Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.

Supplementary Information

Water-dispersed semiconductor nanoplatelets with high fluorescence brightness, chemical and colloidal stability

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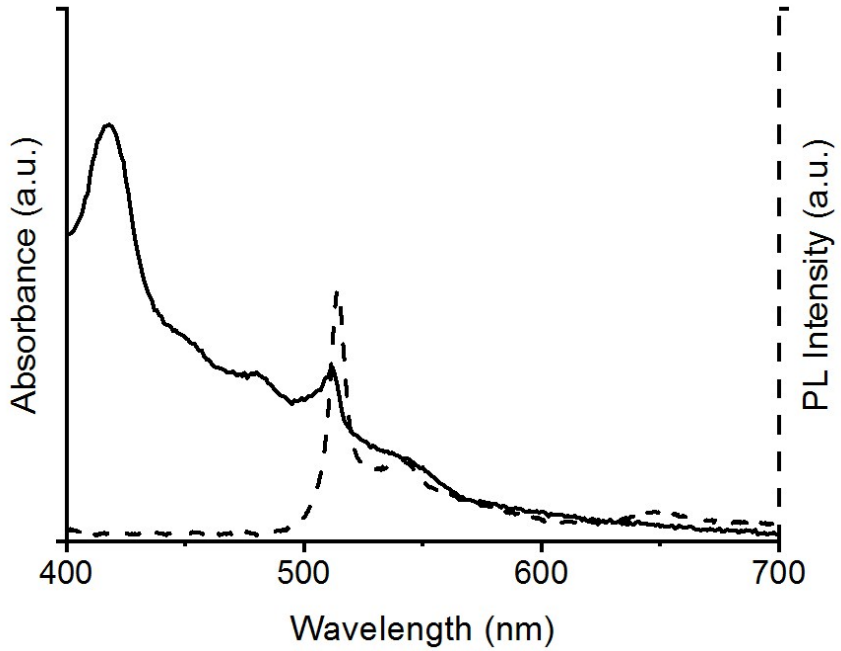

Figure S1. Absorption and fluorescence spectrum of water transferred 4ML core only NPLs. The broadened peaks suggest the NPLs were damaged during the water transfer.

