CHEMPHYSCHEM

Supporting Information

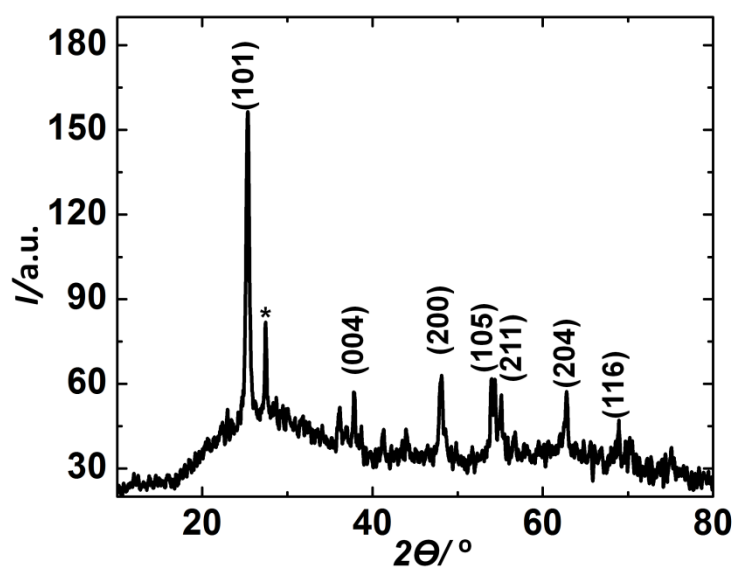# Energy Relay from an Unconventional Yellow Dye to CdS/CdSe Quantum Dots for Enhanced Solar Cell Performance

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Supporting Information

Figure S1 X-ray diffractograms of TiO$_2$ nanoparticles, the hkl values are expressed within parentheses.

The d-values observed by us match well with the body centered tetragonal crystal structure of TiO$_2$ (anatase) in accordance with the PDF file number 894921. The HRTEM lattice scale image of TiO$_2$ is shown below (Figure S2). The interplanar separation is observed to be 0.36 nm which agrees well with the d-spacing of 0.351 nm corresponding to the <101> reflection of the anatase phase. This result is in line with the XRD pattern wherein, the most intense peak also corresponds to the <101> plane.
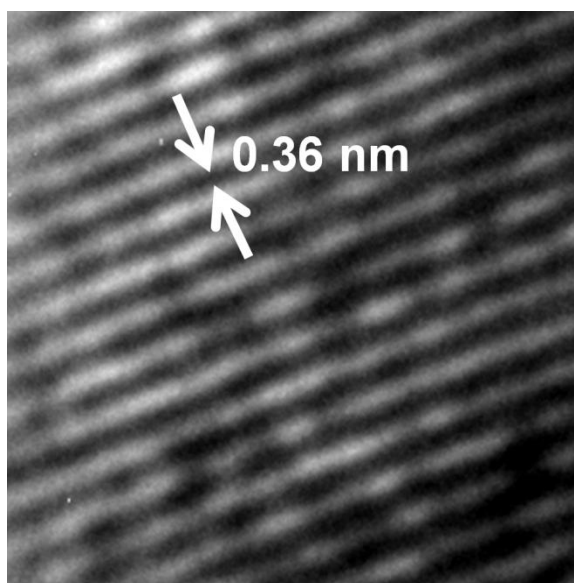
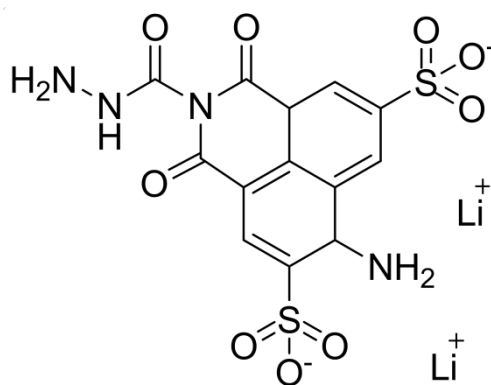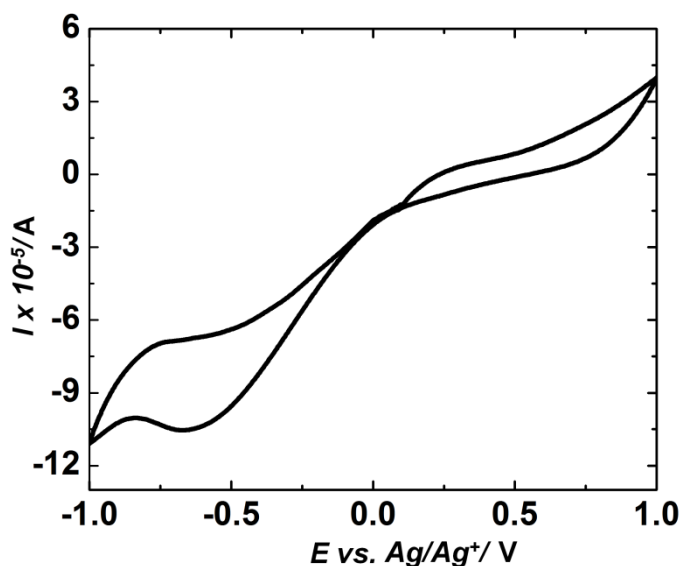**Figure S2** Lattice scale image of TiO$_2$.


