Core-shell designs of photoluminescent nanodiamonds with porous silica coatings for bioimaging and drug delivery I: Fabrication

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Supplementary Information



Supplementary Figure 1. DLS of sample ND-1. z-average=193 nm, PDI=0.096, (Intensity mean=212 nm; volume mean =216 nm; number mean =168 nm)



Supplementary Figure 2. DLS of SiO₂-coated ND-1 (CTAB/TEOS 40/100). z-average=373 nm, PDI=0.067, (Intensity mean=398 nm, volume mean = 428 nm, number mean= 356 nm).



Supplementary Figure 3. DLS of sample ND-2. z-average =84 nm, PDI=0.325, (DLS average size by intensity of main peak=129 nm; intensity mean=198 nm; number mean=15 nm; volume mean=82 nm)



Supplementary Figure 4. DLS of SiO₂-coated ND-2. z-average =262 nm, PDI=0.024, (DLS average size by intensity=272 nm, volume mean = 284 nm, number mean= 248 nm).



Supplementary Figure 5. Fourier transform infrared transmission spectra for pure CTAB, ND@MSN before and after extraction of the CTAB template. The green spectrum corresponds to that of pristine SiO₂.



Supplementary Figure 6. The dependency of integral PL intensity over time for 0.3 mg/ml water suspension of ND-2. The PL intensity was measured every 15 min for 2-hours of irradiation of the suspensions with 488 nm Ar laser light of 10 W/cm² power density.



Supplementary Figure 7. Powder XRD patterns of silica-coated samples a) ND-1@MSN and b) ND-2@MSN. The *d*-values for both peaks are 38.5 Å, characteristic of ordered mesopores in the size range 3-4 nm.





Supplementary Figure 8. Elemental analysis on sample CTAB/TEOS 10/20 confirming the presence of carbon (ND) only.

Nanodiamond/silica ratio in silica-coated ND-1, 230 nm (average from TEM)

 $d(ND_{core}) = 80 \text{ nm} \rightarrow r = 40 \text{ nm}$ $d(ND-SiO_2) = 230 \text{ nm} \rightarrow r = 115 \text{ nm}$

$$\begin{split} \rho_{\text{ND}} &= 3.5 \text{ g/cm}^3 \\ \rho_{\text{np} \text{ SiO2}} &= 2.2 \text{ g/cm}^3 \\ \rho_{\text{mp} \text{ SiO2}} &= 0.73 \text{ g/cm}^3 \ (\sim\!66\% \text{ porosity}) \\ \text{[pore volume} &= 0.795 \text{ cm}^3/\text{g]} \end{split}$$

 $V = \frac{4}{3}\pi r^{3}$ $V_{ND} = \frac{4}{3}\pi * (40nm)^{3} = 2.716 * 10^{4}nm^{3}$ $V_{ND-SiO_{2}} = \frac{4}{3}\pi (115nm)^{3} = 6.455 * 10^{5}nm^{3}$ $V_{SiO_{2}} = V_{ND-SiO_{2}} - V_{ND} = \frac{4}{3}\pi 115^{2} - \frac{4}{3}\pi 40^{2} = 6.1834 * 10^{5} nm^{3}$

$$\rho = \frac{m}{V}$$
 $n = \frac{N}{N_A}$
 $n = \frac{m}{M}$

$$\begin{split} m_{ND} &= \rho V = 3.5 \frac{g}{cm^3} * 2.716 * 10^4 * 10^{-18} cm^3 = 9.506 * 10^{-14} g \\ m_{SiO_2} &= \rho V = 0.73 \frac{g}{cm^3} * 6.1834 * 10^5 * 10^{-18} cm^3 = 4.514 * 10^{-13} g \\ \frac{m_{ND}}{m_{SiO_2}} &= 9.506 * \frac{10^{-14} g}{4.514 * 10^{-13} g} = \frac{1}{4.75} \end{split}$$

Ratio ND/SiO₂ \sim 1/4.75