Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

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

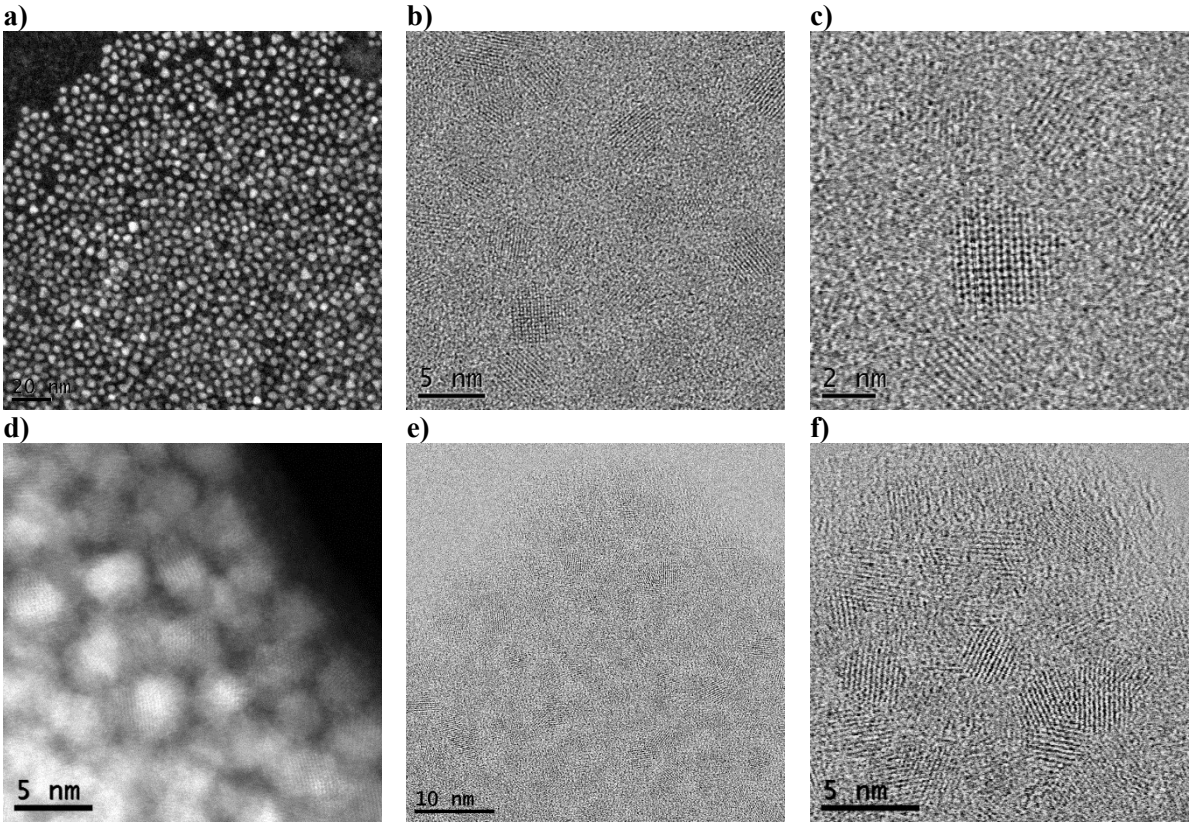


Figure S1. STEM and HRTEM micrographs of ZnO-*una*1 NCs (a-c) and ZnO-*una*2 NCs (d-f) prepared from samples dissolved in DMSO.

