Electronic Supplementary Information

Fluorescent and paramagnetic core-shell hybrid nanoparticles for bi-modal magnetic resonance/luminescence imaging

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1 - **Characterization of the as-synthesized amorphous $Gd(OH)CO_3{\cdot}H_2O$ nanoparticles**

The FT-IR spectrum provides the insight into the chemical composition of the as-prepared sample (Figure S1(a)). A strong and broad absorption bands peaking at 3400 cm^{-1} and a shoulder located at 1645 cm^{-1} are the characteristic absorption of water of hydration in the structure or surface adsorbed water and hydroxyl groups (OH^-).[1] The presence of carbonate anions in the molecular structure was confirmed by the appearance of absorption doublets in the region 1350–1600 cm^{-1} (ν_3 of CO_3^{2-}, peaking at ~1408 and 1504 cm^{-1}) and also by the occurrence of multiple absorptions ranging from 500 to 1000 cm^{-1} (ν_2 and ν_4 of CO_3^{2-}).[2,3] The elemental analysis quantifies the elemental components (mass %) of the as-prepared precursor. Elemental contents of the dried particles analyzed by the inductively coupled plasma (ICP) spectrophotometric method were listed in Table S1, yielding a Gd:C:O molar ratio of about 1:1.01:5.10. Assuming that all the carbon was from CO_3^{2-} and considering molecular neutrality, the chemical formula of the as-prepared product may be expressed as $Gd(OH)CO_3{\cdot}H_2O$. The results are consistent with the pioneering work of Matijevic *et al.* and the recent work by Lechevallier's group.

The thermogravimetric analysis (TGA) curve of the as-prepared sample was shown in Figure S2. The weight loss of $Gd(OH)CO_3{\cdot}H_2O$ undergoes a three-step process. The first one (25-170°C) is due to the desorption of water molecules adsorbed at the particles surface due to the storage in air. The second weight loss (170-550°C) is related to the removal of water molecules due to the dehydration of hydrated compounds and the self-condensation of hydroxyl groups (O-H). This is confirmed by FTIR spectrum of the sample calcinated at 550°C (Figure S1(b)), where the characteristic absorptions of hydration water and hydroxyl groups almost disappear, compared to that of the as-prepared $Gd(OH)CO_3{\cdot}H_2O$ (Figure S1(a), SI). The third one (550-750 °C) originates from the release of CO_2 molecules that is also confirmed by FTIR spectrum of the sample calcinated at 750 °C (Figure. S1(c)), in which we observed the disappearance of the characteristic vibrations of CO_3^{2-}.

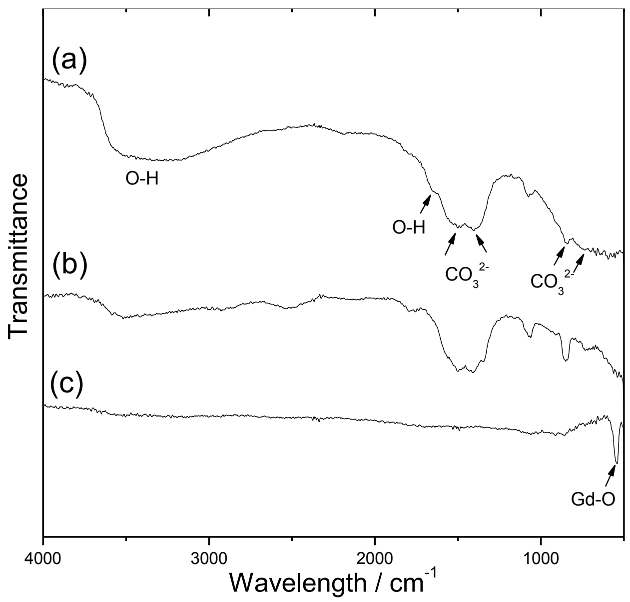

Figure S1. FT-IR spectra of the as-prepared Gd(OH)CO$_3$·H$_2$O (a) and the samples calcinated at 550 ºC (b) and 750 ºC (c), respectively.

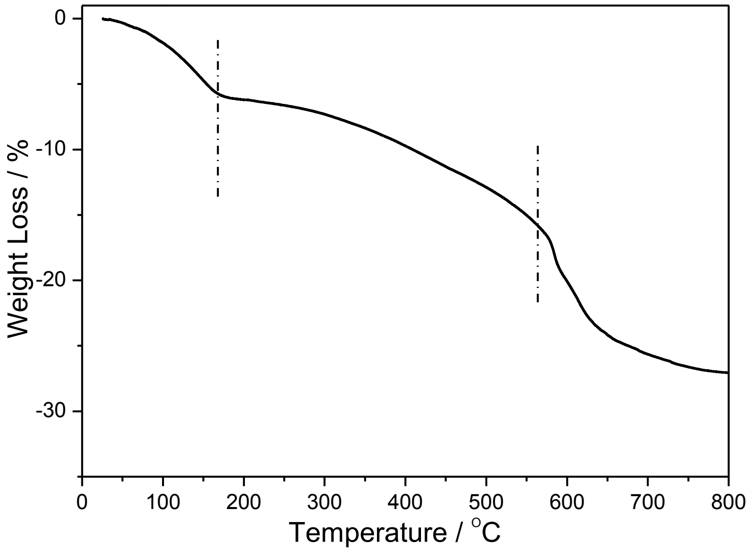

Figure S2. Thermogravimetric analysis curve of the precursor Gd(OH)CO$_3$·H$_2$O measured in air.

Table S1. Elemental content of as-prepared partilcles (mass %).

Gd	C	O
62.1%	4.8%	31.6%

2 – The absorption spectrum of RhB entrapped core-shell nanoparticles.