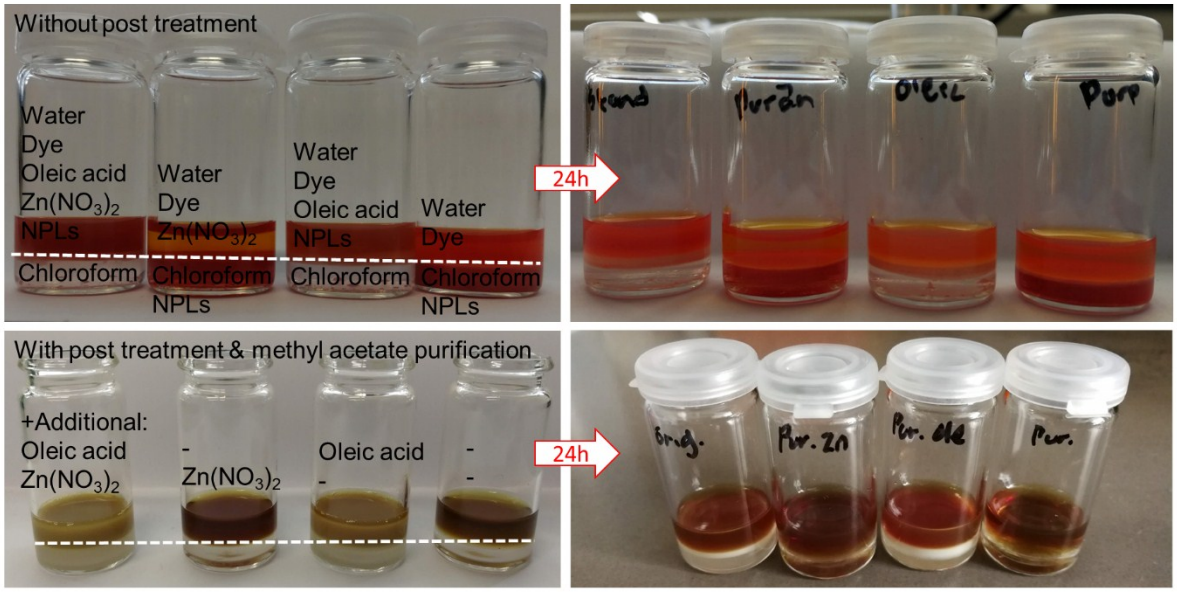

Figure S2. Study of the effect of oleic acid and zinc nitrate on the phase transfer of core/shell NPLs. Top photographs shows the study conducted on the system without post treatment after the core/shell synthesis. Bottom photographs shows the study conducted on the system with post treatment and methyl acetate purification to remove the excess oleic acid introduced in the post treatment step.

In the case without post treatment, samples without oleic acid addition shows red colour in the bottom chloroform layer. This indicates that the NPLs preferentially stays in the organic solvent instead of the aqueous solvent. The samples with oleic acid addition show a colourless chloroform layer. This indicates that the NPLs prefers to stay in the aqueous layer (dyed orange with fluoresceinamine). This effect is independent of the presence or absence of zinc nitrate.

In the post treatment, oleic acid was introduced (bottom row). The oleic acid should bind to the surface of the NPLs and exchange with the octylamine ligands introduced in the core/shell synthesis. The excess oleic acid is removed by precipitating the NPLs with methyl acetate and re-dispersing the NPLs in chloroform. To determine whether an excess of oleic acid is needed for the phase transfer, additional oleic acid was added to two of the four samples containing in the presence and in the absence of zinc nitrate. After the polymer coating and the addition of the basic buffer, all samples dispersed in water. Addition of chloroform layer is colourless which indicates that the NPLs prefer to stay in the aqueous layer.

Note the effect of excess oleic acid on the samples: with excess oleic acid the aqueous layer is cloudy while without the layer is clear. Overnight storage of the samples shows the cloudy aqueous layer become clear with the generation of a white interlayer between the two phases. The white substance is likely to be the precipitated excess polymer mixed with oleic acid micelles. The same is observed for the samples without post treatment.