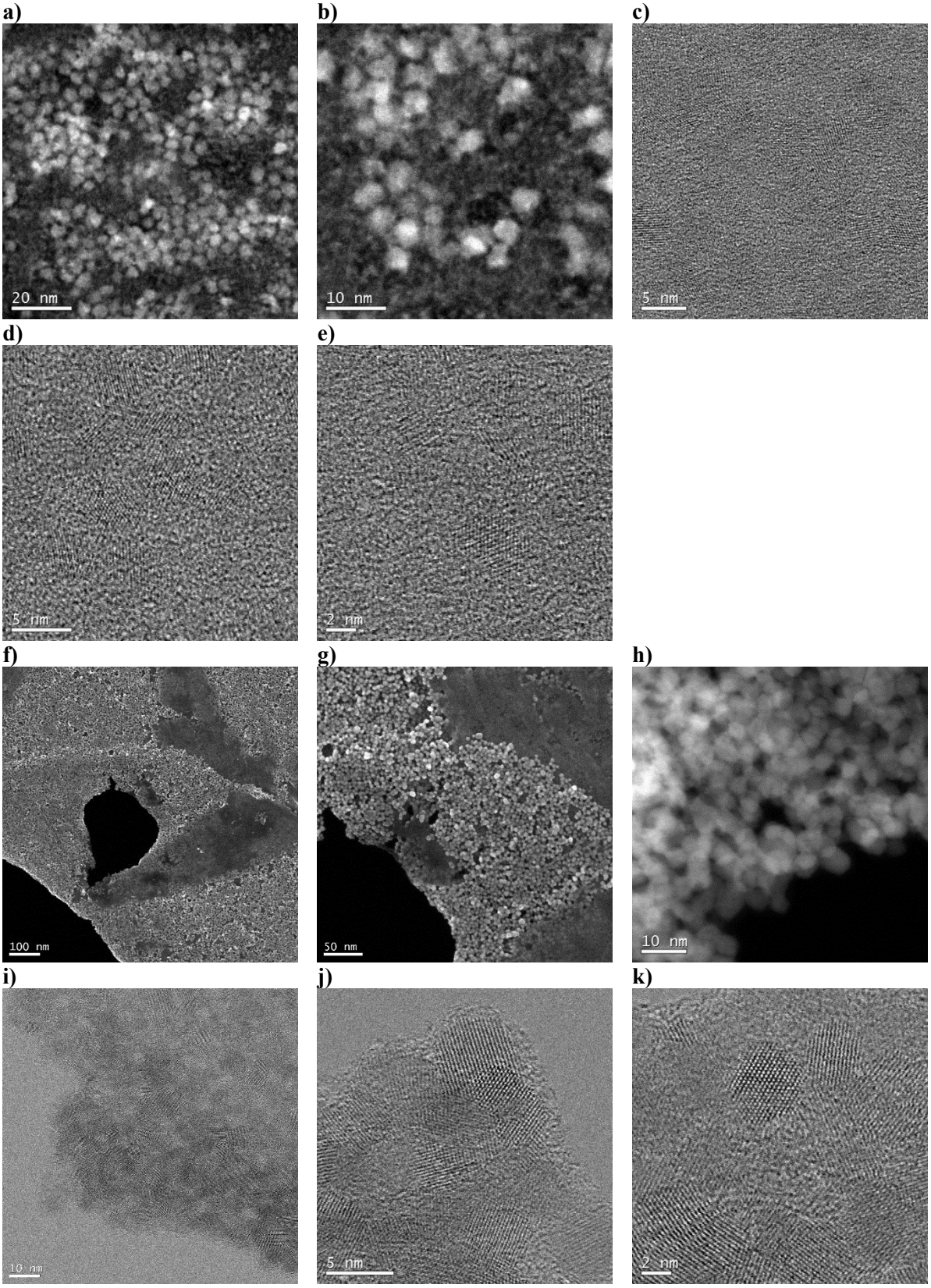


Figure S2. STEM and HRTEM micrographs of ZnO-*hex*1 NCs (in DMSO) (a-e) and ZnO-*hex*2 NCs (in H_2O) (f-k).

2. Size distribution of ZnO NCs

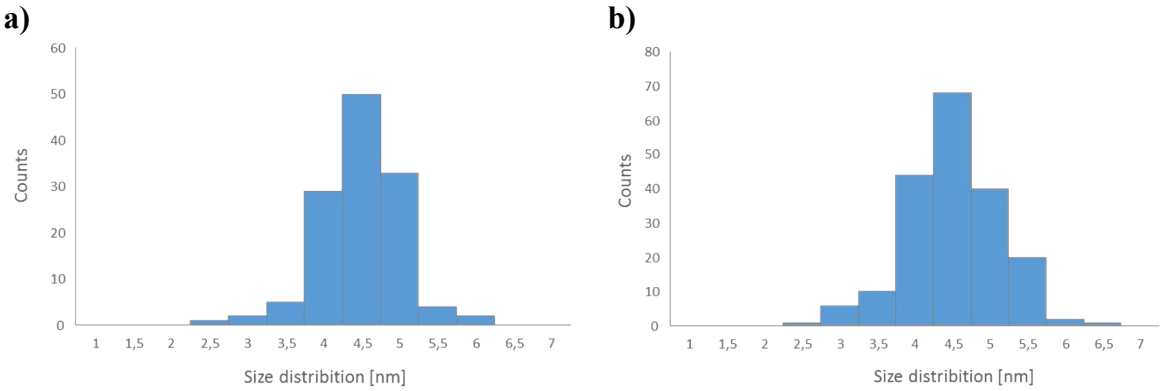


Figure S3. Size distributions of a) ZnO-*hex*1 NCs and b) ZnO-*hex*2 NCs.

