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Highly fluorescent and photostable organic- and water-soluble CdSe/ZnS core-shell quantum dots capped with thiols

Jordi Aguilera-Sigalat, Simon Rocton, Juan F. Sánchez-Royo, Raquel E. Galian* and Julia Pérez-Prieto*

SupportingInformation

TABLE OF CONTENTS

Title page

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Table S1: Physical properties of the CdSe/ZnS QDs capped with thiols and their precursors[a]

		λ_{max} 1st exciton peak (nm)	D [b] (nm)	λ_{max} emission peak (nm)	FWHM [c] (nm)	φ_F [d]
QD-CS1[e]	Evident	509	2.43	531	45 ± 1	0.50
QD-CS2[e]	Evident	521	2.64	539	40± 1	0.61
QD-CS3[e]	Evident	564	3.45	582	34± 1	0.63
QD-CS4[e]	Ocean	503	2.37	517	36± 1	0.58
QD-CS5[e]	Ocean	544	2.93	562	33± 1	0.55
QD-CS6[e]	homemade	535	2.77	543	26± 1	0.45
QD-CS7[e]	homemade	539	2.84	548	26± 1	0.32
CS1@KP	homemade	509		534	44± 1	0.75
CS2@KP	homemade	520		540	38± 1	0.70
CS6@KP	homemade	537	2.80	546	28± 1	0.35
CS7@KP	homemade	538	2.82	547	27± 1	0.30
CS3@MUA	homemade	571		595	30± 1	0.54
CS3@MPA	homemade	566		586	30± 1	0.45

[a] The core-shell QD-CS1- QD-CS3 were commercially available (www.evidenttech.com), QD-CS4 and QD-CS5 were purchased from Ocean Nano Teach LLC. [b] The diameter was calculated according to the method of W. W. Yu, L. Qu, W. Guo, X. Peng *Chem. Mater*. 2003, **15**, 2854. [c] Full width at half maximum (FWHM), [d]Fluorescence quantum yield obtained using fluoresceine as the standard. [e] Capping ligand: fatty amine and monosubstituted olefin (Evident), fatty amine, oleic acid, and monosubstituted olefin (Ocean), TOPO (QD-CS6), and TOPO and octadecylamine (QD-CS7). [f]The ^{1}H-NMR spectrum of the QD showed the presence of monosubstituted olefin.

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***Table S2*:** Maximum in the fluorescence spectra (λ_{max} , nm) and fluorescence quantum yield (Φ_f) of the core-shell QDs upon the addition of the thiol or the thiolate compound.

QD / Thiol System (molar ratio 1:2200)	λ_{max} emission (nm)	Quantum yield (%)
QD-CS4	517	58
QD-CS4/MU	519	50
QD-CS4/MU thiolate	526	20
QD-CS5	561	55
QD-CS5/MU	562	48
QD-CS5/MU thiolate	565	40
QD-CS5/KP-SH	561	53
QD-CS5/KP-SH thiolate	562	46

[a] Fluorescence measured 70 min after the addition of the thiol/thiolate of MU and 140 min for the thiol/thiolate of KP-SH.

Fluorescence Quantum yield Calculation

Quantum dots fluorescence quantum yield ($\varphi_{F,QD}$) was measured by comparing the integrated emission spectra for the QD and fluoresceine according to the following equation (Grabolle, M.; Spieles, M.; Lesnyak V.; Gaponik, N. Eychmüller, A. and Resch-Genger, U.; *Anal.Chem*. 2009, **81**, 6285):

$$\Phi_{F,QD} = \Phi_{F,st} \cdot \frac{F_{QD}}{F_{st}} \cdot \frac{f_{st(\lambda ex)}}{f_{QD(\lambda ex)}} \cdot \frac{n_{QD}^2}{n_{st}^2}$$

where $\Phi_{F,\,st}$ is the fluorescence quantum yield of the standard, F is the area under the fluorescence curve, *f* is the absorption factor at the excitation wavelength (λ_{ex}) and *n* is the refractive index of the solvent.

