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


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 SiO$_2$-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 SiO$_2$-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)**

\[
d(\text{ND}_{\text{core}}) = 80 \text{ nm} \rightarrow r = 40 \text{ nm} \\
d(\text{ND-SiO}_2) = 230 \text{ nm} \rightarrow r = 115 \text{ nm} \\
\rho_{\text{ND}} = 3.5 \text{ g/cm}^3 \\
\rho_{\text{np SiO}_2} = 2.2 \text{ g/cm}^3 \\
\rho_{\text{mp SiO}_2} = 0.73 \text{ g/cm}^3 \ (\sim 66\% \ \text{porosity}) \\
\text{[pore volume} = 0.795 \text{ cm}^3/\text{g}] \\
\]

\[
V = \frac{4}{3} \pi r^3 \\
V_{\text{ND}} = \frac{4}{3} \pi (40 \text{ nm})^3 = 2.716 \times 10^4 \text{ nm}^3 \\
V_{\text{ND-SiO}_2} = \frac{4}{3} \pi (115 \text{ nm})^3 = 6.455 \times 10^5 \text{ nm}^3 \\
V_{\text{SiO}_2} = V_{\text{ND-SiO}_2} - V_{\text{ND}} = \frac{4}{3} \pi 115^2 - \frac{4}{3} \pi 40^2 = 6.1834 \times 10^5 \text{ nm}^3 \\
\rho = \frac{m}{V} = \frac{N}{N_A} = \frac{m}{M} \\
\]

\[
m_{\text{ND}} = \rho V = 3.5 \frac{g}{\text{cm}^2} \times 2.716 \times 10^4 \times 10^{-18} \text{ cm}^2 = 9.506 \times 10^{-14} g \\
m_{\text{SiO}_2} = \rho V = 0.73 \frac{g}{\text{cm}^2} \times 6.1834 \times 10^5 \times 10^{-18} \text{ cm}^2 = 4.514 \times 10^{-13} g \\
\frac{m_{\text{ND}}}{m_{\text{SiO}_2}} = \frac{9.506 \times 10^{-14} g}{4.514 \times 10^{-13} g} = \frac{1}{4.75} \\
\]

Ratio ND/SiO₂ \sim 1/4.75