

**Electronic Supplementary Information (ESI)**  
for

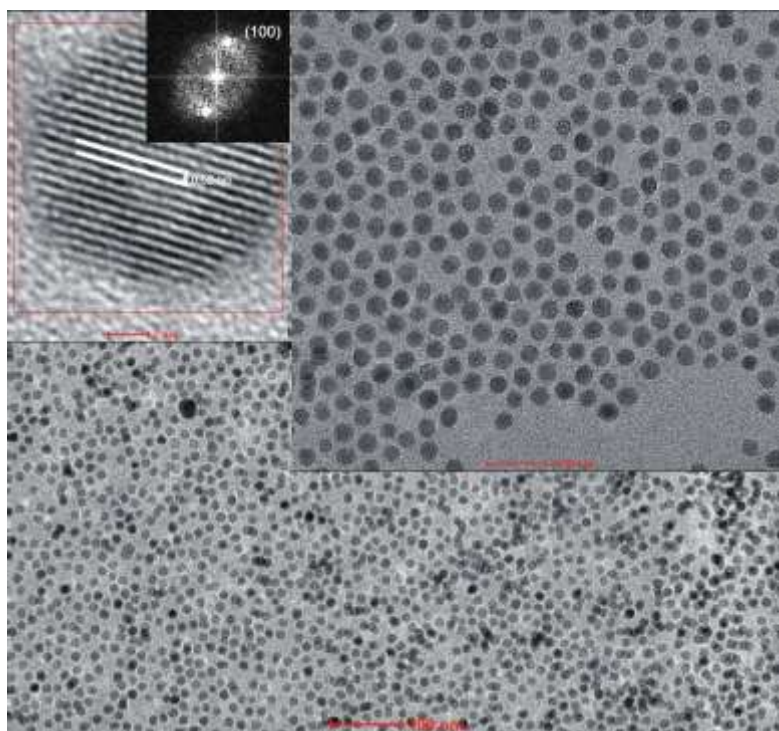
**General and versatile procedure for coating of hydrophobic nanocrystals  
with thin silica layer enabling facile biofunctionalization and dyes  
incorporation.**