Figure S3 Structure of LY dye.

Figure S4 Cyclic voltammogram of an aqueous solution of a LY dye with two platinum rods as the working and counter electrodes and Ag/AgCl/KCl as a reference electrode.

The reduction potential of the LY dye is at ∼ −0.608 V from Figure S4. The potential of the reference electrode is +0.197 V.

Therefore, E_{Red} (*versus* NHE) = −0.608 − (+0.197) V = −0.411 V. The reduction potential of −0.411 V (*versus* NHE) corresponds to the conduction band position of 4.08 eV for the LY dye. The band gap of Lucifer yellow dye obtained from the optical absorption spectrum is 2.88 eV. Therefore the position of valence band is 6.96 eV ($E_g = E_{VB} − E_{CB}$).
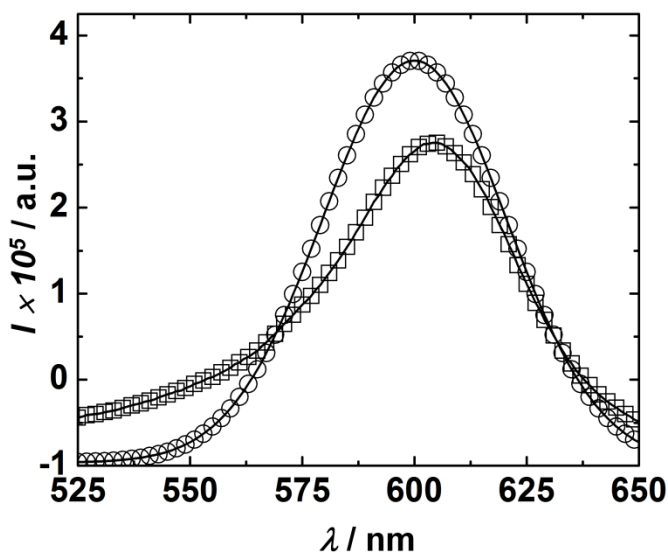
Figure S5 Luminescence spectrum of the pristine TiO$_2$/CdS/CdSe/ZnS electrode (O) is quenched in the presence of an aqueous solution of PEDOT microfibers (□) due to hole transfer from the QDs to PEDOT (λ_{ex} = 370 nm).

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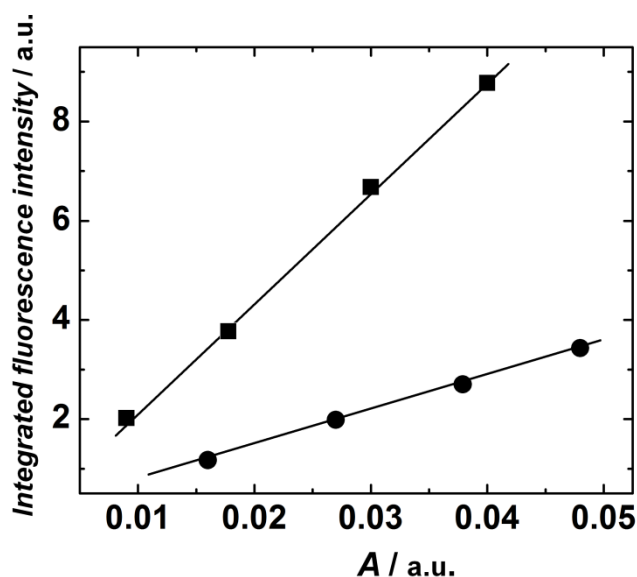
Figure S6 Integrated fluorescence intensity versus absorbance of LY dye (•) and reference: Rhodamine 6G (■). The excitation wavelength was fixed at 430 nm for the LY dye and 480 nm for Rhodamine 6G.

