Supporting Information

Designing green-emissive Cu,N-co-doped carbon dots by pyrolysis of aromatic precursors and application in sensing of Fe(III) and Cr(VI)

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Table S1. Buffer solutions

pH	Salt mixture	Dilute with deionized water to
1	0.3725g KCl and 67mL of 0.20M HCl	100mL
2	0.3725g KCl and 6.5mL of 0.20M HCl	100mL
3	1.021g potassium hydrogen phthalate and 11.15mL of 0.20M HCl	100mL
4	1.021g potassium hydrogen phthalate and 0.05mL of 0.20M HCl	100mL
5	1.021g potassium hydrogen phthalate and 11.3mL of 0.20M NaOH	100mL
6	6.81g potassium dihydrogen phosphate and 23mL of 0.20M NaOH	1000mL
7	**6.81g potassium dihydrogen phosphate and 145.5mL of 0.20M NaOH**	**1000mL**
8	0.681g potassium dihydrogen phosphate and 23.35mL of 0.20M NaOH	100mL
9	0.477g sodium tetraborate and 2.3mL of 0.20M HCl	100mL
10	0.477g sodium tetraborate and 9.15mL of 0.20M NaOH	100mL
11	0.21g sodium bicarbonate and 11.35mL of 0.20M NaOH	100mL
12	0.3725g KCl and 6mL of 0.20M NaOH	100mL
13	0.3725g KCl and 66mL of 0.20M NaOH	100mL

Table S2. QY calculated for Cu,N-CDs

Sample	Intergrated emission intensity (I)	Optical density (A)	Refractive index (n)	Quantum yield (QY)
Quinine sulfate	$104x10^7$	0.207	1.33	0.54 (known)
Cu,N-CDs	$9x10^7$	0.065	1.33	0.15

$$Q = Q' \times \frac{A'}{I'} \times \frac{I}{A} \times \frac{n^2}{n'^2}$$

$$Q = 0.54 \times \frac{0.207}{104x10^7} \times \frac{9x10^7}{0.065} = 0.149$$

Table S3. Reference papers reported carbon dots and its QY

	Precursors	Method	QY (%)	Reference
1	Citric acid, urea	Hydrothermal microwave-assisted pyrolysis	19.0	(1)
2	Morus alba L. leaves	Hydrothermal	9.3	(2)
3	Glucose, ammonia	Continuous hydrothermal flow synthesis (CHFS)	9.6	(3)
4	Tartaric acid, urea	Solid-phase thermal method	10.5	(4)
5	Ammonium citrate	Hydrothermal	13.5	(5)
6	Calcium citrate, urea	Microwave assisted	10.1	(6)
7	**p-Aminosalicylic acid, copper(II) acetylacetonate**	**Solvent-free pyrolysis**	**14.9**	**This work**