3. Dynamic Light Scattering

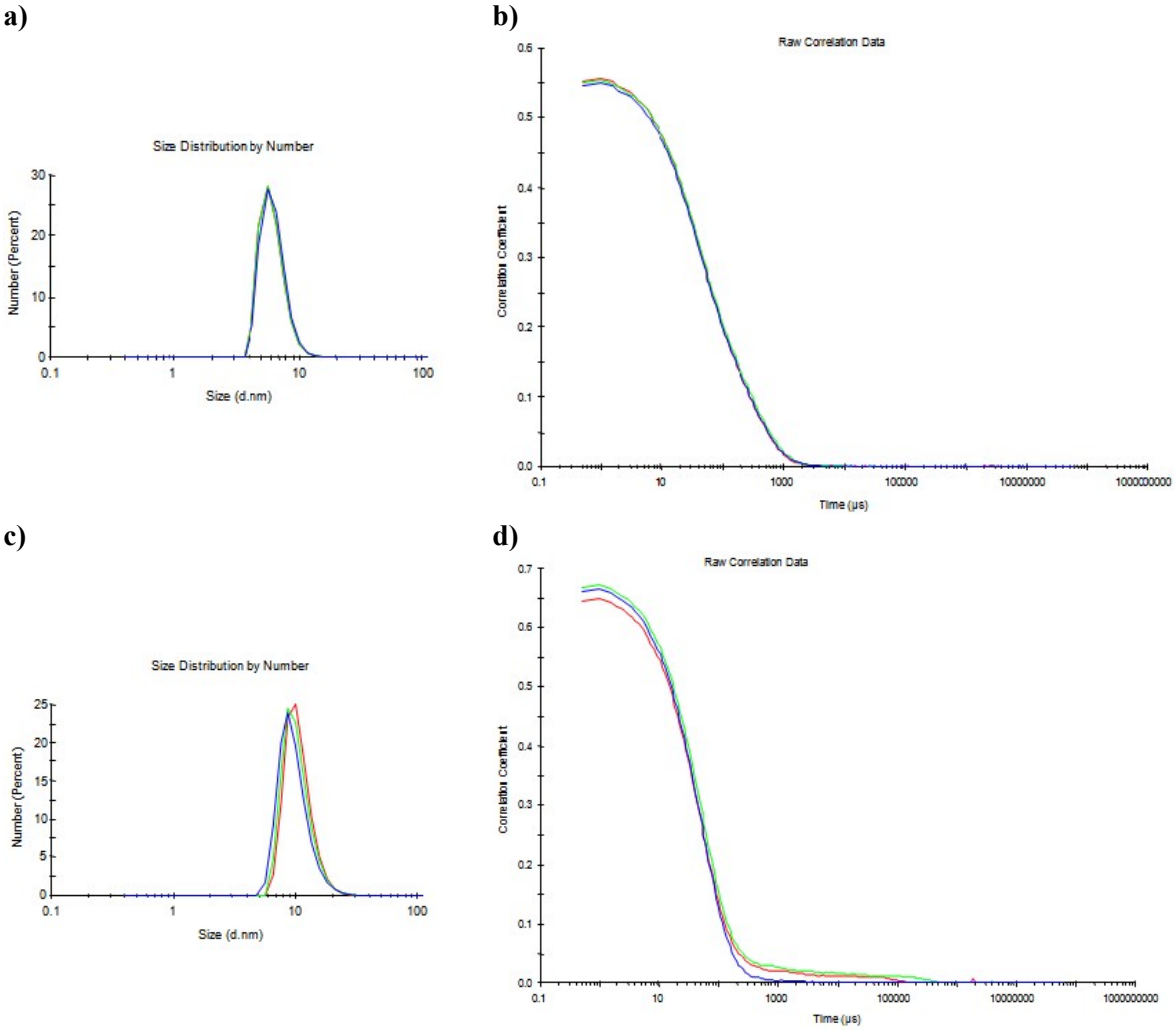


Figure S4. DLS data: size distribution by number and raw correlation data for ZnO-*hex*1 (a-b) NCs and ZnO-*hex*2 NCs (c-d) in DMSO, respectively.

