

## Supplementar Information

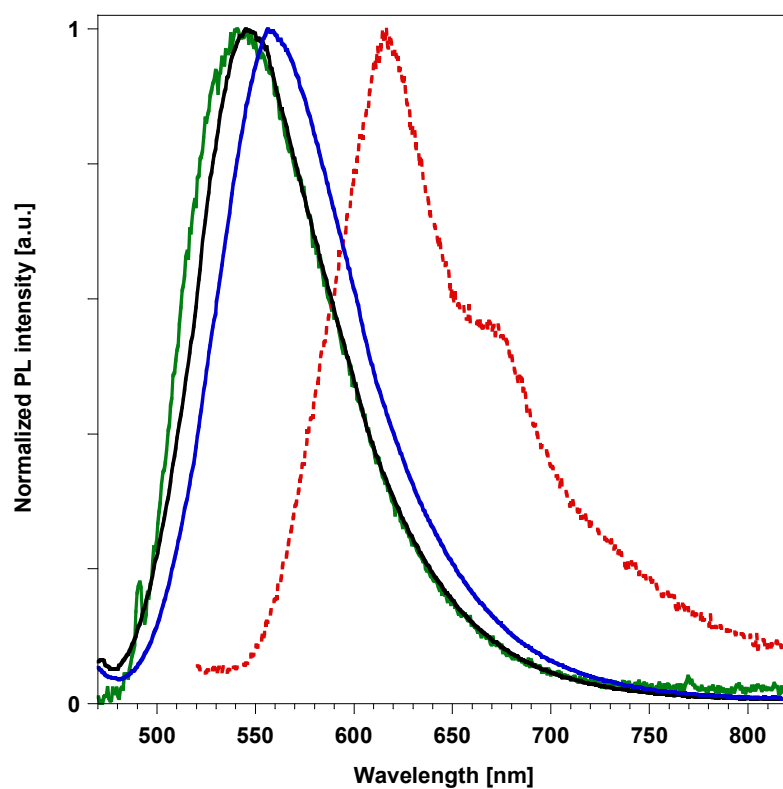
### **Light Harvesting of CdSe/CdS quantum dots coated with $\beta$ -cyclodextrin based host-guests through Resonant Energy Transfer from the nitrobenzoxadiazole guests.**

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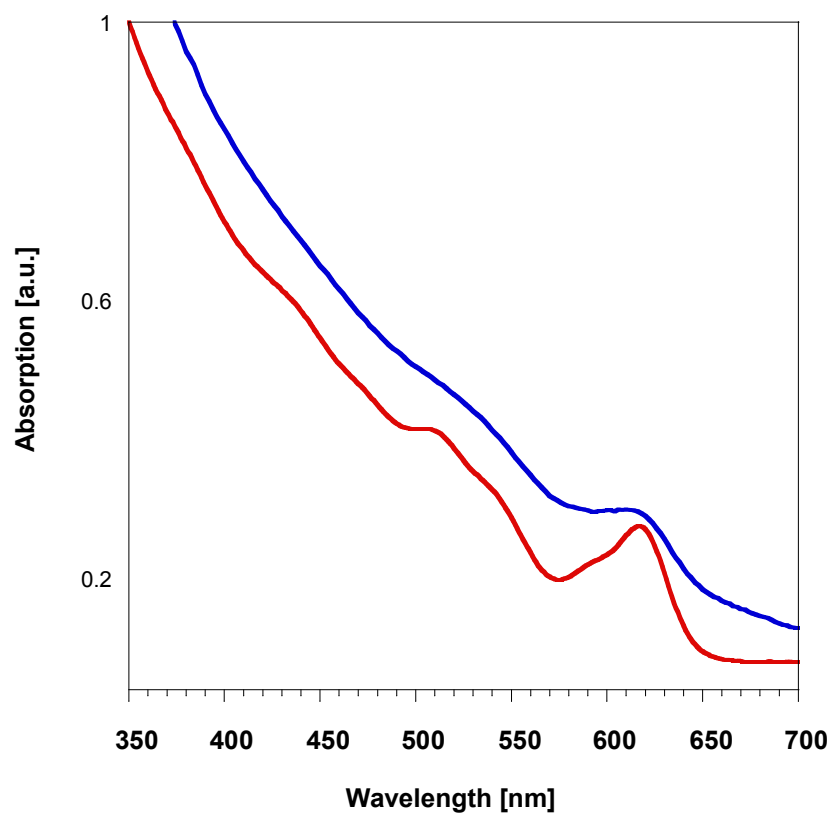
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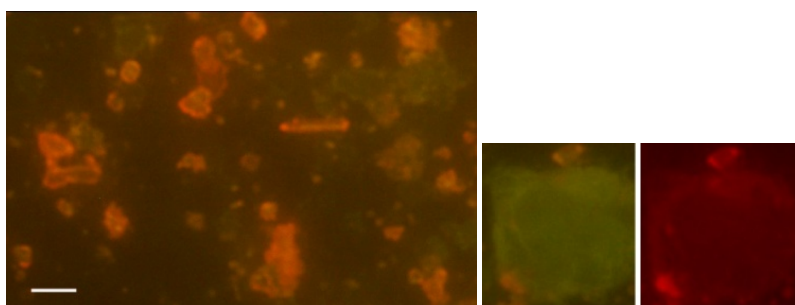
**Figure S1.** Normalized PL spectra of NBD(1) powders (red dotted line); NBD(1) dissolved in methanol (green line); CD/NBD(1) (black line) and CD(3)/NBD(1) (blue line) powders.

