Electronic Supporting Information

Facile Preparation of Gadolinium(III) Chelates Functionalized Carbon Quantum Dots-based Contrast Agent for Magnetic Resonance/Fluorescence Multimodal Imaging

Xianyan Ren, a,b Lihua Liu, c Yu Li, a Qin Dai, c Ming Zhang, c and Xinli Jing* a

a Department of Applied Chemistry, School of Science, Xi’an Jiaotong University, Xi’an, 710049, China.
Fax: +86 29 83237910; Tel.: +86 29 68640809; E-mail: xljing@mail.xjtu.edu.cn, rgfp-jing@mail.xjtu.edu.cn

b State Key Laboratory Cultivation Base for Nonmetal Composite and Functional Material, School of Materials Science and Engineering, Southwest University of Science and Technology, Mianyang, 621010, China.

c First Affiliated Hospital of Xi’an Jiaotong University, Xi’an, 710061, China.

1. Weight extinction coefficient of Gd(III)/CQDs

The weight extinction coefficient of Gd(III)/CQDs at 365 nm and 488 nm were measured according to Lambert-Beer law. In brief, water solutions of Gd(III)/CQDs with different mass concentration of 0.1, 0.25, 0.5, 0.8 and 1 mg·L⁻¹ were prepared, whose absorbances at 365 nm and 488 nm, respectively, were recorded by an UV-vis spectrophotometer (Hitachi U2001). The weight extinction coefficient was calculated through dividing the absorbance by the concentration and the cell length (1 cm). As shown in Figure S1, the weight extinction coefficient (a) of the Gd(III)/CQDs at 365 nm and 488 nm was 1.99 L·g⁻¹·cm⁻¹ and 0.72 L·g⁻¹·cm⁻¹, respectively.

![Figure S1 Absorbances versus weight concentration of Gd(III)/CQDs prepared at 300 °C at 365nm (1) and 488 nm (2).](image)

2. Dispersibility of Py-GdPM, Py-Mx and the mixture of Py-GdPA and Py-Meg.
Figure S2 Water dispersion (1 mg.mL$^{-1}$) of the (a): mixture of Py-Meg and Py-GdPA, (b) Py-Mx, and (c) Py-GdPM (300 °C).

3. TEM images of Gd(III)/CQDs prepared at 250 °C and 300 °C, respectively.

Figure S3 TEM images and size histograms of Gd(III)/CQDs prepared at (a) 250 °C and (b) 300 °C.

4. Wide-scan XPS spectra

Figure S4 Wide-scan XPS spectra (1: GdPM; 2-5: Gd(III)/CQDs prepared at 250 °C, 300 °C, 350 °C and 400 °C, respectively).
5. Dialysis experiment

Two solutions (5 mL) containing Gd$^{3+}$ at a concentration of 0.4 mg·mL$^{-1}$ were prepared by dissolving gadopentetic acid and Gd(III)/CQDs into water, respectively. Each of them was dialyzed against a dialysate of 500 mL deionized water through a 1000D dialysis bag (with a pore diameter of about 1.2 nm). The concentrations of Gd$^{3+}$ in the dialysate at different time passing through dialysis bag during dialysis were detected by an inductively coupled plasma optical emission spectrometer (ICP-ES, Varian 715) (Figure S5).

Figure S5 The concentration of Gd$^{3+}$ ions passing into dialysate at different time during dialysis of gadopentetic acid and Gd(III)/CQDs, respectively. Inset: the UV-vis spectra of dialysate (after dialysis of Gd(III)/CQDs for 24h) and the Gd(III)/CQDs before dialysis.

6. Photoluminescence properties of Gd(III)/CQDs

Table S1 The maximum emission wavelength ($\lambda_{em}$), maximum excitation wavelength ($\lambda_{ex}$), Stokes shift and FWHM of Gd(III)/CQDs prepared at different temperatures.

<table>
<thead>
<tr>
<th>Pyrolysis temperature (°C)</th>
<th>$\lambda_{em}$/nm</th>
<th>$\lambda_{ex}$/nm</th>
<th>Stokes shift/nm</th>
<th>FWHM/nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>250</td>
<td>436</td>
<td>360</td>
<td>86</td>
<td>102</td>
</tr>
<tr>
<td>300</td>
<td>442</td>
<td>375</td>
<td>92</td>
<td>134</td>
</tr>
<tr>
<td>350</td>
<td>434</td>
<td>368</td>
<td>84</td>
<td>110</td>
</tr>
</tbody>
</table>

7. Dispersibility of Gd(III)/CQDs
Figure S6 Gd(III)/CQDs solution in water, phosphate-buffered saline buffer solution and culture medium with a concentration of 2 mg·mL$^{-1}$