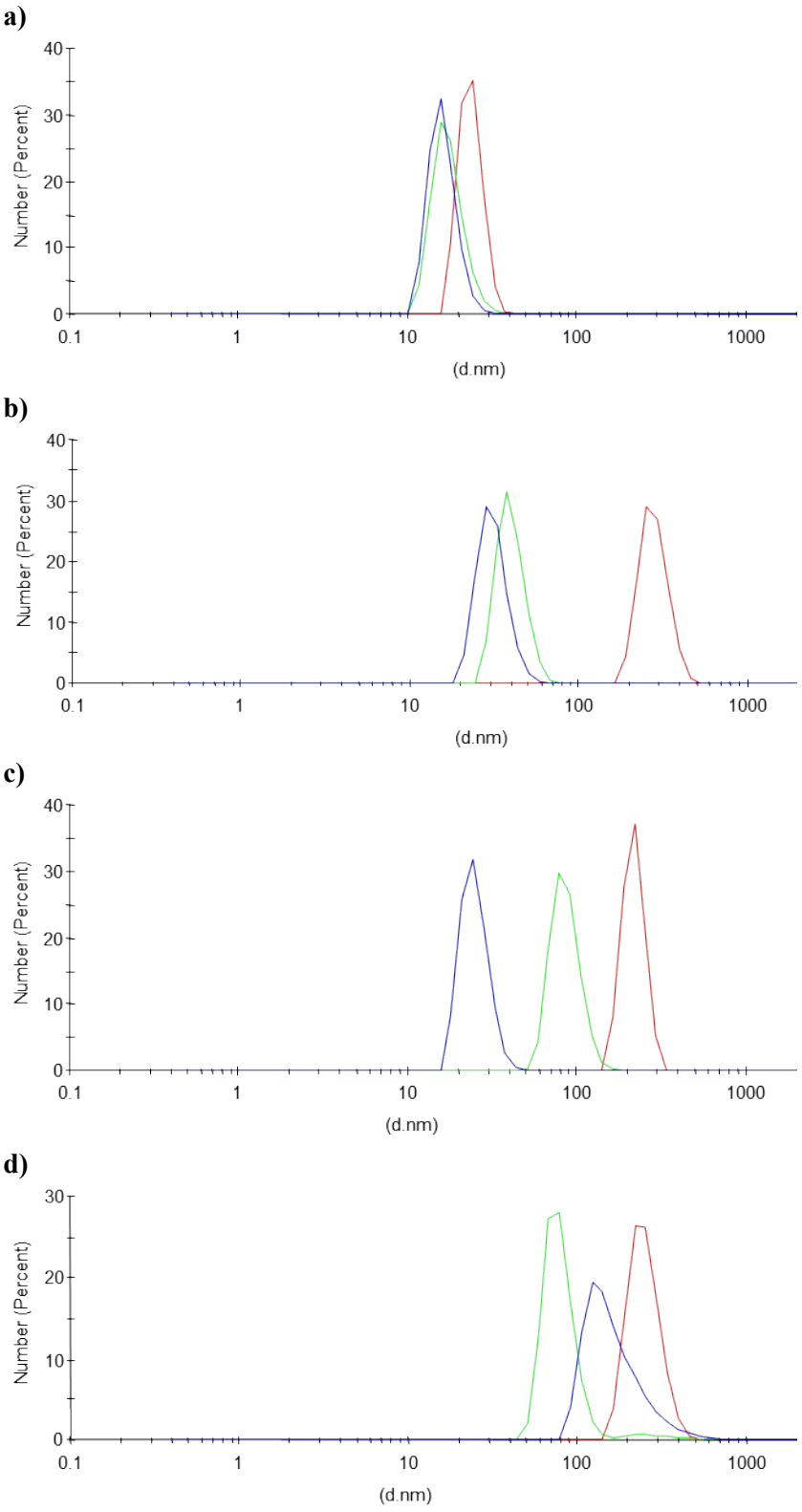


Figure S5. The ZnO-*hex*2 NCs size distribution by number: a) in 50% DMSO/50% H_2O (v/v), b) 50% DMSO/50% H_2O (v/v) after 24 h, c) 10% DMSO/90% H_2O (v/v), and d) 10% DMSO/90% H_2O (v/v) after 5 days. The above data present three individual repeats of the same sample.

4. NMR spectroscopy

4.1 ^{1}H NMR spectra for ZnO-*una*2 NCs

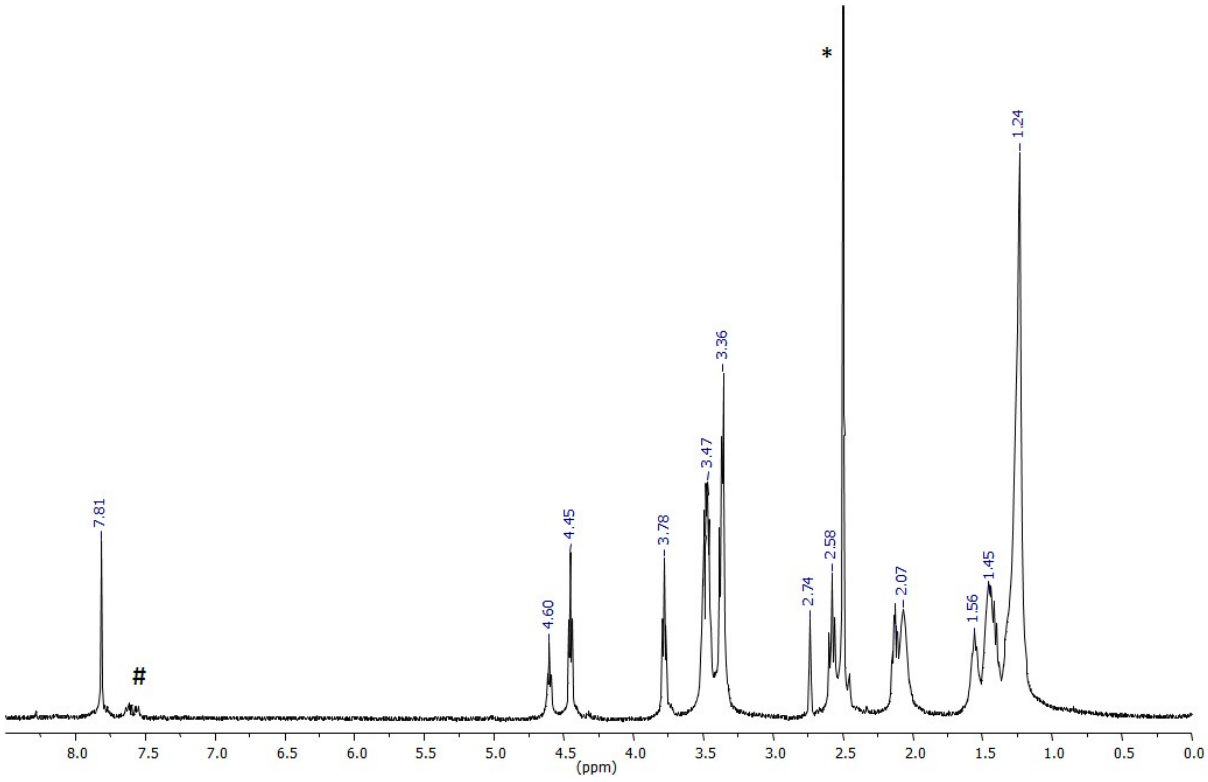


Figure S6. ^{1}H NMR spectra of ZnO-*una*2 NCs after the CuAAC process, the most distinctive signals (ppm) for OH-terminated triazole molecule: 7.81 (=*CH*-N), 4.60 (-OH), 4.45, 3.78, 3.47, 3.36; 2.74 (C≡CH from unreacted *una* acid), *-DMSO-d_6, # - catalyst residue, RT.