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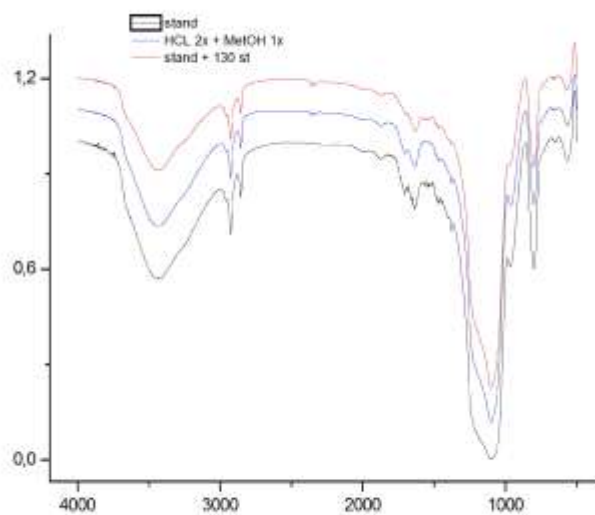
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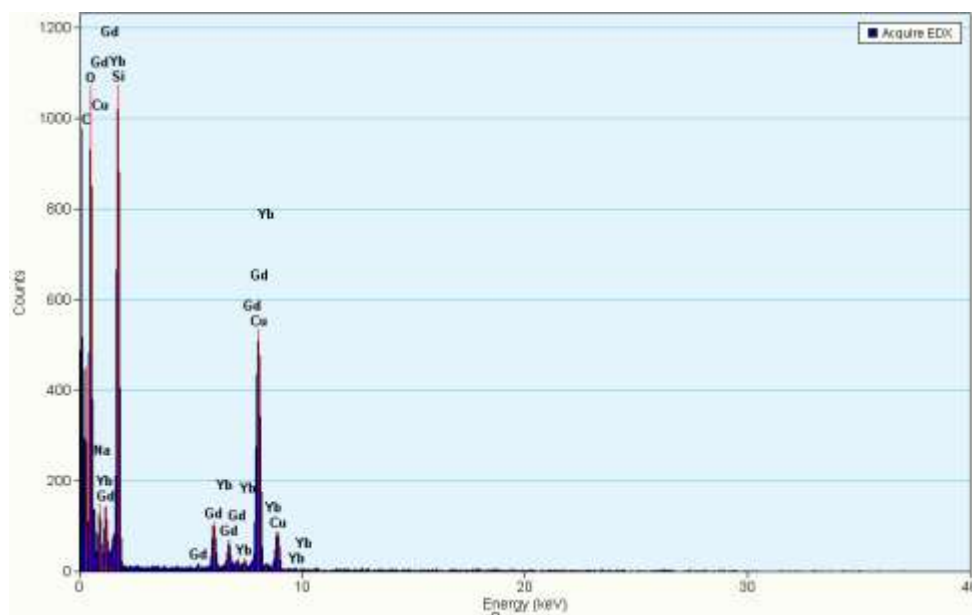
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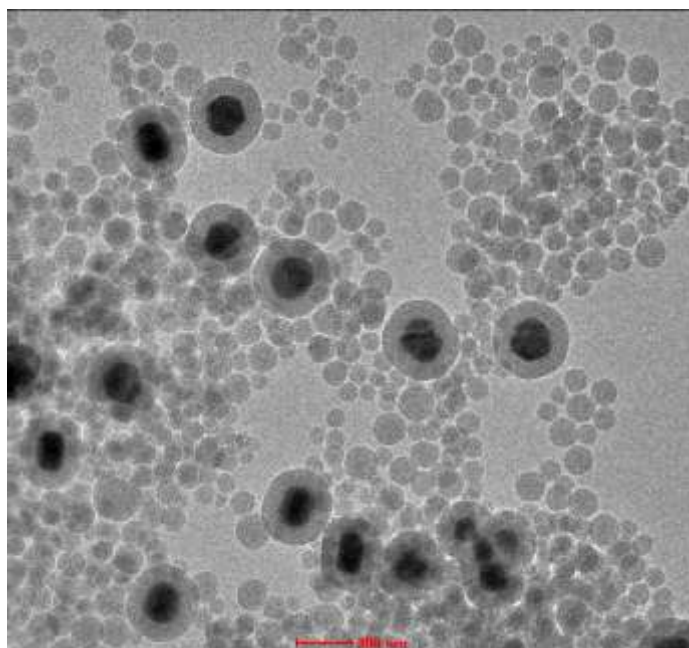
**Figure S1.** TEM images of  $\beta$ -NaGd<sub>0.80</sub>Yb<sub>0.18</sub>Er<sub>0.02</sub>F<sub>4</sub> nanocrystals (12 nm, OA coated). The inset shows HR-TEM image and SAED pattern.



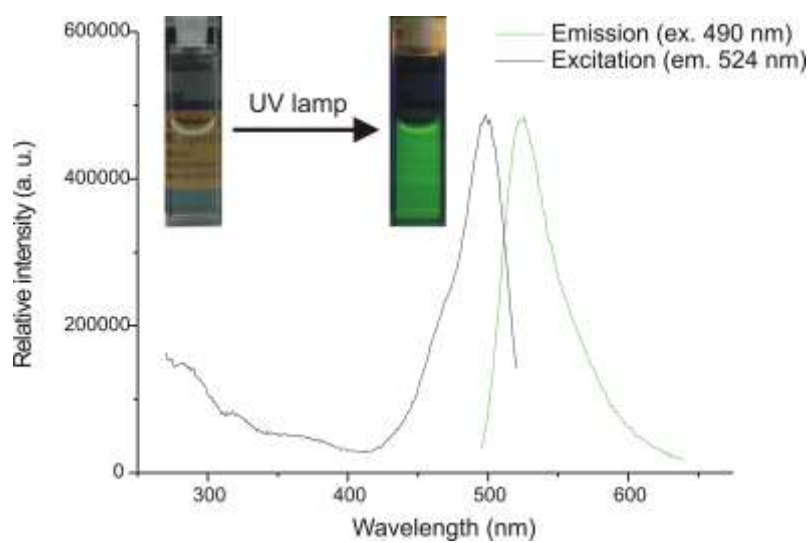
**Figure S2.** FTIR spectra recorded for NGF@mSiO<sub>2</sub> nanoparticles: a) washed with water and ethanol (5 times each); b) washed additionally with HCl solution at pH = 1-2 (2 times) and methanol (1 time); c) washed as in a) and heated at 130 °C in air for 12 hrs.