$$\phi_X = \phi_{ST}\,(Grad_X\,/\,Grad_{ST})\,(\eta^2_X\,/\,\eta^2_{ST}) \tag{1}$$

In equation (1), X and ST denote the test and the standard or reference samples. ϕ, Grad and η respectively denote the quantum yield, slope of the integrated fluorescence intensity *versus* absorbance and the refractive index of the solvent. By substituting the experimental values in equation (1), equation (2) is obtained.

$$Q_D = \phi_X = 95 \times 70\,/(211)\,(1.33^2/\,1.36^2) \tag{2}$$

From equation (2), the quantum yield for LY dye was calculated to be 0.30. In a similar vein the quantum yield of CdS/CdSe QDs was determined to be 0.28.
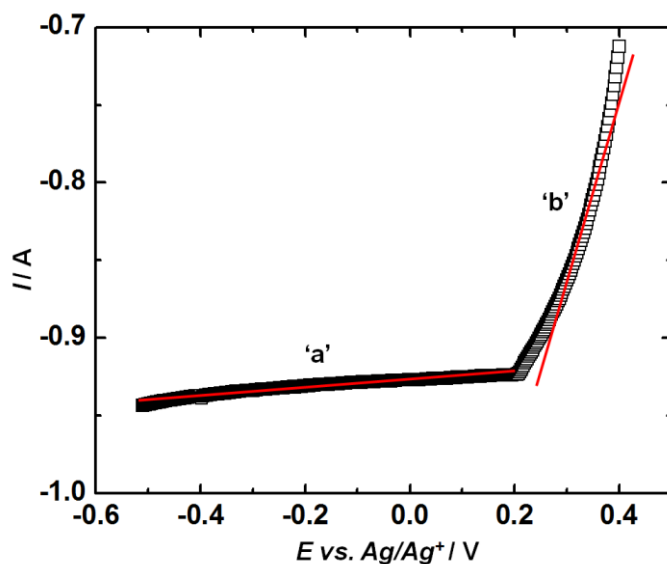

Figure S7 Linear sweep voltammogram of PEDOT microfibers with two Pt electrodes.

The linear sweep voltammogram of PEDOT microfibers in Figure S7, shows different slopes in the region marked as 'a' (between −0.5 to +0.2 V) and in the region marked as 'b' (between +0.2 to +0.4 V) a a function of applied potential. The conductivity (σ) of PEDOT fibers was deduced from the linear fits in the two potential domains, by using σ = Slope (I/V) × l/a, where l is the distance between the