**Table S1** PL QY of NBD(1) dissolved in different solutions; NBD(1), CD/NBD(1) and CD(3)/NBD(1) solid state

	QY
Ethyl acetate	39%
THF	45%
dichloromethane	41%
methanol	20%
acetonitrile	59%
NBD(1) (solid state)	0.7%
CD/NBD(1) (solid state)	26%
CD(3)/NBD(1) (solid state)	14%



**Figure S2.** Absorption spectra of QD (red line) and QD/CD(3) (blue line) in solution



**Figure S3.** Fluorescence microscopy images of QD/CD(3)/NBD(1) complex dispersed in PVA films. Scale bar 10  $\mu\text{m}$ . Left: excitation at 330-380nm. A detail of a film is excited at 330-380nm (centre image) and 510-560nm (right side image) in order to excite the QD selectively and highlight the aggregate homogeneity.

### CD(3)/NBD(1) vs QD molar ratio in films

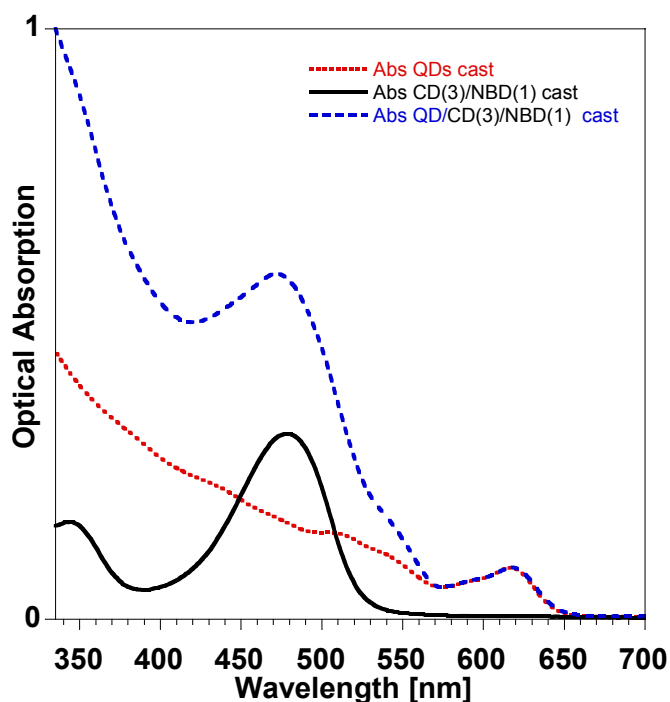
The theoretical number of NBD(1) molecules per QD ( $\#_{ideal}$ ) was determined as the ratio of the QD external surface to the cyclodextrin base area, the former calculated considering the QDs as spherical nanoparticles with radius  $R_{QDs}$  (2.8 nm), and the latter calculated taking into account the cyclodextrin outer radius  $r_{CD}$  (0.765 nm):<sup>1</sup>

