

Electronic supporting information

## Highly Fluorescent Nitrogen and Boron Doped Carbon Quantum Dots for Selective and Sensitive Detection of Fe<sup>3+</sup>

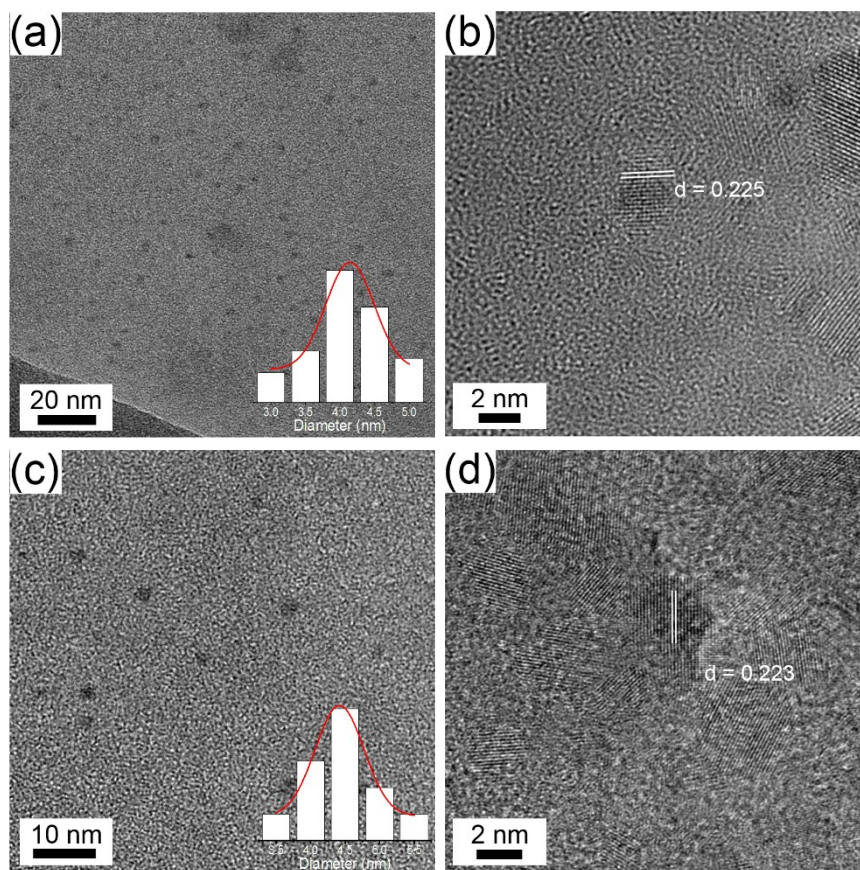
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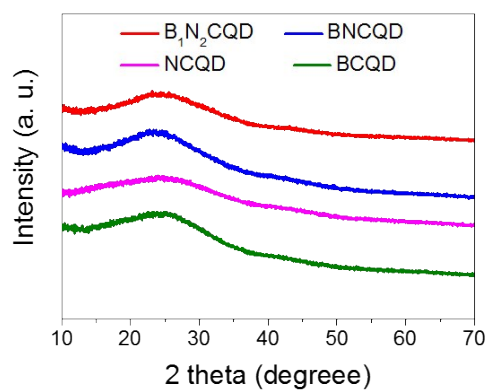
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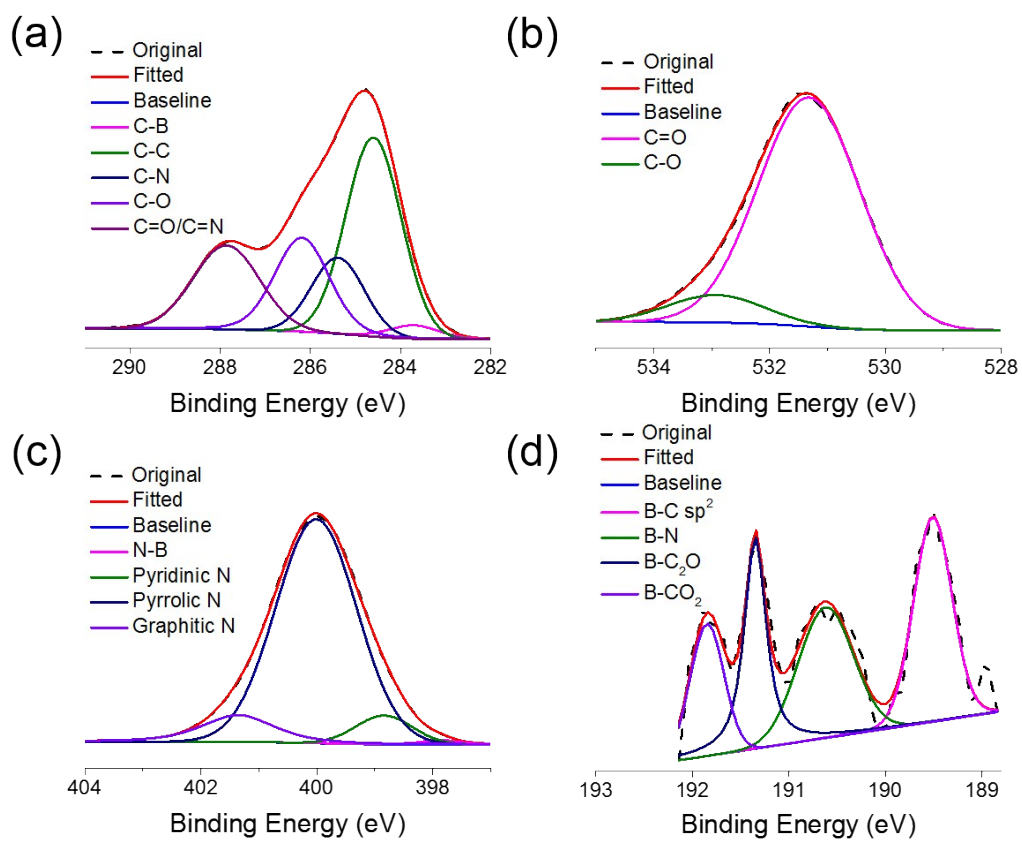
E-mail: lirun@hnu.edu.cn