4.2 ^{1}H NMR spectra for *hex*-H and ZnO-*hex*1 NCs

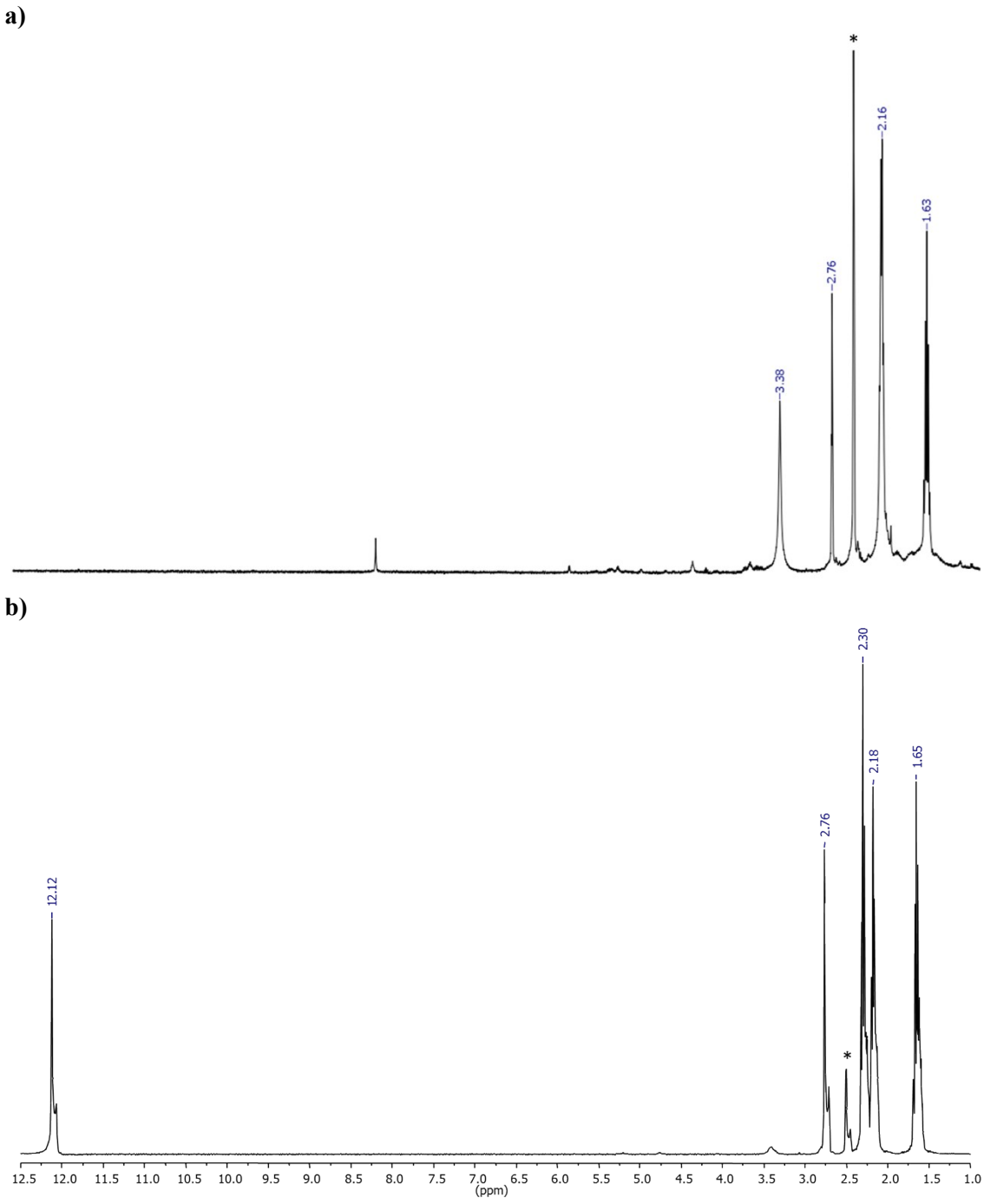


Figure S7. ^{1}H NMR spectra of a) ZnO-*hex*1 NCs and b) *hex*-H, *-DMSO-d_6, RT.