$$\#_{ideal} = \frac{4\pi R_{QDs}^2}{\pi r_{CD}^2} = 53.5$$

Simultaneously, the actual number of dye molecules per QD ( $\#_{experimental}$ ) was extracted from the absorption spectra of the films, knowing the molar extinction coefficient of the two components. Being the dye ( $C_{CD(3)-NBD(1)}$ ) and QDs ( $C_{QD}$ ) molar concentration,<sup>7</sup>

$$\#_{experimental} = \frac{C_{CD(3)/NBD(1)}}{C_{QD}}$$

$C_{QD} = 1.3 \times 10^{-7}$  M was obtained by dividing the optical density at the first excitonic band maximum in the absorption spectrum of a casted film of QDs



$C_{S-CD-NBD}$  was then calculated according to the following formula:<sup>2</sup>

$$\frac{OD_{QD/CD(3)/NBD(1)}^{480nm} - \left( \frac{OD_{QD/CD(3)/NBD(1)}^{615nm}}{OD_{QDs}^{615nm}} \times OD_{QDs}^{480nm} \right)}{\varepsilon_{CD(3)/NBD(1)}^{480nm}} = 1.3 \times 10^{-7} M$$

where the subscripts  $QD/CD(3)/NBD(1)$ ,  $QDs$  and  $CD(3)/NBD(1)$  relate to the complex,  $QDs$  alone and dye alone absorption spectra respectively, and the superscripts 480nm and 615nm relate to the dye and  $QDs$  first excitonic absorption band maxima respectively.

Since the so-calculated  $\#_{experimental}$  (140) is almost two and a half times higher than  $\#_{ideal}$ , we assume that the number of host-guest complexes in excess are not attached to any  $QD$  and do not necessarily participate in the FRET process. Nevertheless, part of these unattached complexes might contribute to the energy transfer, and, in order to understand their role in this process, it is necessary to calculate the Förster radius.

### Förster radius

The Förster radius  $R_0$  can be estimated according to the following formula:

$$R_0 = 8.97 \times 10^{-5} [k^2 n^{-4} QY_D J(\lambda)]$$

where  $k^2$  is the orientation factor, assumed to be 2/3 for randomly oriented dipoles,<sup>3</sup>  $n$  is the refractive index of the medium (assumed to be 1.54 in cyclodextrin-based systems),  $QY_D$  is the quantum yield of the donor in the absence of the acceptor (0.14) and  $J(\lambda)$  expresses the degree of spectral overlap between the donor emission and the acceptor absorbance. The latter can be calculated as follows:<sup>3</sup>

$$J(\lambda) = \frac{\int_0^{\infty} F_D(\lambda) \varepsilon_A(\lambda) \lambda^4 d\lambda}{\int_0^{\infty} F_D(\lambda) d\lambda} \cong 5.8 \times 10^{16} \text{ cm}^{-1} \text{ M}^{-1} \text{ nm}^4$$

where  $F_D$  is the corrected fluorescence intensity of the donor and  $\varepsilon_A$  is the molar extinction coefficient of the acceptor.

The resulting  $R_0$  is 6.7 nm.

It follows that all unattached complexes that fall within this limit contribute to the energy transfer process.

### References

- 1 M. Artemyev, E. Ustinovich, I. Nabiev, JACS 2009, 131, 8061
- 2 E.M.M. Del Valle, Process Biochemistry 2004, 39, 1033

3 J.R. Lakowicz, Principles of Fluorescence Spectroscopy, Kluwer Academic/Plenum Publishers, New York, 1999