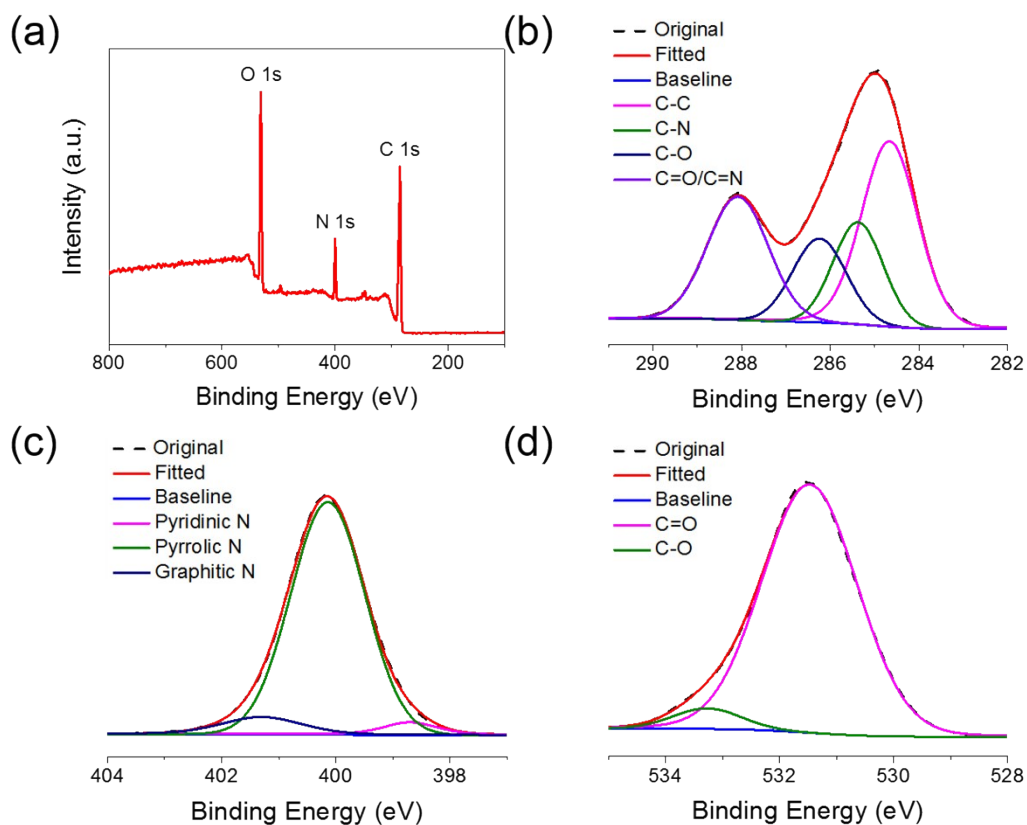
**Fig. S1** TEM and high resolution-TEM images of BNCQD (a, b) and NCQD (c, d). Insert of (a) and (c) are the corresponding size distribution.



