Supplementary Material

Ultrafast and Energy-saving Synthesis of Nitrogen and Chlorine Co-doped Carbon Nanodots via Neutralization Heat for Selective Detection of Cr(VI) in Aqueous Phase

Qin Hu ^{1,2}, Tao Li ³, Lu Gao ^{1,2}, Xiaojuan Gong ⁴, Shengqi Rao ^{1,2}, Weiming Fang ^{1,2}, Ruixia Gu ^{1,2} and Zhenquan Yang ^{1,2,*}

- ¹ College of Food Science and Engineering, Yangzhou University, Jiangsu 225001, China; qinhu1998@outlook.com (Q.H.); gaolu@yzu.edu.cn (L.G.); sqrao@yzu.edu.cn (S.R.); wmfang@yzu.edu.cn (W.F.); rxgu@yzu.edu.cn (R.G.)
- ² Jiangsu Key Laboratory of Dairy Biotechnology and Safety Control, Yangzhou University, Jiangsu 225001, China
- ³ Department of Agronomy, Yangzhou University, Jiangsu 225001, China; taoli@yzu.edu.cn
- ⁴ Institute of Environmental Science, and School of Chemistry and Chemical Engineering, Shanxi University, Taiyuan 030006, China; gxj1124@sxu.edu.cn
- * Correspondence: yangzq@yzu.edu.cn (Z.Y); Tel.: +86-0514-8978-6037

Experimental

Quantum Yield (QY) Measurements

The quantum yield (Φ_s) of the as-fabricated *N*,*Cl*-CDs sample was determined by a comparative method. The quinine sulfate ($\Phi_R = 0.54$) in 0.10 M H₂SO₄ (refractive index, $\eta = 1.33$) was used as the reference to determine the Φ_s of the *N*,*Cl*-CDs sample in ultrapure water ($\eta = 1.33$) at different concentrations. A UV-2550 absorption spectrophotometer (Shimadzu Co., Ltd., Tokyo, Japan) was used to record all the absorbances of the solutions at 380 nm. A RF-5301PC fluorescence spectrophotometer (Shimadzu Co., Ltd., Tokyo, Japan) was used to record their PL spectra with an excitation wavelength (λ_{ex}) of 380 nm. The integrated PL intensity was the area under the PL curve in the wavelength range of

400–600 nm. Then a graph of the integrated PL intensity against the absorbance was plotted. The Φ_s of the *N*,*Cl*-CDs sample was calculated using equation (1):

$$\Phi_{\rm S} = \Phi_{\rm R} \left(\operatorname{Grad}_{\rm S} / \operatorname{Grad}_{\rm R} \right) \left(\eta^2_{\rm S} / \eta^2_{\rm R} \right) \tag{1}$$

where Grad is the gradient from the plot of the integrated PL intensity against the absorbance, and η is the refractive index of the solvent. The subscripts S and R denote the sample and reference, respectively. In order to minimize the self-absorption effect, the absorbances in the 10-mm path-length fluorescence cuvette was kept under 0.01 at the λ_{ex} of 380 nm[1–2].

References:

- 1. Zhu, S.; Meng, Q.; Wang, L.; Zhang, J.; Song, Y.; Jin, H.; Zhang, K.; Sun, H.; Wang, H.; Yang, B., Highly Photoluminescent Carbon Dots for Multicolor Patterning, Sensors, and Bioimaging. *Angewandte Chemie International Edition* **2013**, 52, (14), 3953-3957.
- 2. Tian, T.; He, Y.; Ge, Y.; Song, G., One-pot synthesis of boron and nitrogen co-doped carbon dots as the fluorescence probe for dopamine based on the redox reaction between Cr(VI) and dopamine. *Sensors and Actuators B: Chemical* **2017**, 240, 1265-1271.

Table S1. Elemental analysis of the as-fabricated *N*,*Cl*-CDs: (A) elemental content and (B) relative number of atom in *N*,*Cl*-CDs.

	Elemental content							
Sample	С	Н	N	C1	0			
					(calculated)			
<i>N,Cl</i> -CDs	25.88%	9.40%	25.69%	23.29%	15.74%			

Sample		Relati	Empirical formula			
	С	Н	Ν	Cl	0	C HaN ChO
N,Cl-CDs	6	28	6	2	3	C6H28IN6CI2O3



Figure S2. Plots of integrated PL intensity against the absorbance of (A) *N*,*Cl*-CDs and (B) quinine sulfate at λ_{ex} /emission wavelength (λ_{em}) of 381/468 nm.

Sample name	<i>N,Cl-</i> CDs	N,Cl-CDs/Cr(VI)
$\tau_{l}(ns)/A_{l}(\%)$	4.43/32.86	2.92/21.91
$\tau_2(ns)/A_2(\%)$	10.75/67.14	9.08/78.09
Average $\tau(ns)$	8.67	7.73

Table S2. Double-exponential fitting of *N*, *Cl*-CDs and *N*, *Cl*-CDs/Cr(VI) decay curves.



Figure S3. Cell viability test of *N*,*Cl*-CDs on SiHa cells. The values represent percentage cell viability (mean $\% \pm$ SD, n=6).