5. FTIR spectroscopy

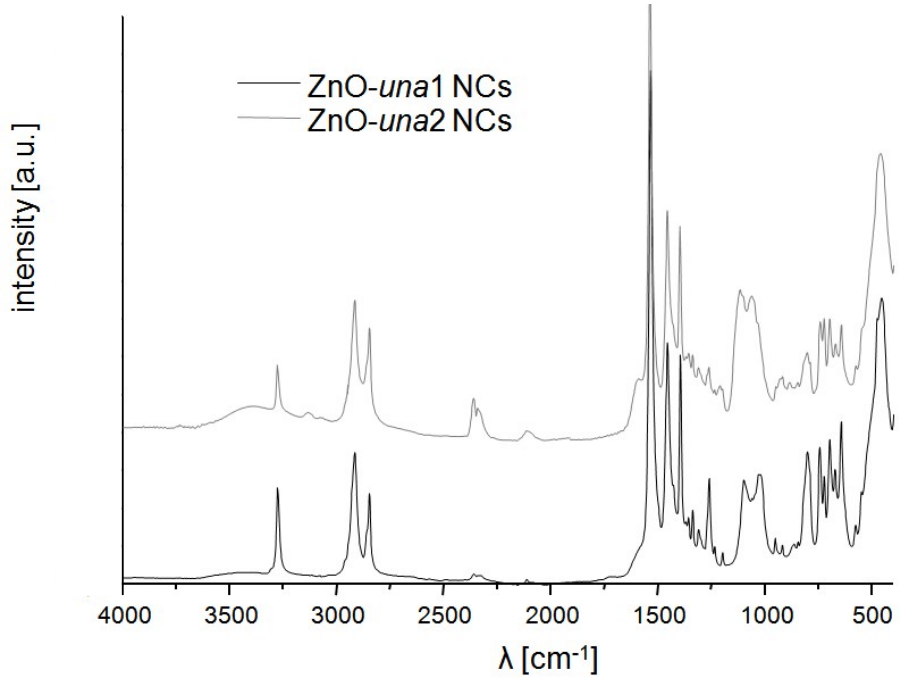


Figure S8. FTIR spectra for ZnO-*una*1 NCs (dark grey line) and ZnO-*una*2 NCs (grey line), respectively.

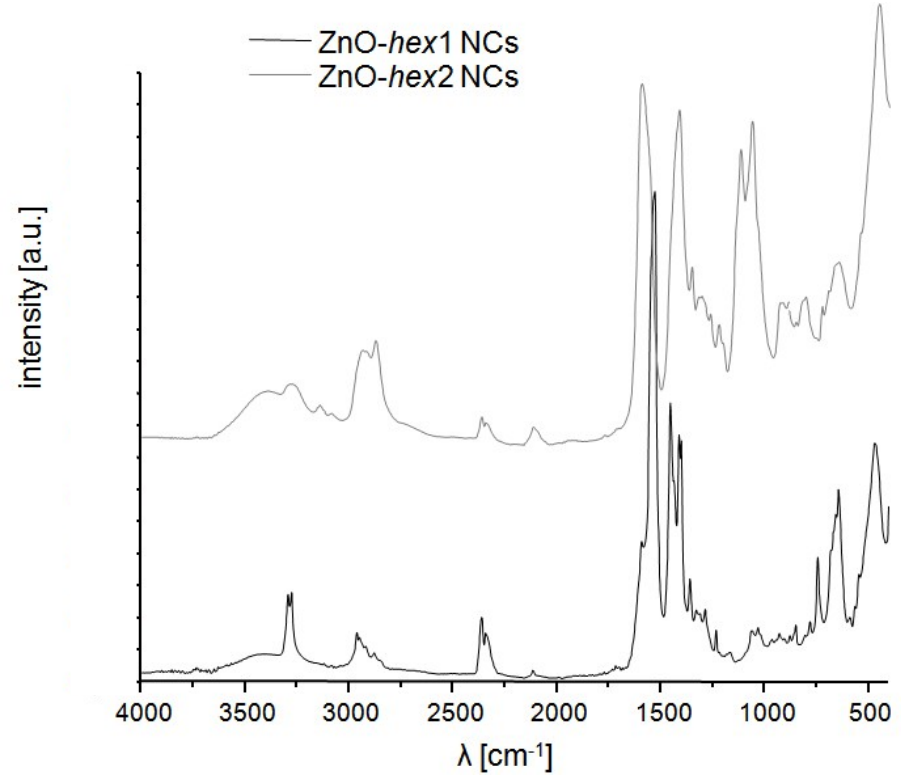


Figure S9. FTIR spectra for ZnO-*hex*1 NCs (dark grey line) and ZnO-*hex*2 NCs (grey line), respectively.

6. Powder X-ray diffraction studies

For XRD data for ZnO-*una*1 NCs see: *Chem. Commun.,* **2016**, *52*, 7340-7343 and the Supplementary Information therein).