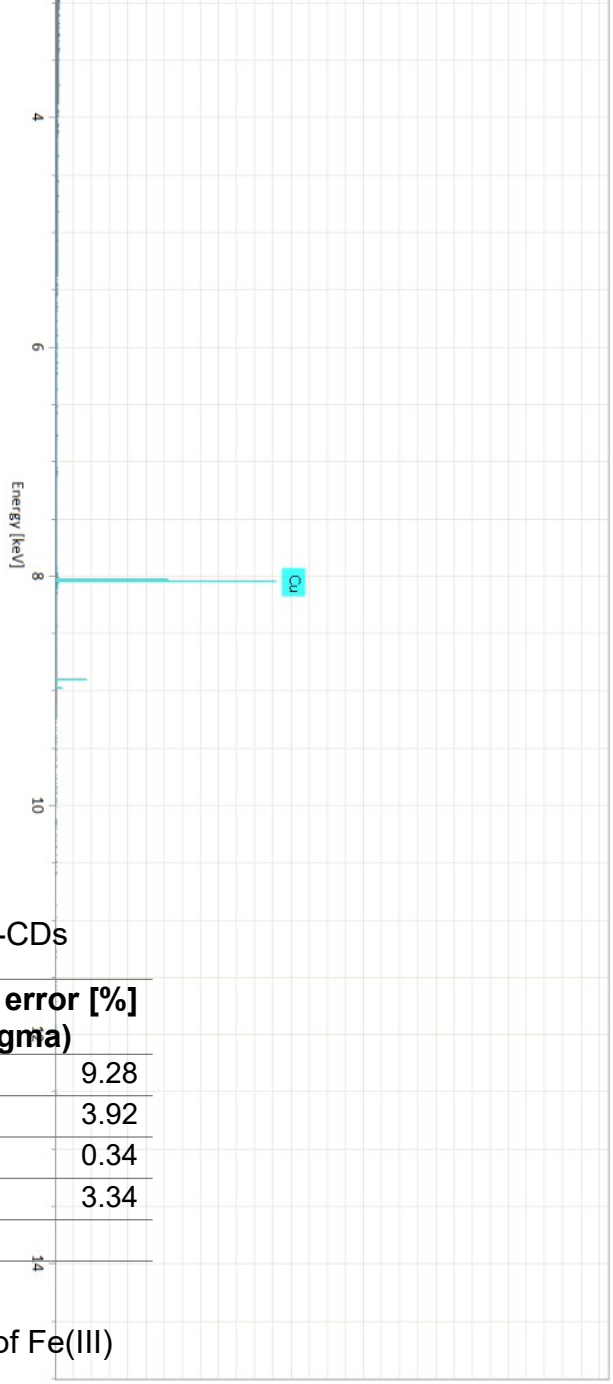

Figure S1. EDX analysis of Cu,N-CDs

Table S4. Results of EDX scan of Cu,N-CDs

Element	Mass Norm. [%]	Atom [%]	abs. error [%] (1 sigma)
C	68.06	75.06	9.28
O	18.28	15.13	3.92
Cu	4.23	0.88	0.34
N	9.43	8.92	3.34
	100.00	100.00	

Table S5. Calculating limit of detection of Fe(III)

Fe(III) (nM)	F_0/F
10	1.09
20	1.11
50	1.18
100	1.25
200	1.3
500	1.25
1000	1.3
2000	1.71
5000	2.58
10000	8.72
20000	15.84
50000	33.19
100000	50.32

Slope	0.000658
Standard error for slope	1.85E-05
R^2	0.992123
F statistic	1259.575
Regression sum of squares	1026.17
Intercept	1.006347
Standard error for intercept	0.294505
Standard error for Y estimate	0.902605
Degrees of freedom	10
Residual sum of squares	8.146952
Ksv (1/M)	6.58E+05
LOD (nM)	1477.591

Table S6. Calculating limit of detection of Cr(VI)

Cr(VI) (nM)	F_0/F
10	1.004678
25	1.012013
50	1.069548
75	1.097959
100	1.182746
250	1.409411

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Slope	0.001732
Standard error for slope	8.85E-05
R^2	0.989663
F statistic	382.9678
Regression sum of squares	0.113968
Intercept	0.982189
Standard error for intercept	0.010304
Standard error for Y estimate	0.017251
Degrees of freedom	4
Residual sum of squares	0.00119
Ksv (1/M)	1.73E+06
LOD (nM)	19.63523

Table S7. Comparison of CD-based fluorescent probes for Fe(III) and Cr(VI) detection

Fe(III) detection					
Material	Synthetic Method	Emission λ (nm)	QY (%)	LOD	Ref.
N-CQDs (citric acid/o-phenylenediamine)	Hydrothermal	483	33.55%	0.177 μM	(7)
N-CDs (citric acid/o-phenylenediamine)	Hydrothermal	535	30.2%	13.8 nM	(8)
N-CDs (carboxymethylcellulose/LPEI)	Hydrothermal	465.5	44%	0.14 μM	(9)
N-CQDs	Microwave-	399	9.5%	2.54 μM	(10)

(pumpkin seeds)	assisted				
CDs (glutamic acid/ethylenediamine)	Microwave-assisted	459	12.45%	3.8 μM	(11)
N-CDs (guanidinium chloride/ citric acid)	Pyrolysis with water, 225°C, 12min	425	19.2	100 nM	(12)
N-CDs (ethylenediamine/citric acid monohydrate)	Pyrolysis with water, 120°C, 48h	450	65.5%	0.703 μM	(13)
Cu,N-CDs (PAS/Cu(acac)$_2$)	**Solvent-free pyrolysis, 170°C, 3h**	**495**	**14.9%**	**1.48 μM**	**This work**
Cr(VI) detection					
Cu-CDs (citric acid/urea/$CuCl_2$)	Hydrothermal	438	27.3	0.186 μM	(14)
CDs (EDTA salt)	Hydrothermal	550	—	10 μM	(15)
N,S-CDs (citric acid/L-cysteine)	Microwave-hydrothermal	420	49.3	58 nM	(16)
N,S-CDs (citric acid/L-glutathione)	Pyrolysis, 270°C, 2h	418	69	102 nM	(17)
N-CDs (citric	Pyrolysis,	448	16.2	0.3 μM	(18)

acid/glutamic acid)	200°C, 40min				
Cu,N-CDs (PAS/Cu(acac)$_2$)	**Solvent-free pyrolysis, 170°C, 3h**	**495**	**14.9%**	**19.6 nM**	**This work**

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