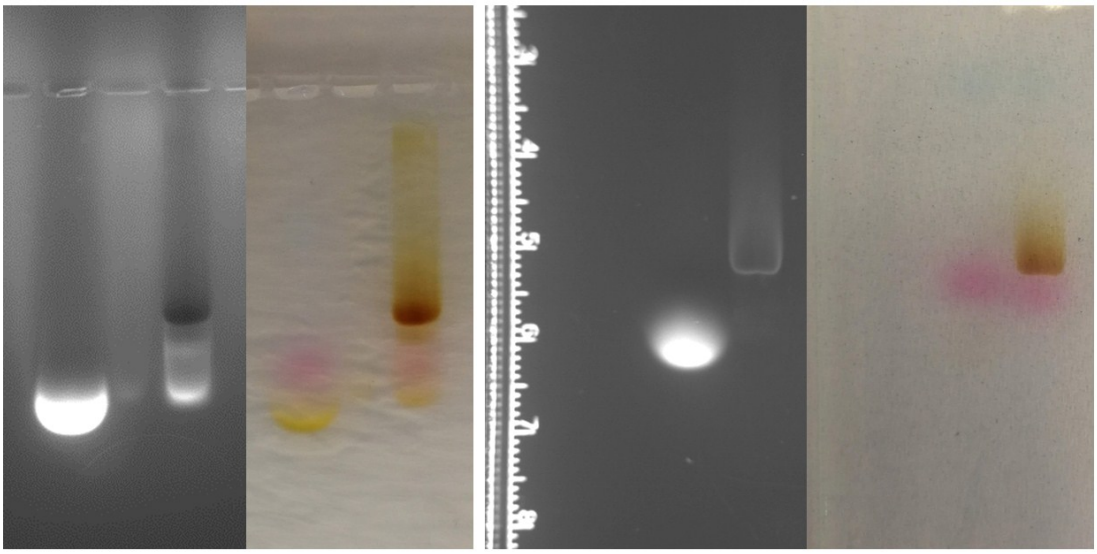

Figure S3. Photographs of samples after gel electrophoresis taken under UV (greyscale) and under ambient conditions (coloured). Brown spots are polymer coated NPLs. Purple spots are standard gel loading dye (purple 6x, typically used for DNA staining). Yellow spots are fluoresceinamine labelled polymer. In the left image, NPLs before sucrose gradient separation in the right lane was compared to the polymer only in the left lane. Based on the image under UV, excess polymer is present. In the right image, the same test was done with NPLs after sucrose gradient separation. Excess polymer was not observed in this case.

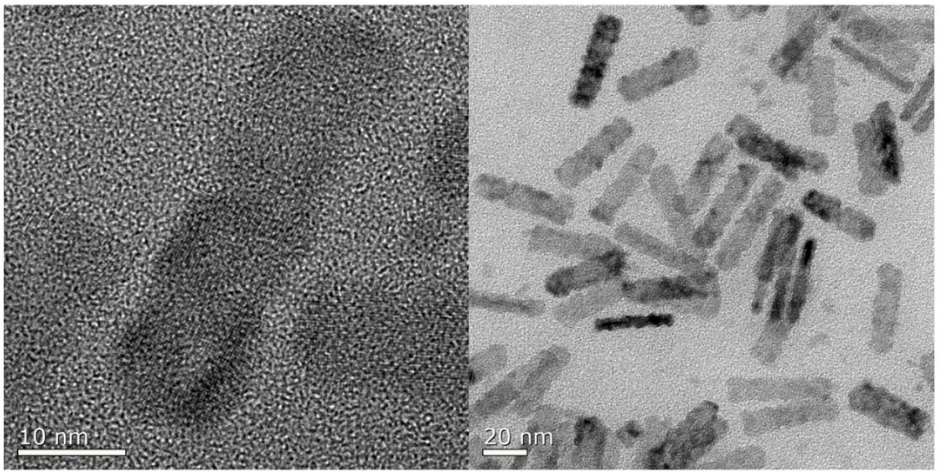

Figure S4. Transmission electron microscopy image of polymer coated core/shell NPLs after phase transfer. NPLs are well distributed which indicates that the NPLs are individually coated (see also Figure S7).