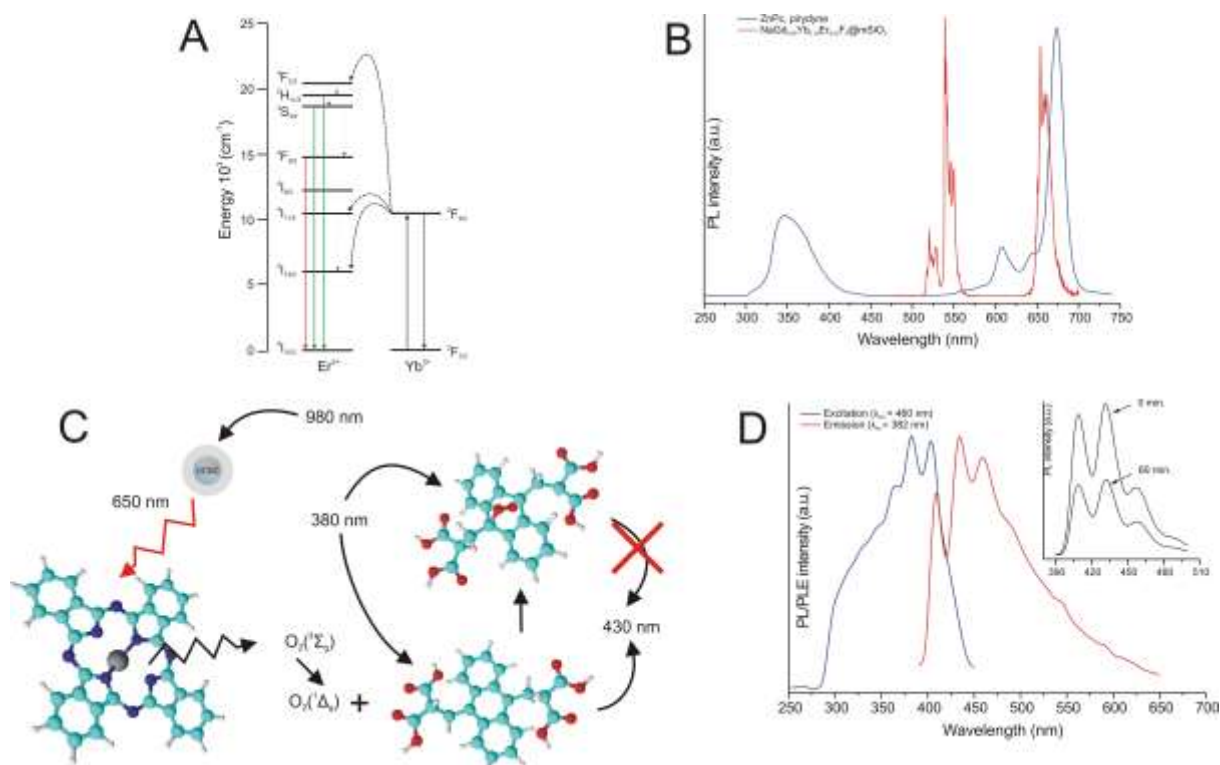
**Figure S3.** EDX spectra of NGF@mSiO<sub>2</sub> nanoparticles washed with water and ethanol (5 times each).



**Figure S4.** TEM images of coated NPs and empty silica spheres obtained when TEOS without organic solvent was used as the top layer.



**Figure S5.** PL ( $\lambda_{\text{ex}} = 490 \text{ nm}$ ) and PLE ( $\lambda_{\text{em}} = 524 \text{ nm}$ ) spectra recorded for FITC-modified NGF@mSiO<sub>2</sub>-FITC NPs dispersed in PBS buffer (pH = 7.4). The inset presents the green fluorescence of FITC-modified NPs observed under UV lamp.