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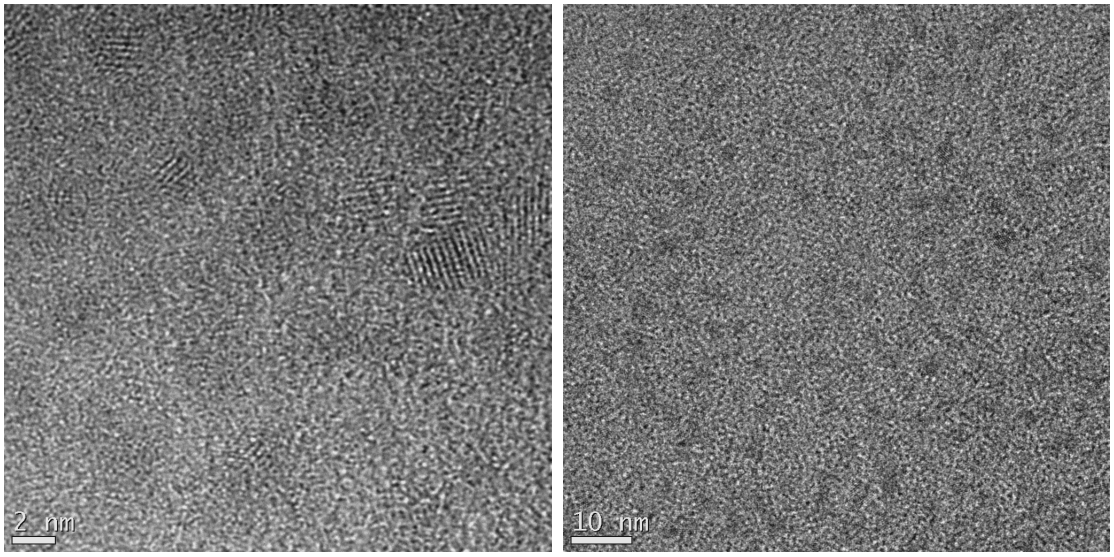

Figure S1: High Resolution Transmission Electron Microscopy images of **CS1** (2.2 ± 0.2 nm)

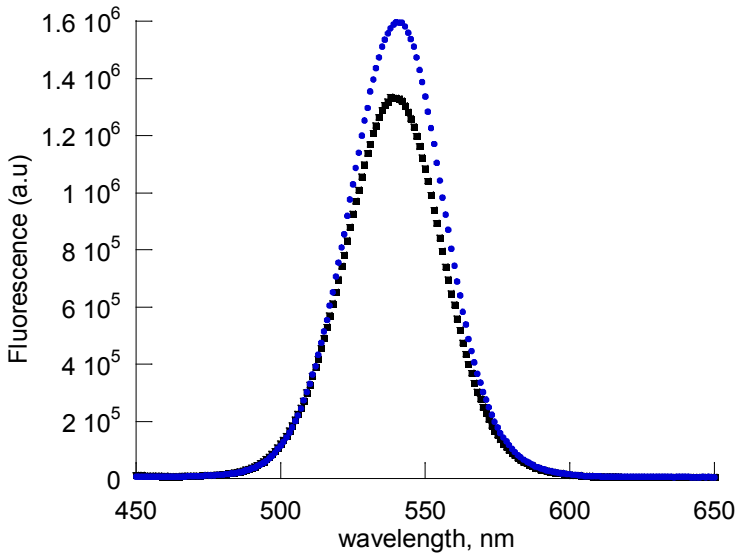

Figure S2: Comparative fluorescence spectra of *deareated* toluene solutions of **QD-CS2** and **CS2@KP**

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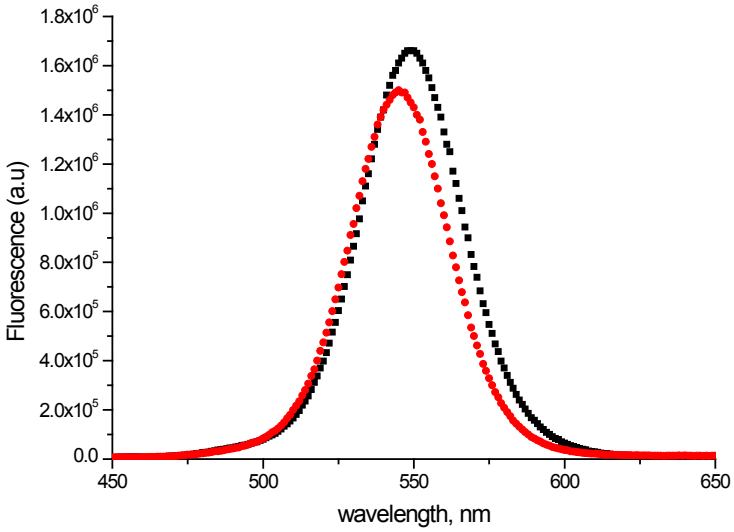

Figure S3 **.** Comparative fluorescence spectra of *deareated* toluene solutions of **QD-CS2** (●) and **CS2@MU** (■).