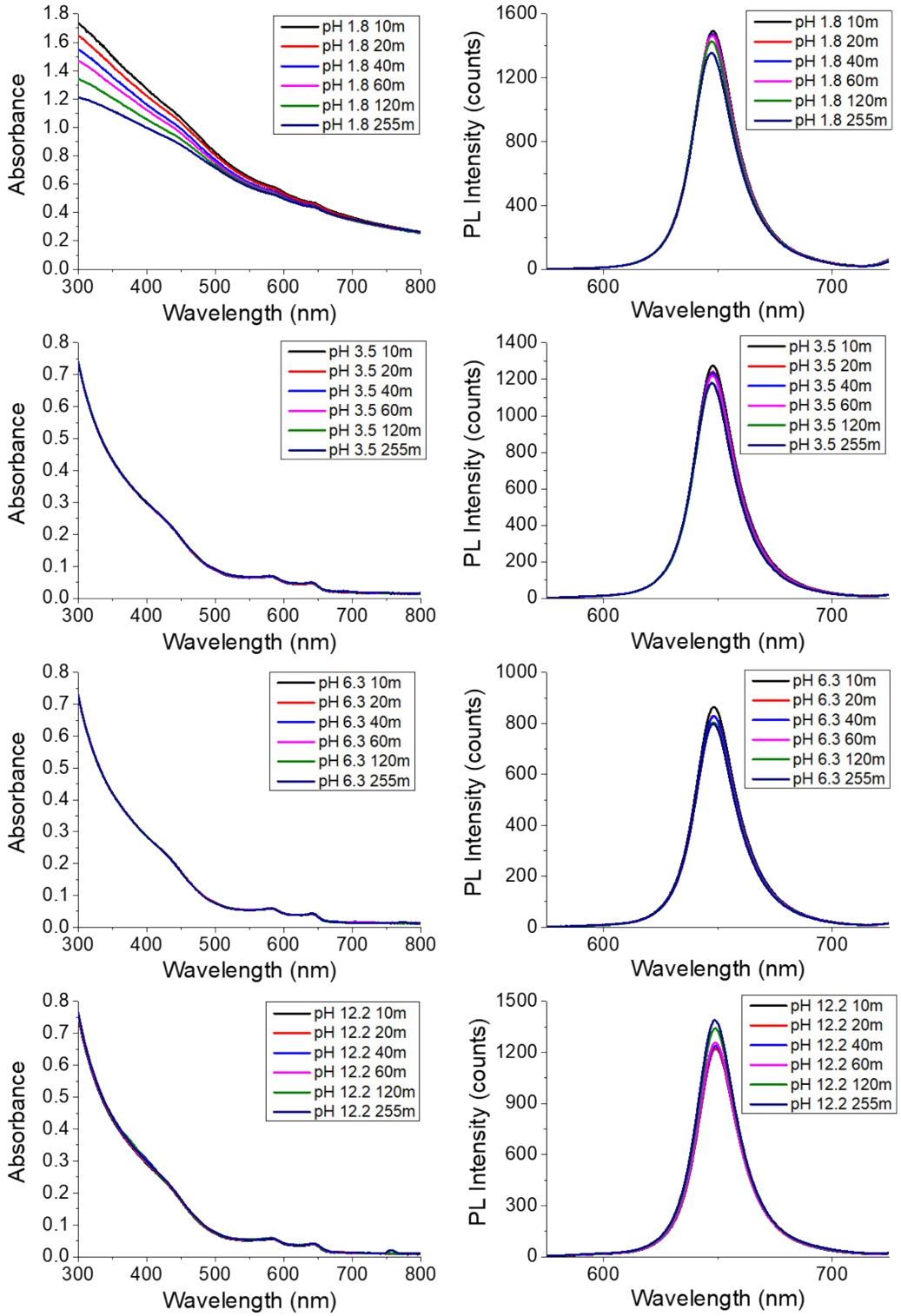

Figure S5. Absorption and PL spectra of water dispersed core/shell NPLs at different pH environments. The spectra remain stable for over 3 hours except in the case in pH 1.8 due to the agglomeration of NPLs over time, caused by the protonation of the COO- groups on the polymer coating.

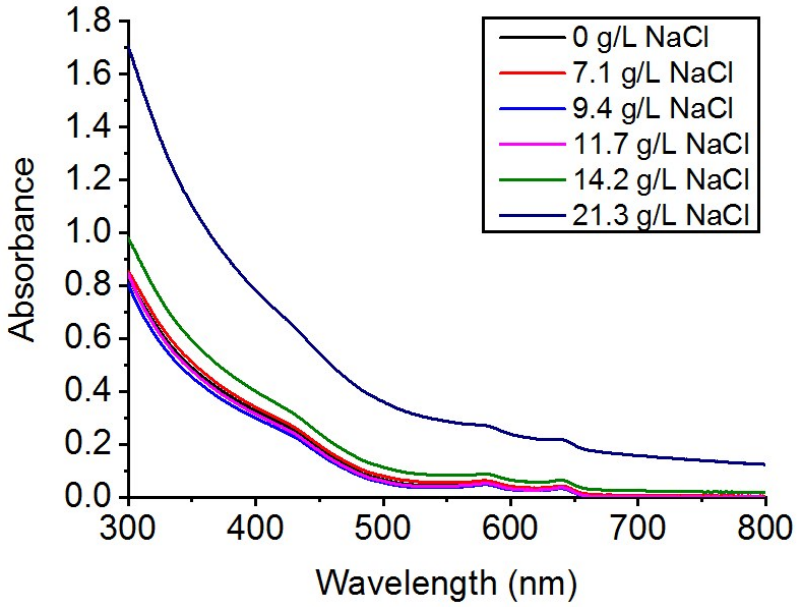

Figure S6. Absorption spectra of NPLs dispersed in Dulbecco's Phosphate Buffered Saline (PBS) buffer at different NaCl concentrations. Signals from scattering are not visible until the NaCl concentration goes over 14 g/L.