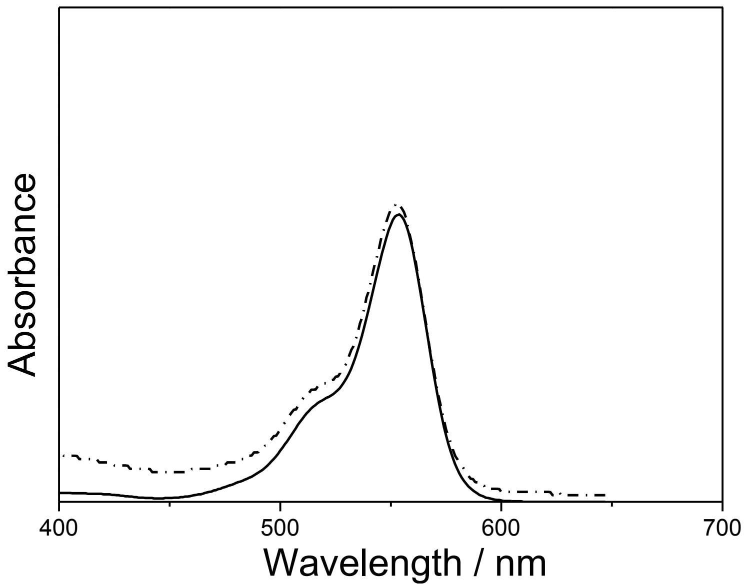

Figure S3. Absorption spectra of pure RhB (full line) and RhB entrapped $Gd(OH)CO_3 \cdot H_2O@SiO_2$ core-shell particles (dash dotted line).

3 - Cell imaging of RhB entrapped core-shell nanoparticles.

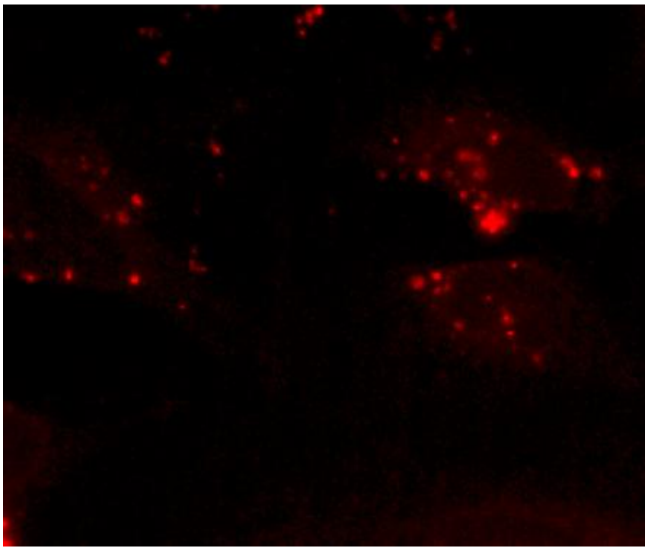

Figure S4. A representative fluorescence image taken from an internal slice of the HeLa cell incubated with RhB entrapped core-shell nanoparticles.

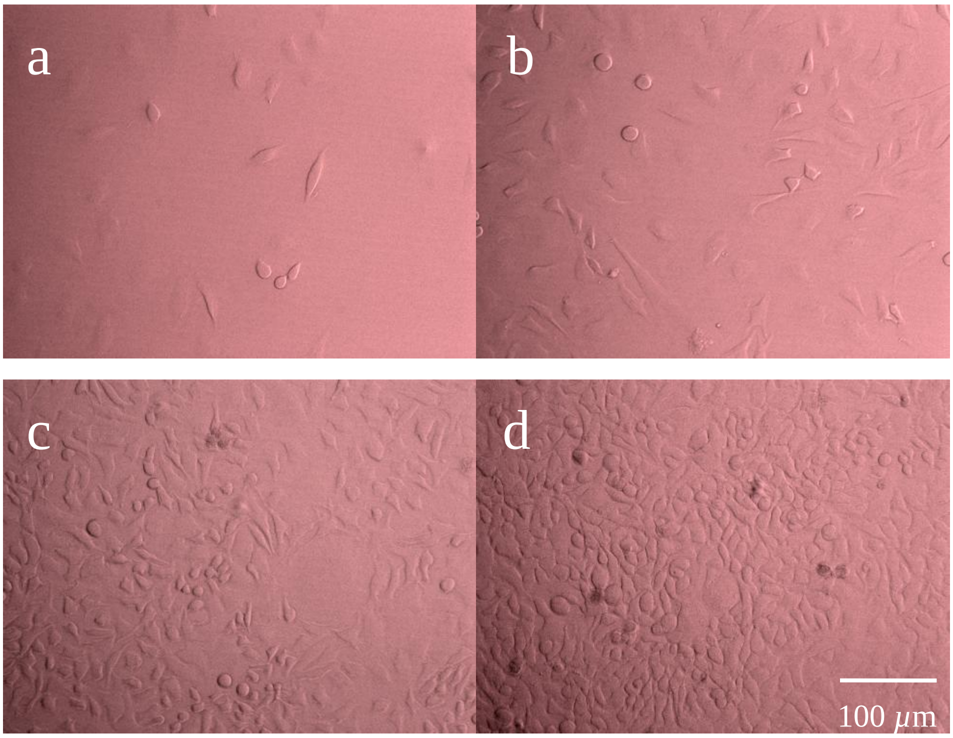

Figure S5. Bright-field microscopy images of HeLa cells alone with incubation time of 4h (a), 24 h (b), 48 h (c) and 72 h (d).

References

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2. W. Matijevic and W. Hsu, *J. Colloid. Interface Sci.* 1987, **118**, 506.

3. K. Makamoto, Infrared spectra of inorganic and coordination compounds. New York: John Wiley & Sons; 1963.