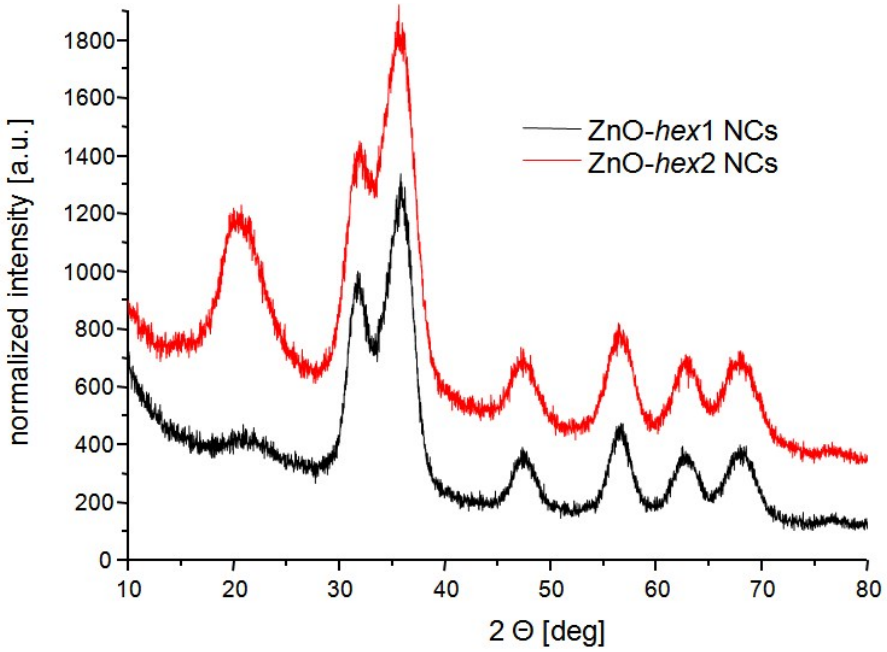


Figure S10. The powder X-ray diffraction patterns for ZnO-*hex*1 NCs (black line) and ZnO-*hex*2 (red line).

7. Optical spectroscopy

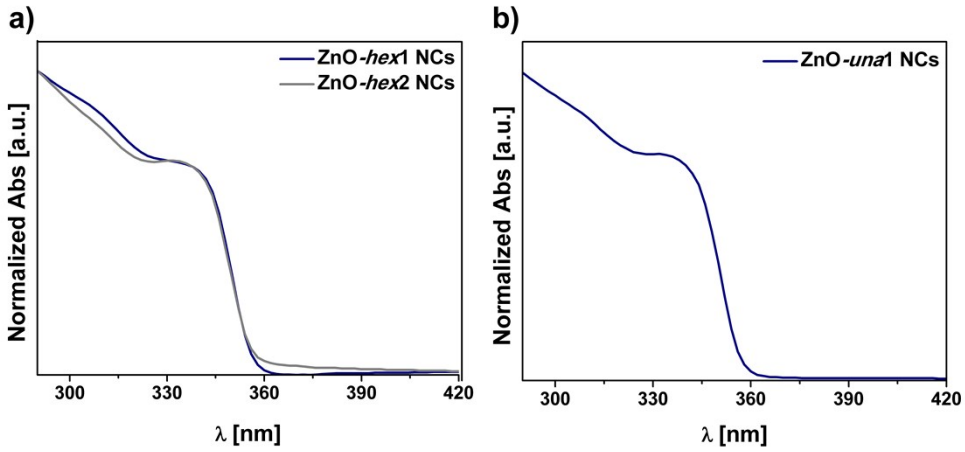


Figure S11. a) Absorption spectra of ZnO-*hex*1 NCs (before the CuAAC reaction) and ZnO-*hex*2 NCs (after the CuAAC) in DMSO; b) absorption spectrum of ZnO-*una*1 NCs in DMSO.

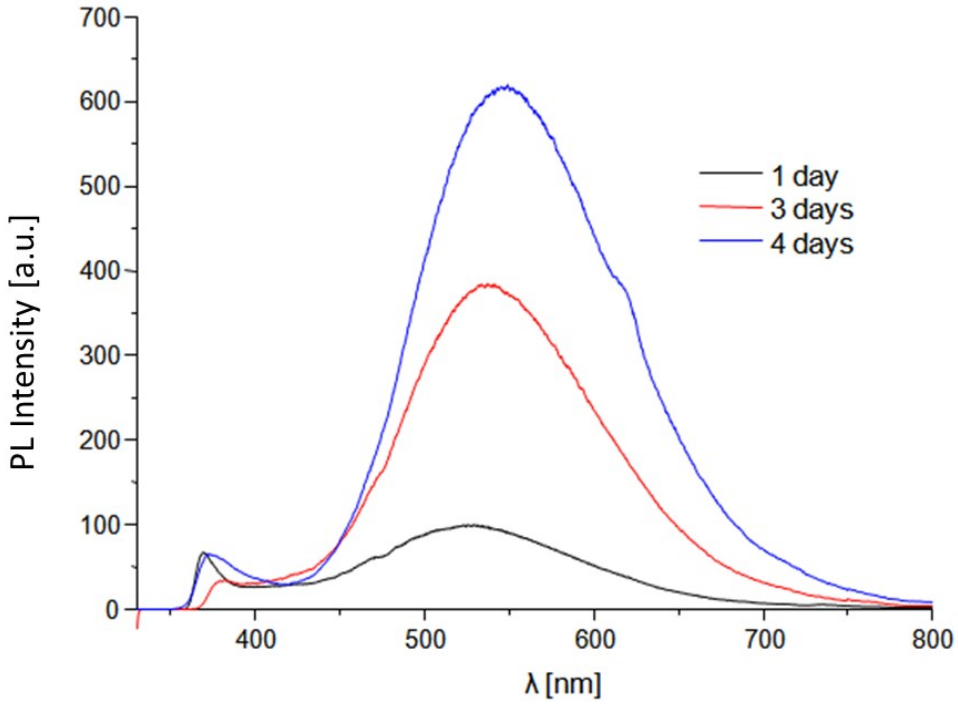


Figure S12. Time-dependent emission of ZnO-*hex*2 NCs in water.