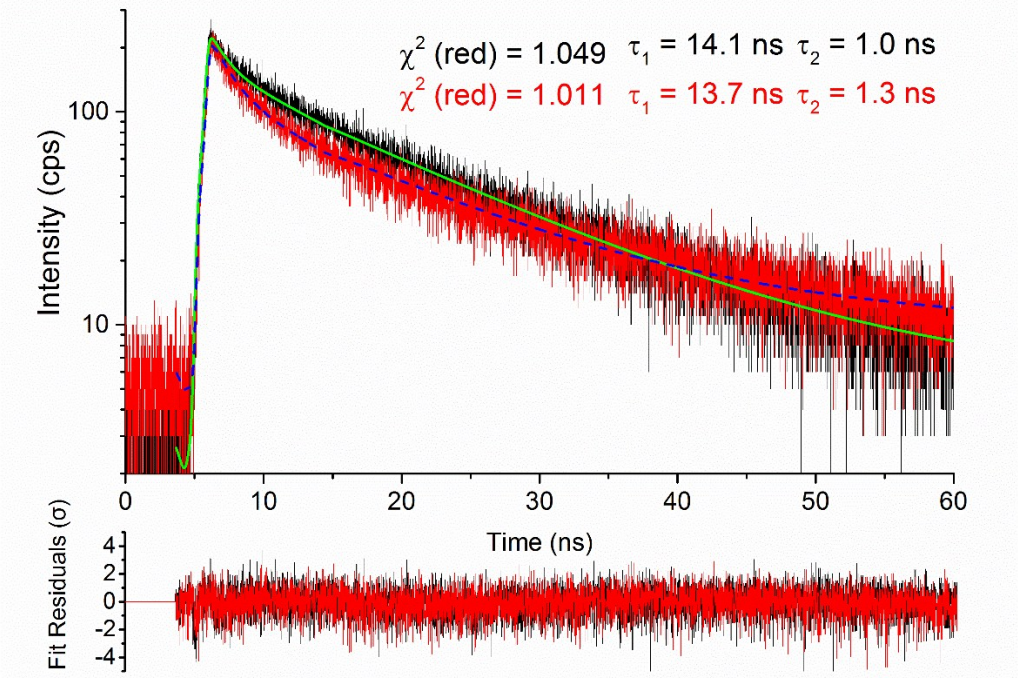

Figure S7. Fluorescence lifetime measurements of core/shell NPLs before phase transfer (in hexane, black) and after phase transfer (in water, red). Green solid line shows double exponential fitting of the fluorescence decay of the core/shell NPLs in hexane. Lifetimes obtained from fit were 14.1 ns and 1.0 ns. Blue dashed line shows double exponential fitting of the fluorescence decay of the core/shell NPLs in water. Lifetimes obtained from fit were 13.7 ns and 1.3 ns.

The fitting was done with the following equation:

$$I(t) = \int_{\infty}^{t} IRF(t') \sum_{i=1}^{2} A_i e^{-\frac{t-t'}{\tau_i}} dt'$$

Where:

IRF Instrument response function

A_i Amplitude of the i^{th} component, in counts

τ_i Lifetime of the i^{th} component, in nanoseconds

X^2 Quality of fitting

Sample	**X^2(reduced) [σ]**	**A_1 [counts]**	**τ_1 [ns]**	**A_2 [counts]**	**τ_2 [ns]**
Core/Shell NPLs in hexane	1.049	169.0	14.1	126.7	1.0
Core/Shell NPLs in water	1.011	129.1	13.7	142.6	1.3