**Fig. S2** XRD patterns of  $B_1N_2CQD$ , BNCQD, NCQD and BCQD.



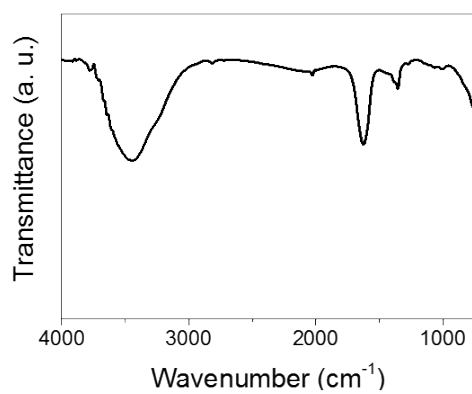
**Fig. S3** High-resolution XPS C 1s (a), O 1s (b), N 1s (c) and B 1s (d) peaks of BNCQD.



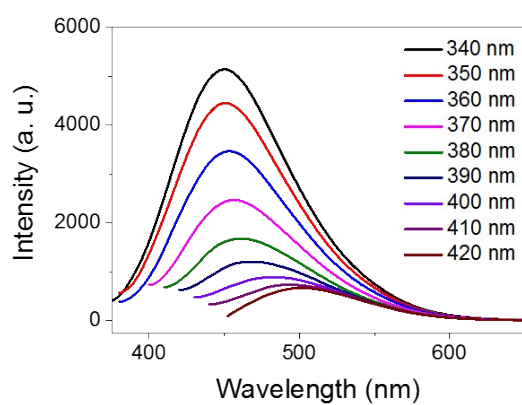
**Fig. S4** XPS survey spectra (a) and detailed high-resolution C 1s (b), N 1s (c) and O 1s (d) peaks of NCQD.

**Table S1.** Elementary composition of three different carbon quantum dots based on XPS measurement.

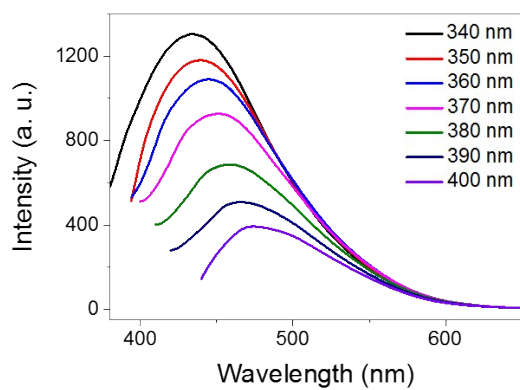
Sample name	Carbon (at%)	Oxygen (at%)	Nitrogen (at%)	Boron (at%)
B <sub>1</sub> N <sub>2</sub> CQD	67.02	19.75	13.04	0.20
BNCQD	68.44	19.12	12.33	0.11
NCQD	66.61	23.69	9.7	-