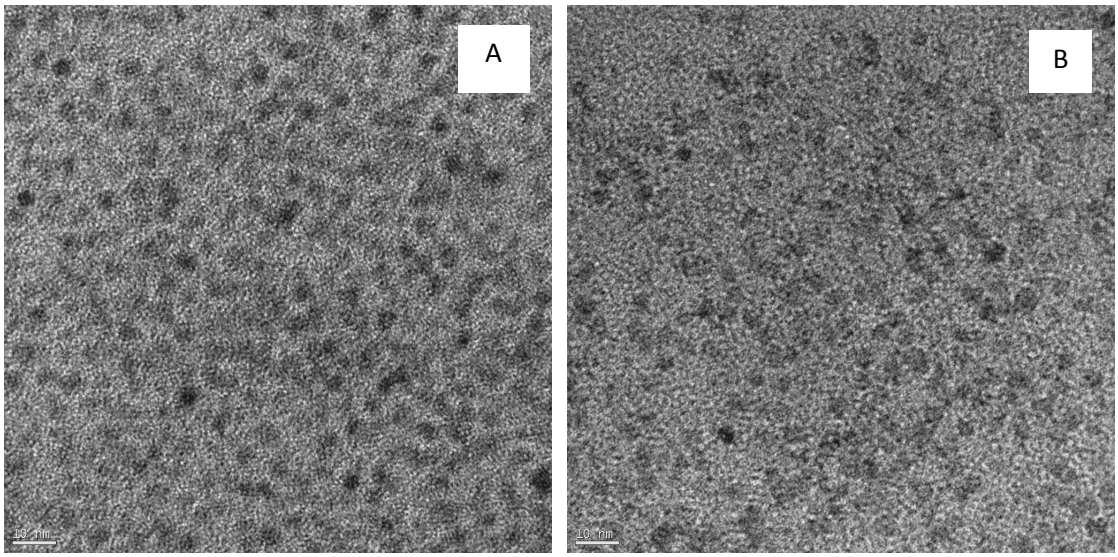

Figure S4: High resolution transmission electron microscopy images of **CS3** (**A**, 3.1 ± 0.3 nm) and **CS3@MPA** (**B**, 3.3 ± 0.3), the scale bar is 10 nm.

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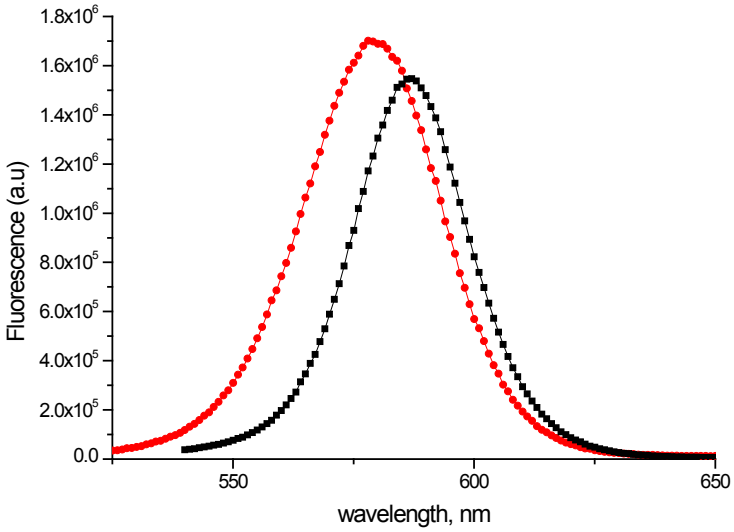

Figure S5. Comparative fluorescence spectra of a *deareated* solution of **QD-CS3** (●) and a water solution **CS3@MPA** (■).

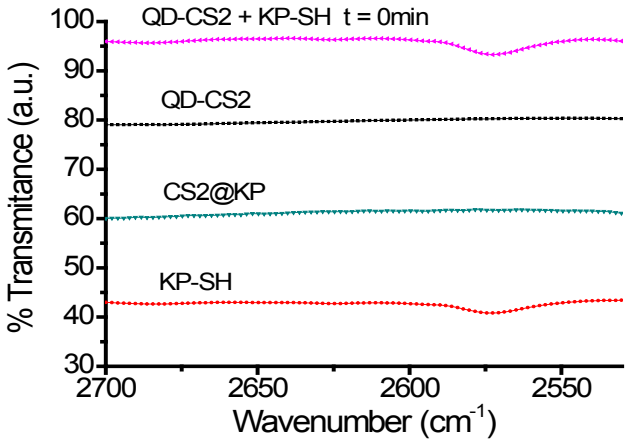

Figure S6. Comparative IR spectra a freshly-prepared mixture of **QD-CS2** and KP-SH, **QD-CS2**, **CS2@KP**, and of KP-SH.

