Supporting Information

Spectral and photochemical properties of hybrid organic-inorganic nanosystems based on CdS quantum dots and merocyanine ligand

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Measurement and characterisation.

TEM. A transmission electron microscopy (TEM) imaging, high-resolution TEM (HRTEM) imaging and selected area electron diffraction (SAED) were performed on JEOL JEM-2100 transmission electron microscope operated at 200 kV. The TEM samples were prepared by placing a drop of the dilute chloroform solution of nanoparticles on the carbon coated copper grids and allowing the solvent to evaporate at room temperature.

XRD. X-ray diffraction measurements on powder samples were performed with a Siemens D500 diffractometer (CuKα1 radiation).

IR. ATR-FTIR measurements were collected using Perkin-Elmer Spectrum 100 FTIR spectrometer equipped with ATR accessory.

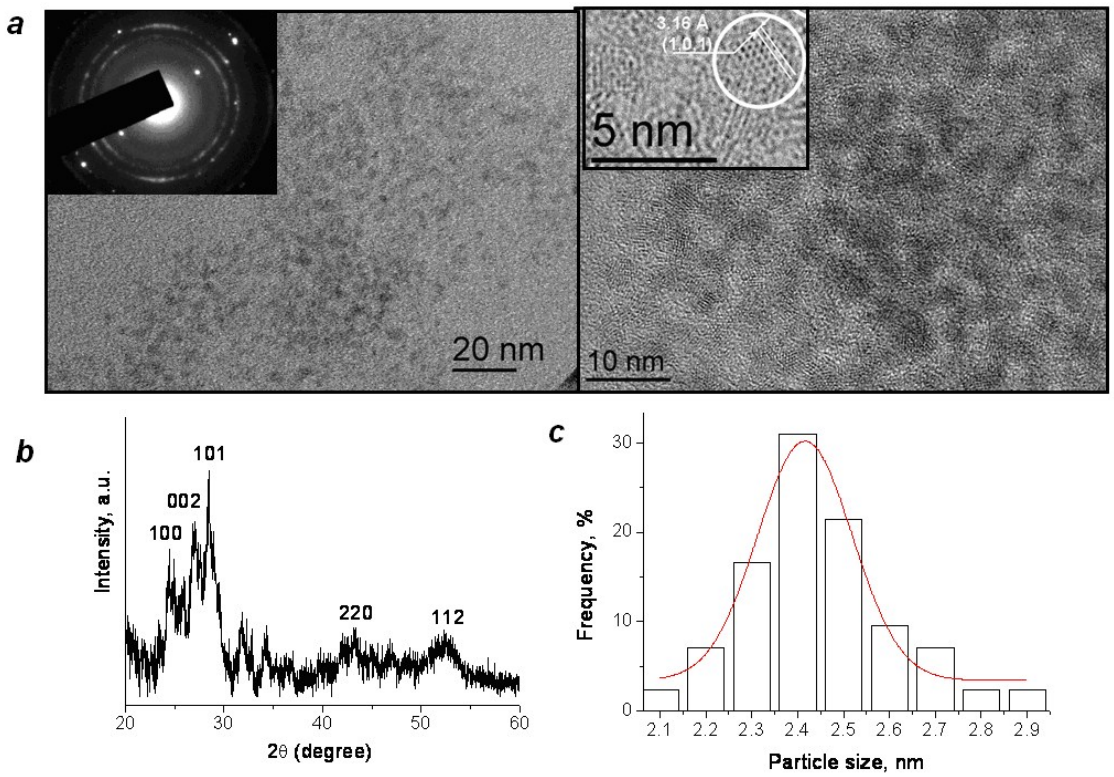

Fig. SI-1 Characterisation of the BM capped CdS nanocrystallites: *a* – TEM (insets: left – SAED, right - HRTEM), *b* – XRD, *c* – size distribution (histogram).

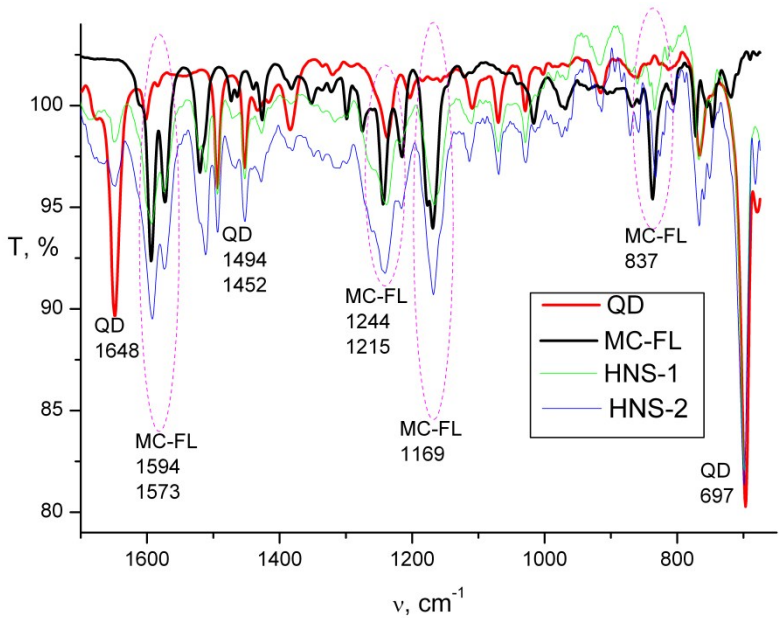

Fig. SI-2. ATR-FTIR spectra of the "free" CdS nanocrystallites (QD), merocyanine functional ligand (MC) and consisting of them investigated hybrid nanosystems (HNS-1, HNS-2).

Distance between QD and MC in HNSs calculation.

The distance between the QD and MC-FL in HNSs was calculated supposing the mechanism of energy transfer in this case being FRET (see discussion in the text).

Efficiency of the FRET from QD to MC (E_{FRET}) was calculated following the formula (1)[1]

$$E_{FRET} = 1 - \frac{\varphi_{DA}}{\varphi_D} \qquad (1)$$

where φ_D is the PL QY of the free QD (energy donor), φ_{DA} – QY of QD in the HNS (in the presence of energy acceptor – MC). Calculated E_{FRET} (lower bounds) are 38% for the HNS-1 and 50% for the HNS-2.

Calculated Forster radius (R_0) of the QD-MC donor-acceptor pair is 1.9 nm. Distance between donor (QD) and acceptor (MC) in HNS may be calculate from the E_{FRET} by the formula (2)

$$r = \sqrt[6]{\frac{1 - E_{FRET}}{E_{FRET}} * N} * R_0 \qquad (2)$$

where N is a number of the MC-FL in HNS.[1] Formal calculation for the HNS-1 (N = 1) gives an upper bound of the distance between QD and FL of 2.07 nm. However, it should be considered that in fact the HNSs of the different compositions are present in solution. According to the Poisson distribution,[2] in case of the average N = 1, the shares of the HNSs containing 0, 1, 2, 3, and 4 molecules of the FL are 37, 37, 18, 6 и 1.5 %, respectively. Hence, the observed for the HNS-1 φ_{DA} = 0.0025 is a superposition of the QYs for the set of HNSs. Considering the composition distribution, the real distance between donor and acceptor in HNS-1 is calculated to be 1.89 nm.

1. Medintz L., Mattoussi H., *Phys. Chem. Chem. Phys.*, 2009, **11**, 17
2. Budyka M.F., Chaschikhin O.V., Nikulin P.A., *Nanotechnol. Russ.*, 2016, **11**, 78.