electrodes and a is the area of the electrode. The conductivities in regions 'a' and 'b' were found to be 0.025 and 0.97 S cm^{-1}. The average value of conductivity was therefore 0.5 S cm^{-1}, which is acceptable for use of PEDOT fibers as a hole transport layer.
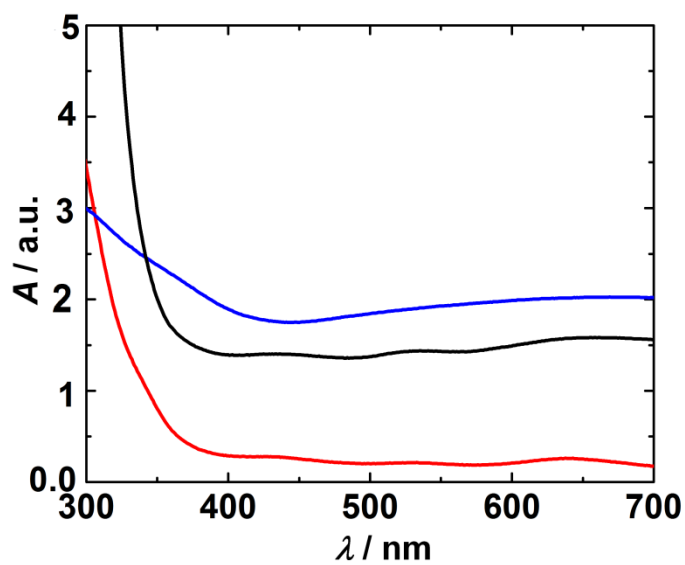
Figure S8 Absorption spectra of an aqueous solution of PEDOT microfibers (━), PEDOT/Na$_2$S gel (━) and Na$_2$S gel (━).
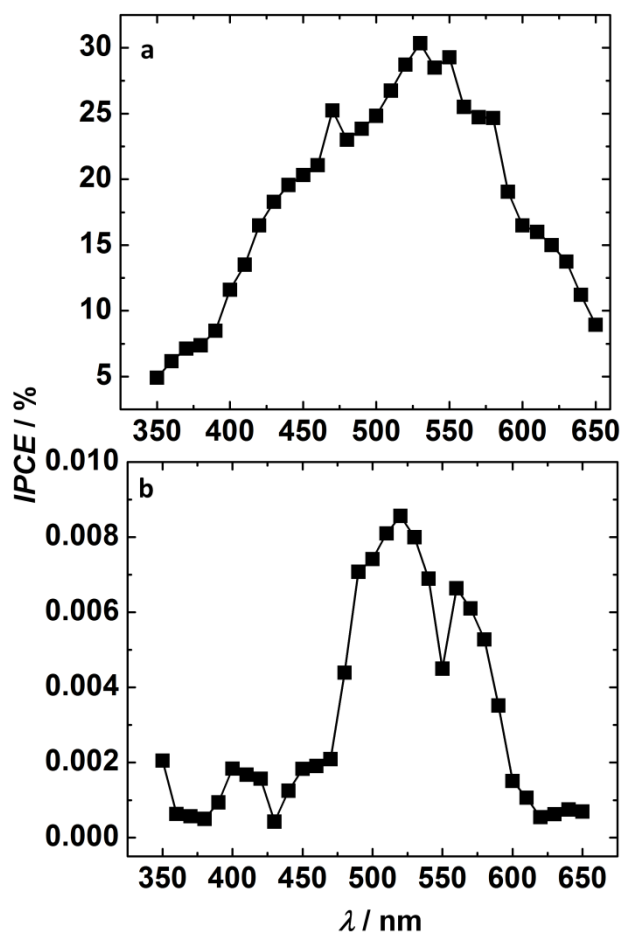
Figure S9 (a) IPCE spectra of the donor-acceptor cell: $TiO_2/CdS/CdSe/ZnS–LY/S^{2-}–MWCNT$ with 2 layers of ZnS and (b) the donor only cell: $TiO_2/LY–S^{2-}–MWCNT$.

It is known that the FRET efficiency is maximum when the donor is separated from the acceptor by a distance ranging between 1 to 10 nm. The reason for restricting to only one layer of ZnS is based on the decrease in IPCE ongoing from one to two layers of ZnS, while all other components remain the same. IPCE of the donor acceptor cell: $TiO_2/CdS/CdSe/ZnS–LY/S^{2-}–MWCNT$ cell with 2 layers of ZnS is 30 % (at 530 nm) whereas it is 53 % for the same cell with one layer of ZnS. The IPCE of the donor only cell: $TiO_2/LY–S^{2-}–MWCNT$, was abysmal, with a value of only 0.009 %, thus ratifying the sole LY dye in the absence of an appropriate acceptor does not transfer excited electrons to TiO_2, and is absolutely incapable of harvesting solar radiation. The donor only cell was fabricated by dipping the TiO_2 electrode in a LY dye solution for 16 hours; the superfluous dye was washed off by repeated rinsing in deionized water; the yellow colored TiO_2/LY electrode was dried prior to assembling the cell. The sulfonate groups on the dye bind to TiO_2 via electrostatic interaction with the Ti^{4+}.