Electronic Supplementary Information

Phase-transfer Preparation of Ultrasmall MnS Nanocrystals with High Performance of MRI Contrast Agent

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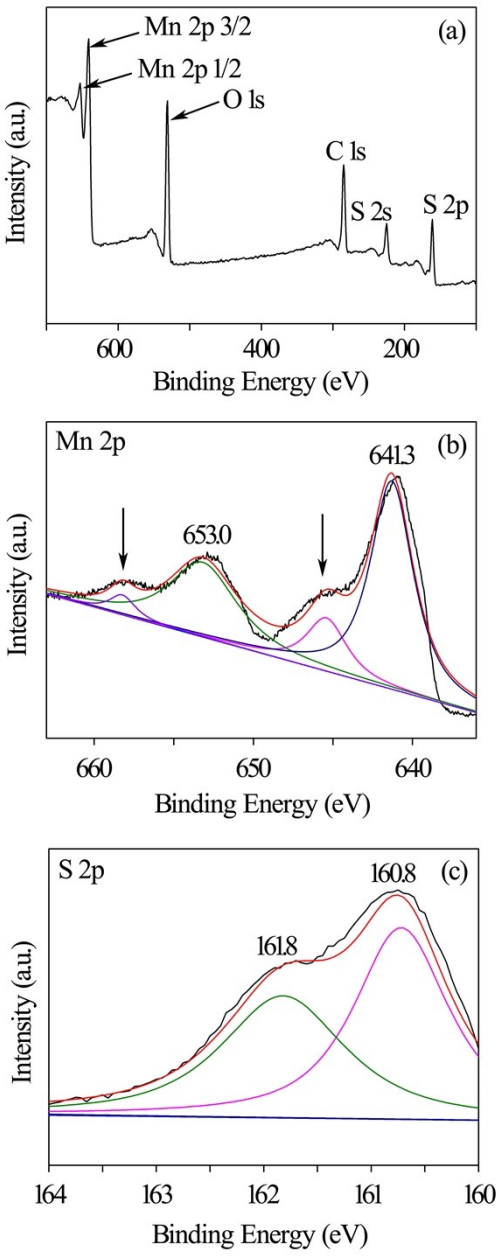
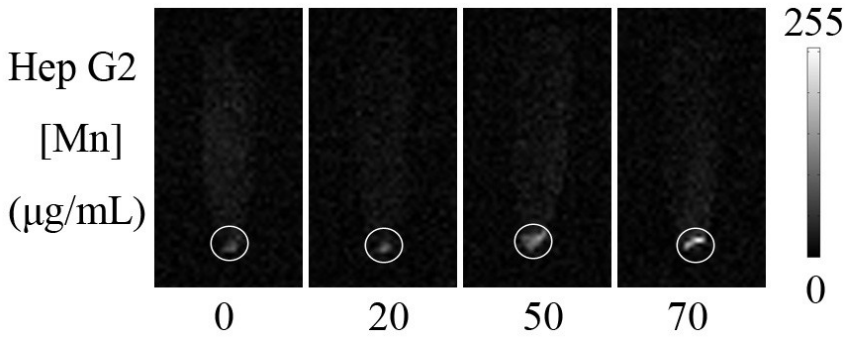
Figure S1. XPS patterns for survery (a), Mn 2p (b) and S 2p (c) of the obtained MnS aggregations.



The X-ray photoelectron spectrometry (XPS) analysis of the MnS aggregations is shown in Figure S1. The molar ratio of Mn and S was calculated to be approximately

1:1 from the XPS peak areas of Mn and S, which was consistent with their stoichiometry within expected error margins. The high-resolution XPS spectra of Mn 2p and S 2p were also measured (Figure S1b and Figure S1c) .The peaks at about 653.0eV and 641.3 eV (Figure S1b) can be assigned to the $2p_{1/2}$ and $2p_{3/2}$ binding energies of Mn^{2+}, including the satellites at about 645.4eV and 658.2 eV. Figure S2c shows the binding energy of S 2p peaks. The deconvoluted binding energies of 161.8 eV and 160.8 eV could be assigned to S $2p_{1/2}$ and S $2p_{3/2}$, indicating the presence of S^{2-}. The binding energies of Mn 2p and S 2p were in accordance with the data reported for MnS.[1\]

Figure S2. T_1-weighted MR images of MnS nanocrystals in Hep G2 cells for 6 h incubation time (0.47 T).



To evaluate the potential application of the MnS nanocrystals as a probe for MR imaging *in vitro*, T_1-weighted MR images were also collected incubated with Hep G2 cells. Hep G2 cells were seeded into culture dishes at a density of 10^7/plate and then cultured over night at 37°C under 5% CO_2. Then, MnS nanocrystals were added with different concentrations of 0, 20, 50, 70 μg mL^{-1}. After co-incubation for 6 h, the cells were washed three times with PBS and detached by adding 1 mL of trypsin/EDTA. After centrifugation, the cells containing MnS nanocrystals in PBS were precipitated at the bottom of the 1.5 mL centrifuge tubes. As shown in Figure S2, it is obvious that

the T_1-MRI signal at the bottom of tubes (marked by the white circles) show a distinct MR signal enhancement with an increase in the incubation concentration of MnS nanocrystals, which was attributed to the dose-dependent cellular uptake. Our results further suggested that the MnS nanocrystals have the potential for the use as MRI T_1 contrast agents *in vivo*.

References

1. Lu J.; Qi P.; Peng Y.; Meng Z.; Yang Z.; Yu W.; Qian Y. *Chem. Mater.* **2011**, *13*, 2169-2172.