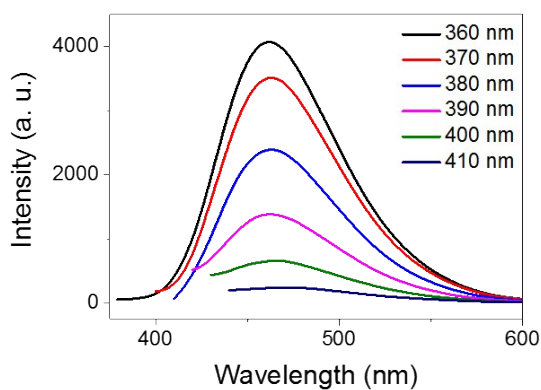
**Fig. S5** FTIR spectrum of BCQD



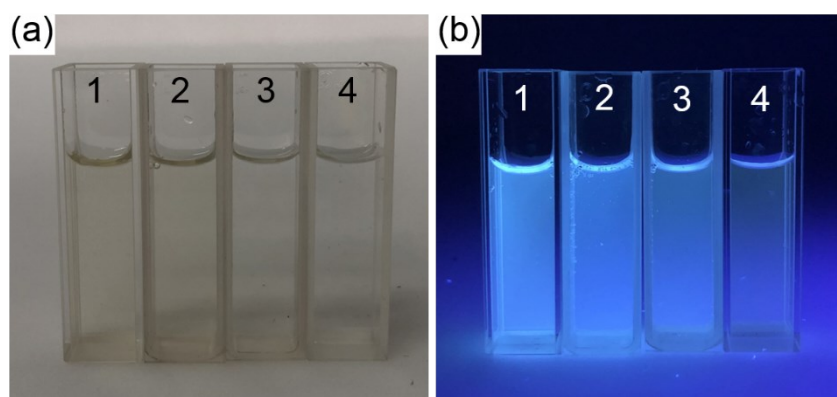
**Fig. S6** Steady-state fluorescence spectra of BNCQD under various excitation wavelengths.



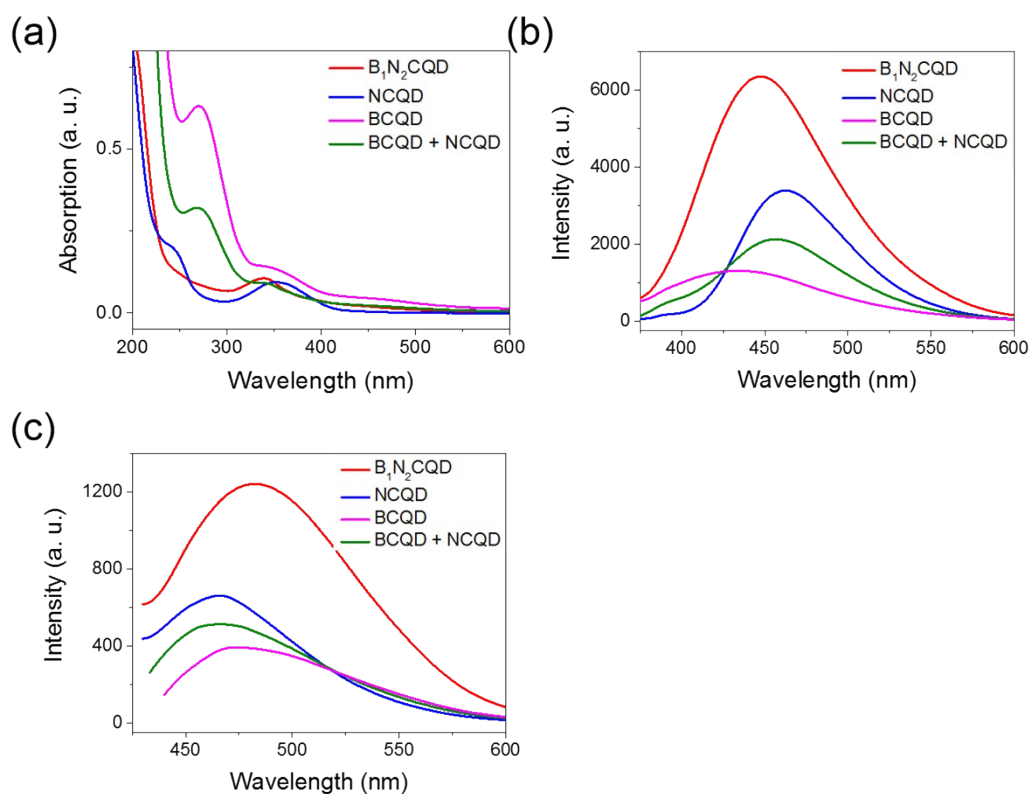
**Fig. S7** Steady-state fluorescence spectra of BCQD under various excitation wavelengths.