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 (λ_{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.

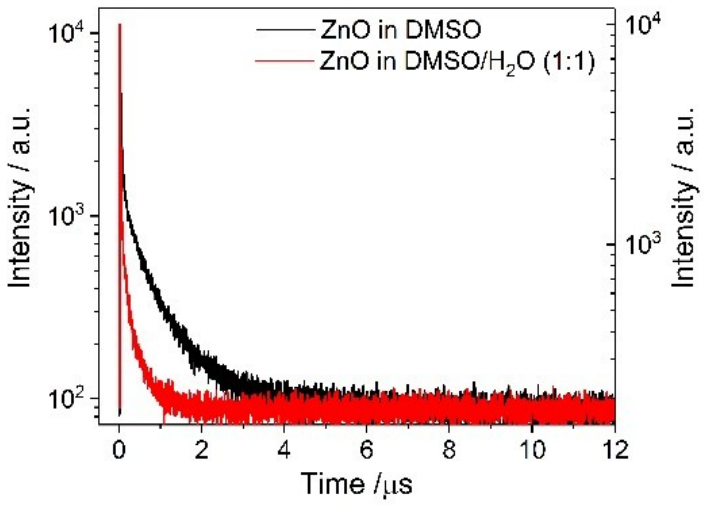
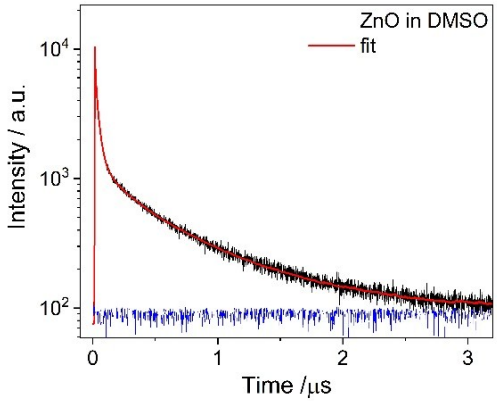
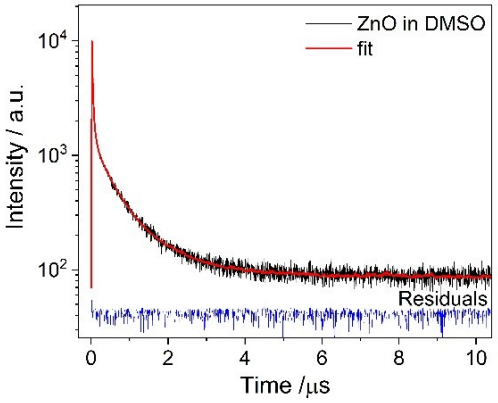


Figure S13. Photoluminescence decays taken for ZnO-*hex*2 NCs in DMSO and in in the mixture of 50% DMSO/50% H_2O (v/v).

a)

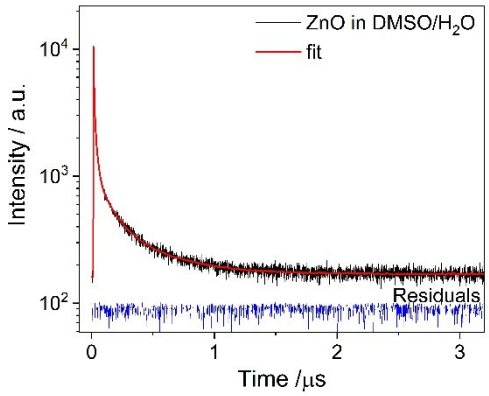


b)

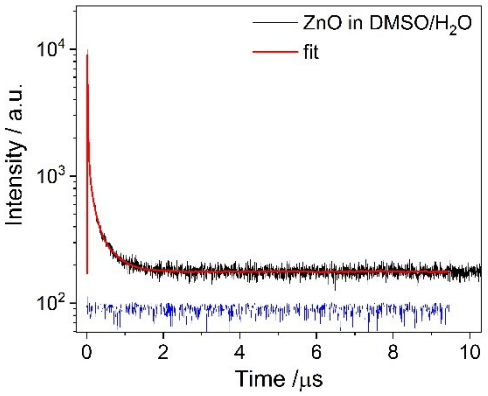


ZnO-*hex*2 in DMSO	τ (lifetime)	S.Dev	a (amplitude)	Normalized a	Relative contribution
1	**1,80E-08**	**1,80E-09**	**0,714**	0,655	**0,116**
2	**5,39E-08**	**2,84E-09**	**0,253**	0,232	**0,123**
3	**4,54E-07**	**1,58E-08**	**0,090**	0,083	**0,370**
4	**1,30E-06**	**2,27E-08**	**0,033**	0,030	**0,390**

c)



d)



ZnO-*hex*2 in DMSO/H_2O	τ (lifetime)	S. Dev.	a (amplitude)	Normalized a	Relative contribution
1	**5,07E-09**	**1,85E-10**	**1,187**	0,683	**0,150**
2	**1,99E-08**	**5,42E-10**	**0,435**	0,250	**0,216**
3	**1,28E-07**	**3,44E-09**	**0,083**	0,048	**0,266**
4	**4,46E-07**	**9,57E-09**	**0,033**	0,019	**0,368**