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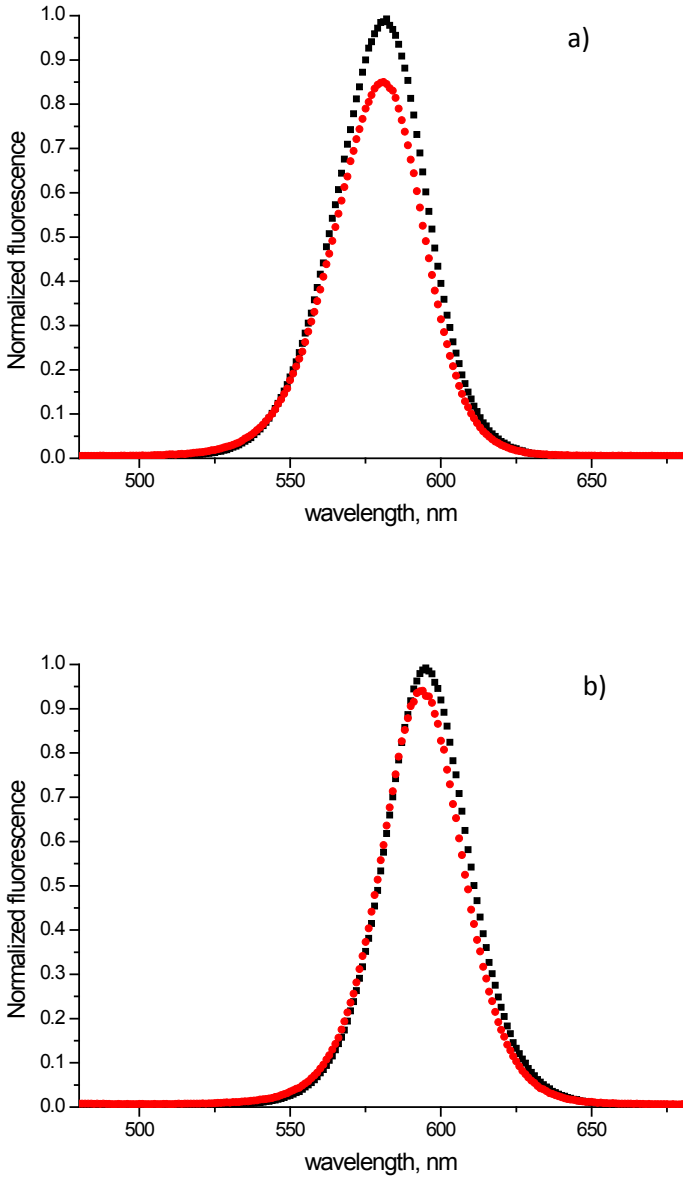

Figure S7. Normalized fluorescence spectra of **deaerated** solutions of a) **QD-CS3** (toluene) and b) **CS3@MUA** (water), before (■) and after (●) 270 min irradiation under 420 nm lamps.

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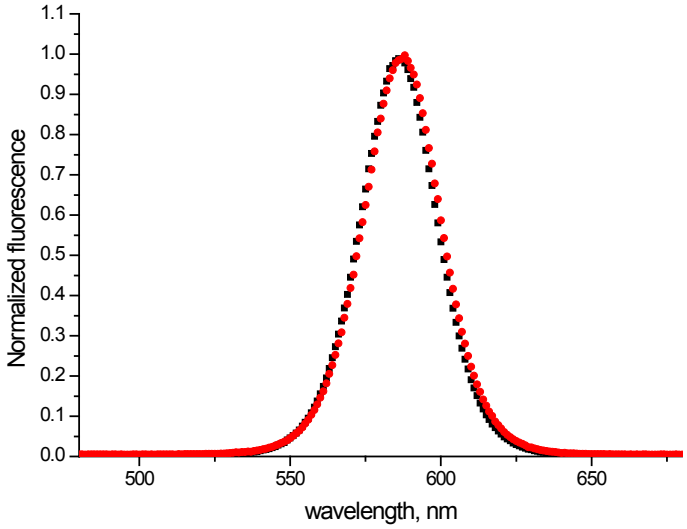

Figure S8. Normalized fluorescence spectra of ***deaerated*** aqueous solution **CS3@MPA**, before (■) and after (●) 270 min irradiation under 420 nm lamps.