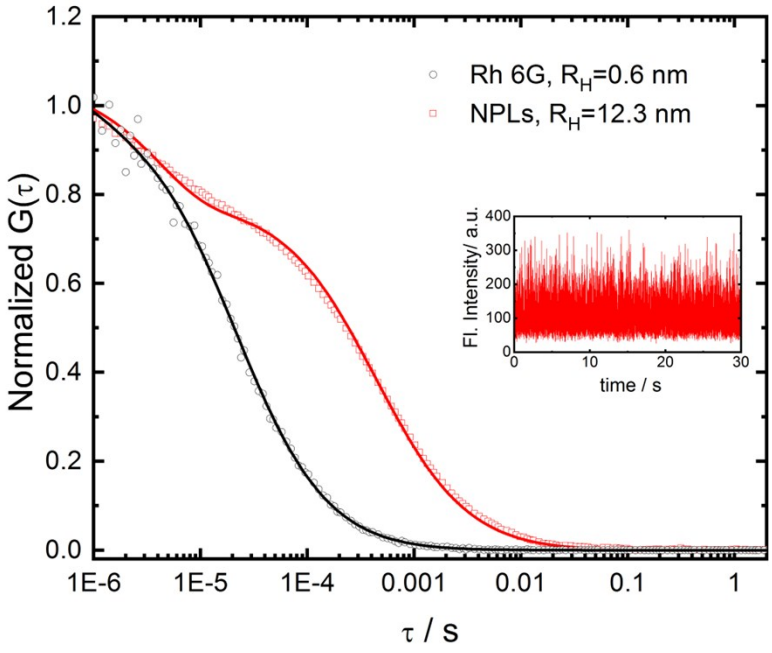

Figure S8. FCS data of core/shell NPLs and Rh 6G used as reference standard. Normalized experimental autocorrelation curves of the NPLs (red squares) and Rh 6G (black circles) measured upon one photon excitation at 488 nm in water. The solid lines represent the corresponding fits with eq. (2). . Inset shows the fluorescence intensity time trace of the NPLs with no spikes from agglomerates.

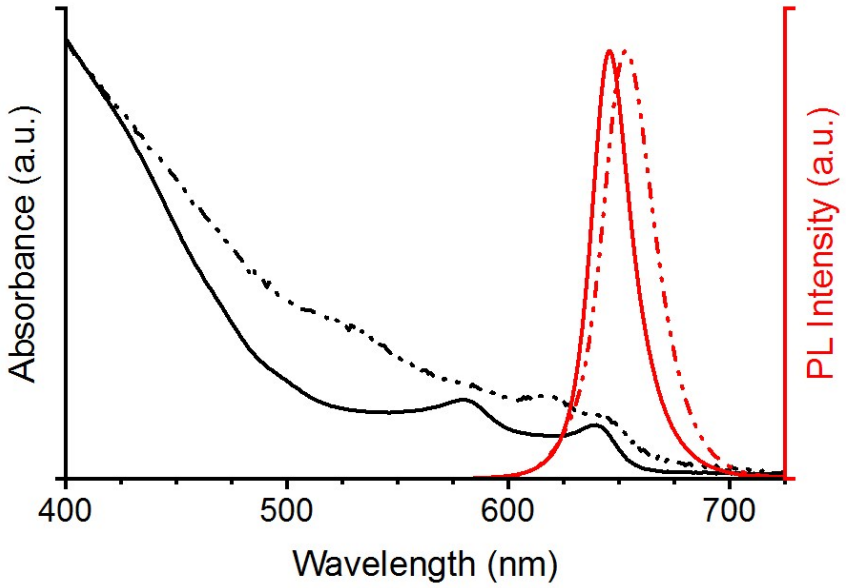

Figure S9. Absorption spectra (black) and fluorescence spectra (red) of CdSe/CdZnS core/shell NPLs (solid line) and commercial Qdot™ 655 ITK™ Carboxyl QDs (dotted line) in water.

