Electronic Supplementary Information

for

N-doped carbon dots as robust fluorescent probes for the rapid detection of hypochlorite

Kai Wang,* Zongling Ru, Jiwei Shi, Yuezhao Zhu, Liguo Yang, Mengxue Wei,

Mengli Xiao, Nana Liu and Fang Wang

Table of Contents

1.	Preparation of N-doped carbon dotsS2
2.	Quantum yield (QY) measurements of four N-doped carbon
	dotsS2
3.	UV-vis Absorption Spectra AnalysisS4
4.	Density Functional Theory (DFT) calculationS5
5.	QYs of NCDs in the presence of hypochlorite

1. Preparation of N-doped carbon dots

Citric acid (0.50 g, 2.6 mmol) and 4-methoxybenzene-1,2-diamine (0.5 g, 3.6 mmol) were dispersed in 20 mL deionized water. Then, the solution was transferred to a poly(tetrafluoroethylene) autoclave (50 mL), and heated at 180 °C for 6 h. Afterwards, the autoclave was cooled to room temperature naturally. The crude products were centrifuged (at 10000 rpm for 10 min) and filterd with 0.22 µm filter membrane to remove agglomerated larger particles. The filtrate was dialyzed with dialysis membrane (MWCO: 1000 Da) for 24 h to get rid of salt and impurities. Finally, the sample was freeze-dried and the MeO-NCDs was obtained thereby.

CF₃-NCDs and NO₂-NCDs were prepared using similar synthetic method.

2. Quantum yield measurements of four N-doped carbon dots

Quinine sulfate (0.1 M H₂SO₄ as solvent, $\Phi_F = 54\%$) was employed as the standard to measure the quantum yields (QYs) of NCDs through slope method ^{S1}. The QYs were calculated by comparing the integrated fluorescence intensity (excited at 360 nm) and the absorbance value (the value was below 0.1 at the excitation wavelength). The slope method equation was as follows:

 $\Phi_{\rm x} = \Phi_{\rm st} (K_{\rm x}/K_{\rm st}) (\eta_{\rm x}/\eta_{\rm st})^2$

Where Φ is the quantum yield, K is the slope of linear fitting curves and η is the refractive index of the corresponding solvent. The subscript "st" refers to standard substance (quinine sulfate) and "x" refers to the tested sample. For the diluted solutions, $\eta_x/\eta_{st} = 1$.



Figure S1 Fluorescence and absorbance of the (a) NCDs, (b) MeO-NCDs, (c) CF_3 -NCDs, (d) NO₂-NCDs and (e) quinine sulfate, respectively.

3. UV-vis Absorption Spectra Analysis



Figure S2 Absorption of the mixed system of NCDs (10 μ g/mL) and NaClO (7 μ M) under the different temperatures (25 °C, 35 °C and 50 °C).

3. Density Functional Theory (DFT) calculation



Figure S3 (a) The optimized molecular geometry of another possible fluorophore unit3 of Ox-NCDs. (b) HOMO-LUMO energy levels of 1 and 3, respectively.

The optimized molecular geometry of another possible fluorophore unit **3** are shown in Figure S5. According to the LUMO levels of **1** and **3**, the electron transfer (ET) process of excited light from **1** to **3** hardly took place due to the higher energy level difference (2.48 eV). Moreover, the energy gap **3** ($E_g = 1.414 \text{ eV}$) is much lower than that of **1** ($E_g = 2.187 \text{ eV}$), indicating **3** can emit fluorescence of much longer wavelength than that of **1** ($\lambda = 370 \text{ nm}$). Unfortunately, this phenomenon is not observed. Therefore, **3** is not proposed as the most possible fluorophore of Ox-NCDs.

4. QYs of NCDs in the presence of hypochlorite



Figure S4 Fluorescence and absorbance of NCDs with the addition of 615 nM NaClO (a), NCDs in the presence of 6.15 μ M NaClO (b), respectively.

References

S1. S. Zhu, Q. Meng, L. Wang, J. Zhang, Y. Song, H. Jin, K. Zhang, H. Sun, H. Wang and B. Yang, *Angew. Chem. Int. Ed.*, 2013, **52**, 3953-3957.