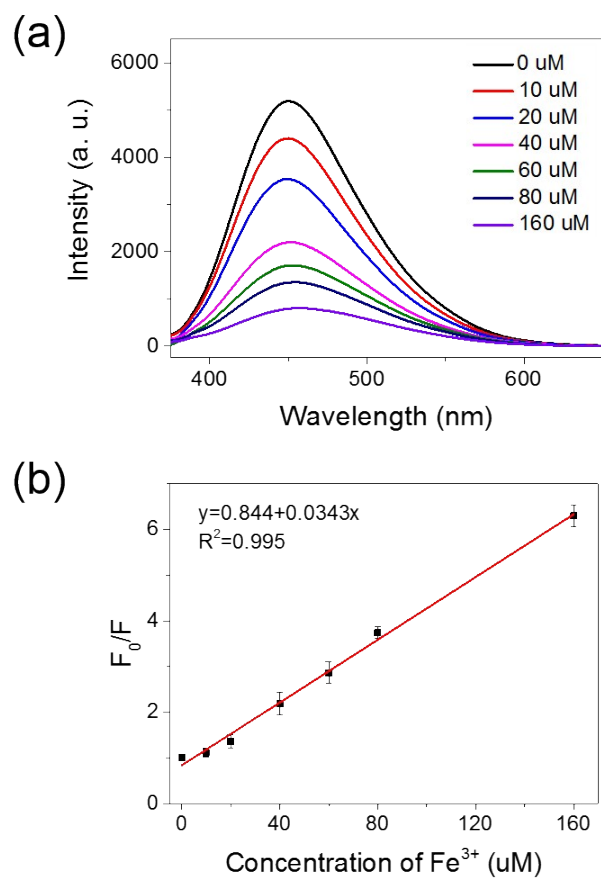
**Fig. S8** Steady-state fluorescence spectra of NCQD under various excitation wavelengths.



**Fig. S9** Photographs of CQDs in aqueous solution under visible light (a) and UV beam of 365 nm. From left to right are  $B_1N_2CQD$  (1),  $BNCQD$  (2),  $NCQD$  (3) and  $BCQD$  (4), respectively.