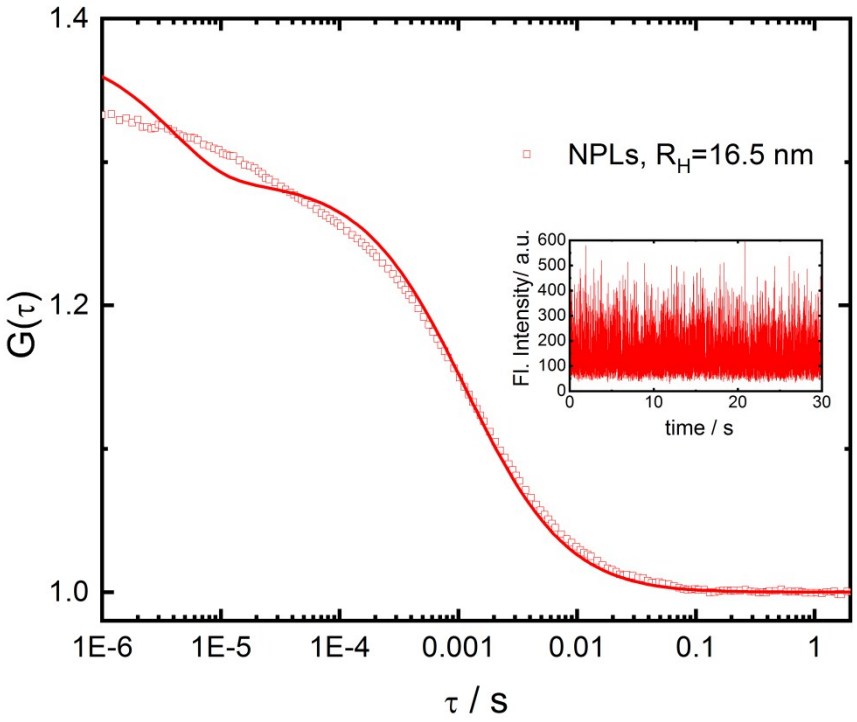

Figure S10. FCS data of core/shell NPLs in human serum. Experimental autocorrelation curve of the NPLs (red squares) measured upon one photon excitation at 488 nm in human serum. The solid line represents the corresponding fit with eq. (2). The deviation at short lag times is probably caused by a more complex photo-physics (blinking behaviour) of the NPLs upon formation of protein corona that cannot be described well with the single exponent term in eq. (1). Inset shows the fluorescence intensity time trace of the NPLs with no spikes from agglomerates.

