Supporting Information

for

The influence of phthalocyanine aggregation in complexes with CdSe/ZnS quantum dots on the photophysical properties of the complexes

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Estimation of the extinction coefficients of the PcS_z molecules in monomeric and aggregated states

Figure S2 shows UV–vis absorption spectra of the PcS_z and QD solutions, which were used for the estimation of the extinction coefficients of the PcS_z molecules in monomeric and aggregated forms.

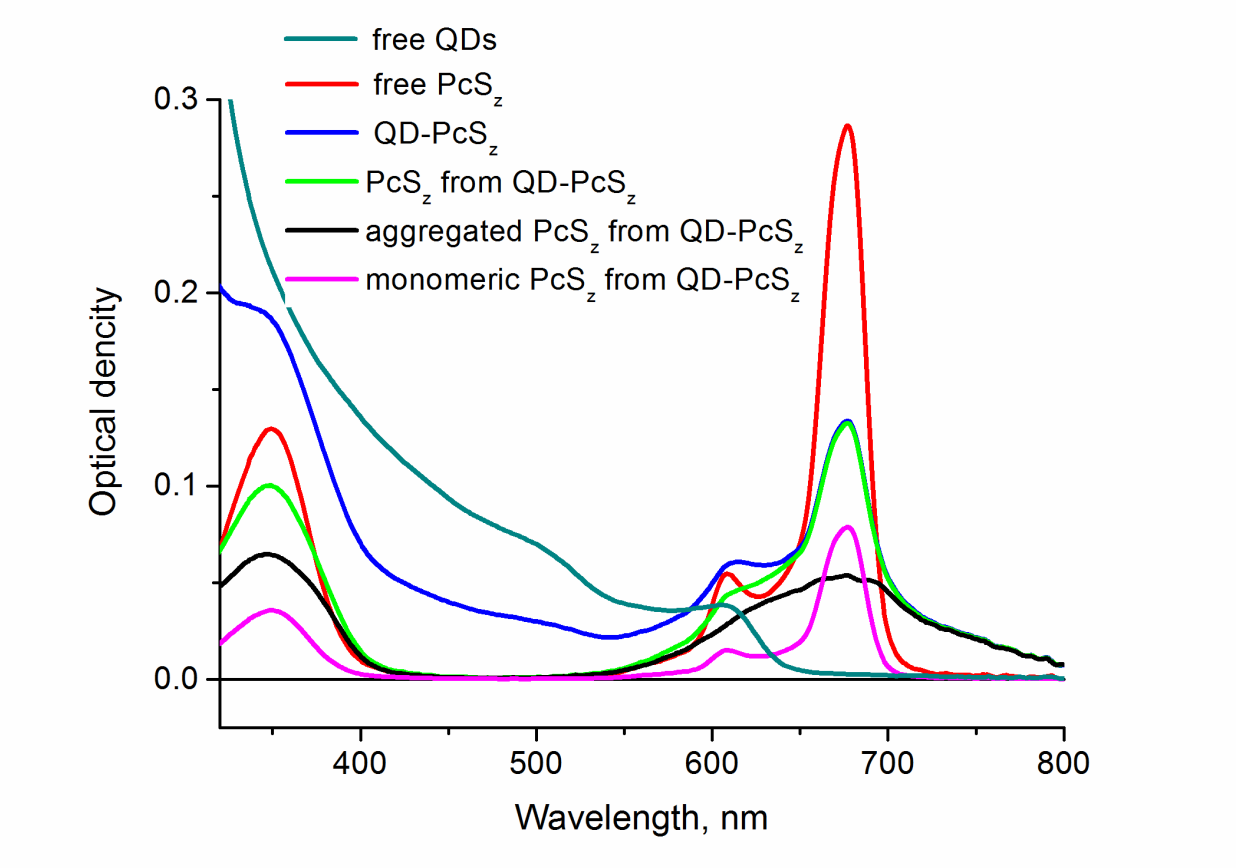

Figure S2: UV–vis absorption spectra of the PcS_z and QD solutions under study.

Complexes of quantum dots with phthalocyanine molecules with a high relative concentration of PcS_z, n ~ 50, were produced by the addition of the stock QD solution to the free PcS_z solution.

Analysis of the absorption spectrum of the mixture solution (blue curve, Figure S2) revealed PcS_z aggregation in the complexes with QDs. A decrease in the intensities of the Pc Soret band (350 nm) and the Q band (675 nm), as well as the appearance of the dimer band at 644 nm, were observed.

An absorption spectrum of the PcS_z in complexes with QDs (green curve) was obtained as a result of subtracting the QD absorption spectrum from the QD/PcS_z mixture absorption spectrum. The absorption spectrum of aggregates (black curve, Figure S2) was derived after subtracting the contribution of the monomeric PcS_z (pink curve, Figure S2) to the absorption spectrum of the PcS_z in the complexes with QDs.

Using a value for the monomeric PcS_z extinction coefficient of 1.75×10^5 $mol^{-1}cm^2$ for the Q band, the total PcS_z concentration C_a and PcS_z monomer concentration C_a^M were calculated from the free PcS_z (red curve, Figure S2) and monomeric PcS_z (pink curve, Figure S2) optical densities according to the Beer–Lambert law.

The concentration of the aggregated PcS_z molecules C_a^A was calculated from mass balance:

$$C_a^A = C_a - C_a^M . \quad \text{(S1)}$$

The extinction coefficients of the PcS_z molecules in monomeric and aggregate forms were calculated for direct PcS_z photoexcitation at a wavelength of 640 nm.

The data obtained are listed in Table S1.

Table S1: Concentrations and extinction coefficients of monomeric and aggregated PcS_z in the complexes with QDs.

C_a, μmol/L	1.64 ± 0.08
C_a^M, μmol/L	0.45 ± 0.018
C_a^A, μmol/L	1.19 ± 0.047
$\varepsilon_a^M(640)$, $mol^{-1}cm^2$	$(3.167 \pm 0.13) \times 10^4$
$\varepsilon_a^A(640)$, $mol^{-1}cm^2$	$(3.64 \pm 0.14) \times 10^4$

The ratio of the extinction coefficients of PcS_z molecules in aggregate and monomeric forms $\varepsilon_a^A / \varepsilon_a^M$ was found to be 1.15 for PcS_z photoexcitation at a wavelength of 640 nm.