Supporting information for:

Remarkable Water-Soluble ZnO Nanocrystals: From ‘Click’ Functionalization to Supramolecular Aggregation Enhanced Emission Phenomenon

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1. STEM and HRTEM analysis

Figure S1. STEM and HRTEM micrographs of ZnO-una1 NCs (a-c) and ZnO-una2 NCs (d-f) prepared from samples dissolved in DMSO.
Figure S2. STEM and HRTEM micrographs of ZnO-\textit{hex} 1 NCs (in DMSO) (a-e) and ZnO-\textit{hex} 2 NCs (in H\textsubscript{2}O) (f-k).
2. Size distribution of ZnO NCs

![Size distribution of ZnO NCs](image)

**Figure S3.** Size distributions of a) ZnO-hex1 NCs and b) ZnO-hex2 NCs.

3. Dynamic Light Scattering

![Dynamic Light Scattering](image)

**Figure S4.** DLS data: size distribution by number and raw correlation data for ZnO-hex1 (a-b) NCs and ZnO-hex2 NCs (c-d) in DMSO, respectively.
Figure S5. The ZnO-hex2 NCs size distribution by number: a) in 50% DMSO/50% H₂O (v/v), b) 50% DMSO/50% H₂O (v/v) after 24 h, c) 10% DMSO/90% H₂O (v/v), and d) 10% DMSO/90% H₂O (v/v) after 5 days. The above data present three individual repeats of the same sample.
4. NMR spectroscopy

4.1 $^1$H NMR spectra for ZnO-una2 NCs

Figure S6. $^1$H NMR spectra of ZnO-una2 NCs after the CuAAC process, the most distinctive signals (ppm) for OH-terminated triazole molecule: 7.81 (=CH-N), 4.60 (-OH), 4.45, 3.78, 3.47, 3.36; 2.74 (C≡CH from unreacted una acid), *-DMSO-d$_6$, # - catalyst residue, RT.
4.2 $^1$H NMR spectra for hex-H and ZnO-hex1 NCs

Figure S7. $^1$H NMR spectra of a) ZnO-hex1 NCs and b) hex-H, *-DMSO-d$_6$, RT.
5. FTIR spectroscopy

**Figure S8.** FTIR spectra for ZnO-una1 NCs (dark grey line) and ZnO-una2 NCs (grey line), respectively.

**Figure S9.** FTIR spectra for ZnO-hex1 NCs (dark grey line) and ZnO-hex2 NCs (grey line), respectively.
6. Powder X-ray diffraction studies

For XRD data for ZnO-una1 NCs see: *Chem. Commun.*, 2016, 52, 7340-7343 and the Supplementary Information therein).

![Figure S10](image)

**Figure S10.** The powder X-ray diffraction patterns for ZnO-hex1 NCs (black line) and ZnO-hex2 (red line).

7. Optical spectroscopy

![Figure S11](image)

**Figure S11.** a) Absorption spectra of ZnO-hex1 NCs (before the CuAAC reaction) and ZnO-hex2 NCs (after the CuAAC) in DMSO; b) absorption spectrum of ZnO-una1 NCs in DMSO.
8. PL lifetimes measurements

The PL lifetimes were measured at 20 °C using a single-photon counting system UV-VIS-NIR Fluorolog 3 Spectro-fluorimeter (Horiba Jobin Yvon). The solid-state pulsed NanoLED ($\lambda_{\text{max}} = 336$ nm) was used as an excitation source. PL decay signals with a nanosecond resolution were obtained using photomultiplier tube. The instrument response function was acquired with a LUDOX scatterer. The obtained luminescence decay curves were fitted using four-exponential function.
**Figure S13.** Photoluminescence decays taken for ZnO-hex2 NCs in DMSO and in the mixture of 50% DMSO/50% H₂O (v/v).

**a)**

![Graph a](image1)

**b)**

![Graph b](image2)

**Table:**

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<th>Relative contribution</th>
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**c)**

![Graph c](image3)

**d)**

![Graph d](image4)

**Table:**

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