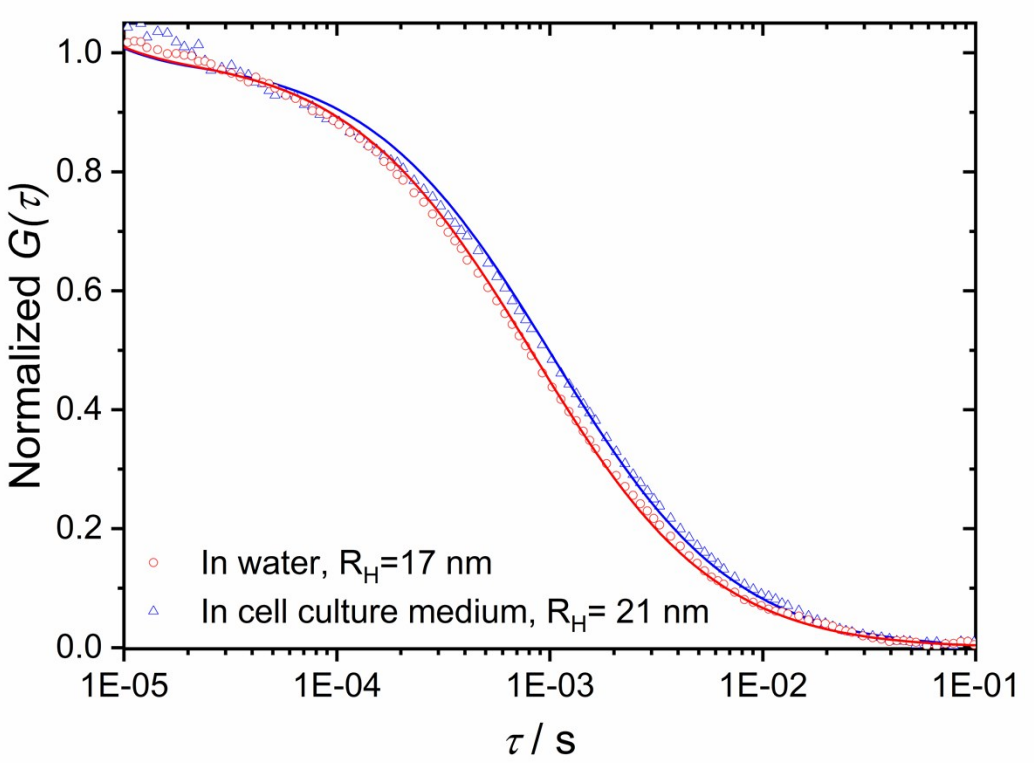

Figure S11. FCS data of core/shell NPLs in water and cell culture medium (DMEM + 10% FBS). NPLs were incubated in the medium for around one hour. Experimental autocorrelation curve of the NPLs (red circles and blue triangles respectively) measured upon one photon excitation at 488 nm. The solid lines represent the corresponding fit with eq. (2). The deviation at short lag times is probably caused by a more complex photo-physics (blinking behaviour) of the NPLs upon formation of protein corona that cannot be described well with the single exponent term in eq. (1). Size increase due to protein corona (+ 4 nm) is consistent with what was observed in human serum (Figure S10).

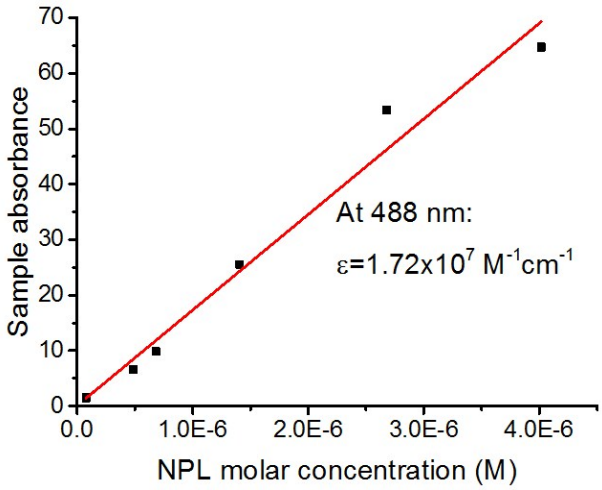

Figure S12. Calibration curve used to determine the molar extinction coefficient of the NPLs at 488 nm. The concentrations were calculated from ICP-OES data.

The QDs' extinction coefficient at 488nm (provided by the supplier) is 3.0×10^6 M^{-1} cm^{-1}.

Since:

$$FB \propto \varepsilon \cdot \varphi$$

$$Estimated\ ratio\ of\ FB = \frac{\varepsilon_{NPL}}{\varepsilon_{QD}} \times \frac{\varphi_{NPL}}{\varphi_{QD}} = \frac{1.72 \times 10^7}{3.00 \times 10^6} \times \frac{0.2}{0.7} = 1.64$$

The measured ratio of fluorescence brightness obtained from FCS = 26/16 = 1.63, which agrees well with the calculation.

Sample	QY ± 10%	Sample	QY ± 10%
Rhodamine 6G (Ethanol)	94%	Sulforhodamine 101 (Ethanol)	95%
Core only NPLs (Hexane)	50%	Core/Shell NPLs (Water)	21%
Core/Shell NPLs (Hexane)	30%	QDs (Water)	65%
Core/Shell NPLs (Water)	25%		

Table S1. Quantum Yields measured in this study. Samples in the first row are the standards used.

Additional references:

Further details regarding the QDs can be found in the data sheet from the supplier's website https://assets.thermofisher.com/TFS-Assets/LSG/manuals/mp19020.pdf