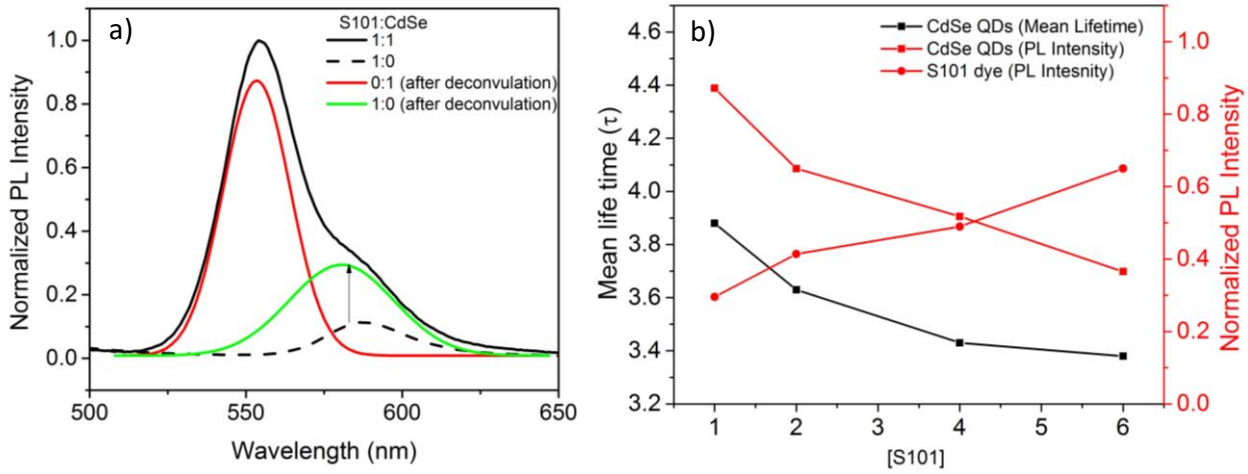

Figure S3: (a) Normalized PL Spectra of RBCP/S101 composite solution in the absence (Dashed line) and presence of CdSe QDs (Solid line). Spectra have been deconvoluted into two separate contributions from the QDs and dye. The red line is the contribution only from CdSe whereas green line is the contribution only from S101, as obtained after deconvulation of the solid black line for S101:CdSe 1:1 case. (b) Quenching of PL emission and mean lifetime of CdSe QDs, and enhancement in PL emission of S101 dye at different dye to QD ratio.

Calculation S1: Calculation of the Distance between QDs and S101 from the Decay curves in Figure 7 of the main article[1]

First, FRET efficiency (E) was calculated using $E = 1 - \tau_{DA}/\tau_D$, where, τ_{DA} and τ_D denotes the lifetime of the donor in the presence and absence of the acceptor, respectively. Then, the distance (r) between the CdSe QDs donor and the S101 dye acceptor were calculated, considering single donor and single acceptor interaction, by the following expression as eq. (1)

$$E = \frac{{R_0}^6}{{R_0}^6 + r^6} \qquad (1)$$

Where, R_0 is the Förster radius (4.21 nm). Accordingly, the calculated distance (r) was 5.63, 5.28, 5.06 and 5.02 for 1:1, 2:1, 4:1 and 6:1 molar ratio of S101 dye:CdSe QD, respectively.

Calculation S2: The rate constant (k_q) of energy transfer process was calculated by the following expression:

$$k_q = \frac{1}{\tau_D}\left(\frac{R_0}{r_n}\right)^6 \qquad (2)$$

Where the value for lifetime of the donor in the absence of acceptor (τ_D) and Förster distance (R_0) were constant and found to be 4.56 ns and 4.21nm, respectively. The τ_D was calculated from eq. (3) described in the experimental section of the manuscript whereas R_o was found using PHOTOCHEMCAD software and is explained in the main manuscript (page 19). Furthermore, the value for average distance (r_n), for the single donor-multiple acceptor case, was 5.89, 5.64, 5.45 and 5.54 for 1:1, 2:1, 4:1 and 6:1 molar ratio of S101 dye: CdSe QD, respectively. This was found using eq. (9) given in the manuscript. Using all the above respective values, the rate constant (k_q) of energy transfer process was calculated as summarized in Table S3.

Table S1: Composition details of BCP/CdSe/S101 composites

Sample[a]	f_{PS}[b]	f_{P4VP}[c]	f_{CdSe}[d]	f_{S101}[e]
BCP	0.7350	0.2649	0	0
(0:1)	0.6916	0.2493	0.059	0
(1:1)	0.6915	0.2493	0.059	0.0002
(2:1)	0.6913	0.2492	0.059	0.0005
(4:1)	0.6909	0.2490	0.058	0.0010
(6:1)	0.6906	0.2489	0.058	0.0015

[a]composition in terms of molar ratio of CdSe/S101

[b]volume fraction of PS block

[c]volume fraction of P4VP block

[d]volume fraction of CdSe QDs

[e]volume fraction of S101 dye

Table S2: The values of quenching parameters of CdSe QDs in the presence of dye using kinetic model

Sample	τ_0 (ns)	m_{dt}	τ_{dt} (ns)	m_{st}	τ_{st} (ns)	m_q	τ_q (ns)
(0:1)	48.6	2.72	0.004	1.74	13.28	-	-
(1:1)	48.6	2.04	0.004	1.89	13.28	1.32	0.56

(2:1)	48.6	0.28	0.004	1.96	13.28	1.48	0.48
(4:1)	48.6	1.67	0.004	2.77	13.28	1.54	0.43
(6:1)	48.6	0.60	0.004	0.99	13.28	1.80	2.79

Table S3: Average number of S101 dye molecules around the single CdSe QDs and the average distance (r_n) considering single donor-multiple acceptor system for different concentration of S101 using the FRET theory

Sample	**R_0**	**τ_{DA} (ns)**	**τ_D (ns)**	**E(FRET)=1-(τ_{AD}/τ_A)**	**m_q (no. of dye molecules)**	**r_n(distance btw A and D) (nm)** $= R_0 \left(\frac{m_q(1-E)}{E}\right)^{1/6}$	k_q (rate constant) (ns^{-1}) $= \frac{1}{\tau_D}\left(\frac{R_0}{r_n}\right)^6$
(1:1)	4.21	3.88	4.56	0.15	1.32	5.89	0.03
(2:1)	4.21	3.63	4.56	0.20	1.48	5.64	0.04
(4:1)	4.21	3.43	4.56	0.25	1.54	5.45	0.05
(6:1)	4.21	3.38	4.56	0.26	1.80	5.54	0.04

1) Sadhu, S.; Haldar, K. K.; Patra, A. Size Dependent Resonance Energy Transfer Between Semiconductor Quantum Dots and Dye Using FRET and Kinetic Model. *The Journal of Physical Chemistry C* **2010**, *114* (9), 3891–3897. https://doi.org/10.1021/jp911801m.