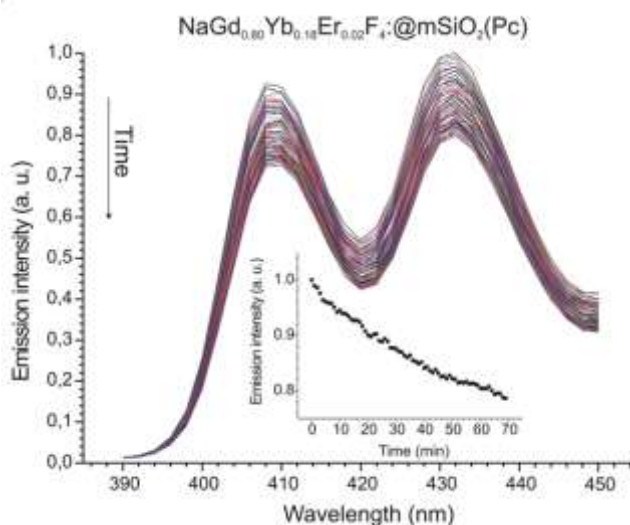


**Figure S6.** A) Schematic energy level diagram illustrating up-conversion energy transfer process from  $\text{Yb}^{3+}$  to  $\text{Er}^{3+}$  ions; B) PL spectrum of  $\text{NaGd}_{0.80}\text{Yb}_{0.18}\text{Er}_{0.02}\text{F}_4@m\text{SiO}_2$  NPs (red line) recorded under excitation with 980 nm and absorption spectrum of ZnPc in pyridyne (blue line); C) Schematic representation of singlet-oxygen generation under irradiation of  $\text{NaGd}_{0.80}\text{Yb}_{0.18}\text{Er}_{0.02}\text{F}_4@m\text{SiO}_2(\text{Pc})$  nanoparticles with 980 nm laser diode and detection of  $^1\text{O}_2$  using ABDA; D) PL ( $\lambda_{\text{ex}} = 382 \text{ nm}$ ) and PLE ( $\lambda_{\text{em}} = 460 \text{ nm}$ ) spectra of ABDA. The inset presents quenching of ABDA fluorescence in the presence of  $^1\text{O}_2$ .

### Singlet oxygen generation.

In the standard procedure 0.81 mg of NGF@OA NCs is used to obtain 10 mg of silica coated NGF@mSiO<sub>2</sub>(Pc) hybrid material. Moreover, the TGA data reveal that NGF cores make about one third of the total mass of NGF@OA nanocrystals. Hence, the concentration of NGF cores in 10 mg/cm<sup>3</sup> solution of NGF@mSiO<sub>2</sub>(Pc) can be evaluated as about 0.001 M. Qian et al.<sup>1</sup> obtained NaGdF<sub>4</sub>:Yb<sup>3+</sup>,Er<sup>3+</sup> up-converting NPs coated with porous silica using microemulsion method and then incorporated ZnPc into silica layer by soaking. Similarly, as in our case, ABDA fluorescence was used as a probe of  $^1\text{O}_2$  generation. The ABDA fluorescence intensity after 10 minutes exposure time to NIR laser radiation decreased to about 75 % of its initial value in Ref. [1], and to about 80 % in our experiment. It is, however, difficult to compare directly results reported here and in Ref. [1]. In both cases the ABDA concentration in nanoparticles dispersion was kept at the same level (20  $\mu\text{M}$ ), but the output power of the laser used in our experiment was lower (400 mW) than in Ref. [1] (500 mW) and the concentration of upconverting nanoparticles was 10 times lower (10 mg mL<sup>-1</sup> here and 100 mg mL<sup>-1</sup> in Ref. [1]). Moreover, the sizes of upconverting cores and silica shells were different.

### The kinetic of singlet oxygen generation.



**Figure S7.** Kinetics of singlet oxygen generation. ABDA fluorescence intensity ( $\lambda_{\text{ex}} = 382 \text{ nm}$ ) was monitored as a function of exposure time of the sample to NIR laser irradiation (980 nm); all samples were prepared by dispersing of 10 mg of appropriate nanoparticles in 1 ml of 20  $\mu\text{M}$  ABDA solution in DI.

The kinetic of singlet oxygen generation detected through ABDA fluorescence quenching is presented in Figure S7. The ABDA fluorescence spectra under excitation at 382 nm were collected every one minute during over an hour under continues irradiation of NGF@mSiO<sub>2</sub>(Pc) dispersion with 980 nm laser diode. Since the laser beam spot size was reduced in this experiment the fluorescence intensity decays slower than in Figure 7. It has been observed that emission of ADPA, employed as a probe of single oxygen generated when merocyanine 540 (M-540) incorporated into silica shell of NaYF<sub>4</sub>:Er<sup>3+</sup>,Yb<sup>3+</sup> NPs was used as a photosensitizing molecule, followed an exponential decay over time<sup>2</sup>. In Figure S7 the dependence of ABDA emission intensity as a function of exposure time is closer to linear than exponential function.

### References.

- (1) Qian, H. S.; Guo, H. C.; Ho, P. C. L.; Mahendran, R.; Zhang, Y. *Small* **2009**, *5*, 2285–2290.
- (2) Zhang, P.; Steelant, W.; Kumar, M.; Scholfield, M. *J. Am. Chem. Soc.*, **2007**, *129*, 4526–4527.