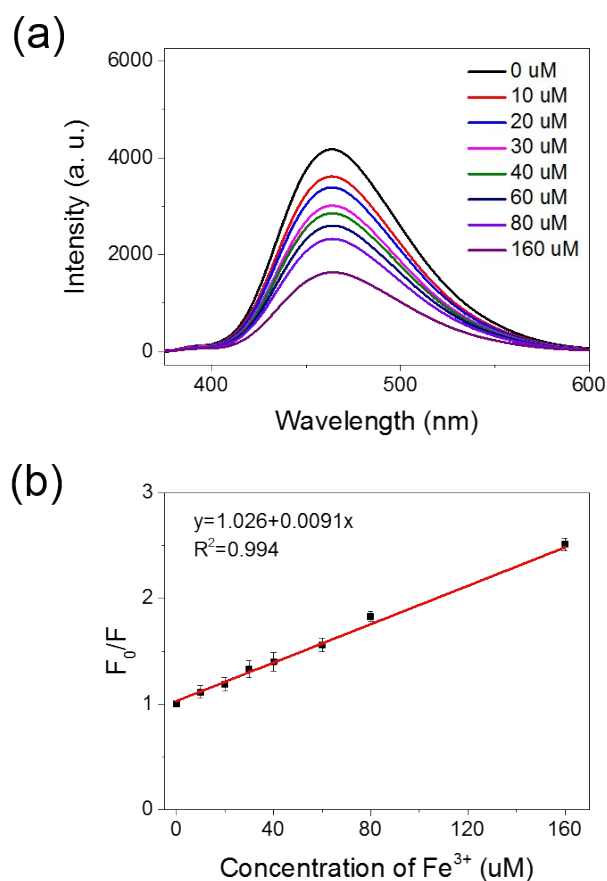


**Fig. S10** UV-Vis (a) and steady-state fluorescence (b, c) spectra of  $B_1N_2CQD$ ,  $NCQD$ ,  $BCQD$  and the mixture of  $BCQD$  and  $NCQD$ . (b) and (c) are excited at 340 and 400 nm, respectively. The mixture of  $BCQD$  and  $NCQD$  consist of 50%  $BCQD$  and 50%  $NCQD$ .

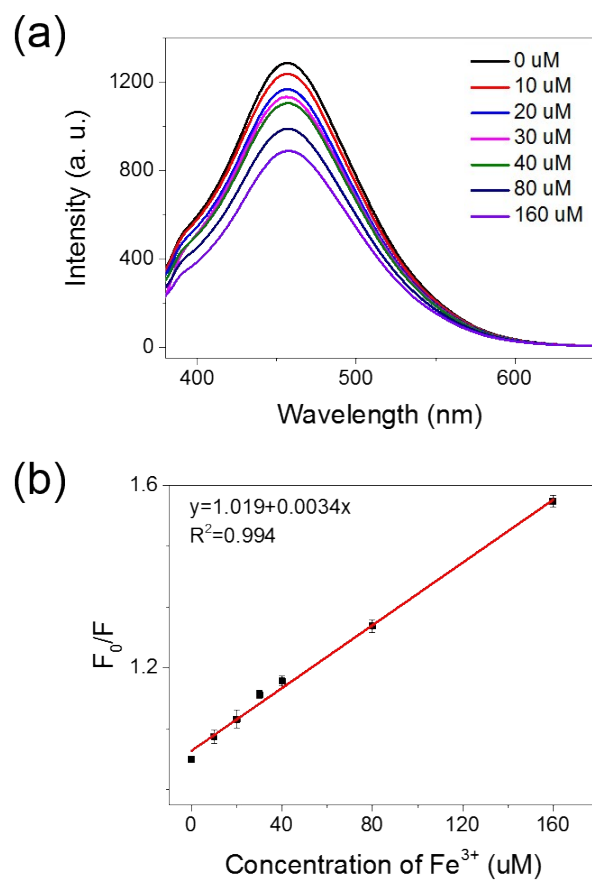


**Fig. S11** (a) Fluorescence spectra of BNCQD upon the addition of various concentrations of Fe<sup>3+</sup> from 0 to 160 uM. (b) Linear relationship between  $F_0/F$  and the concentration of Fe<sup>3+</sup>, where  $F_0$  and  $F$  are the emission intensity in the absence and presence of Fe<sup>3+</sup>, respectively.

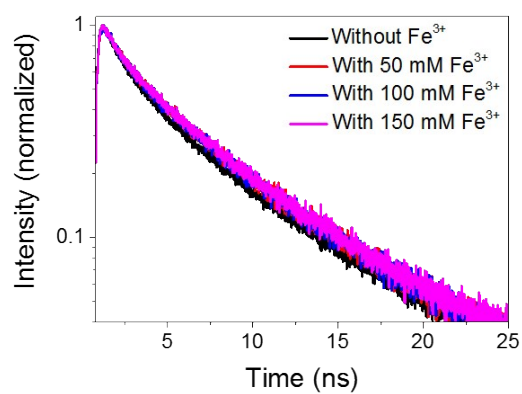




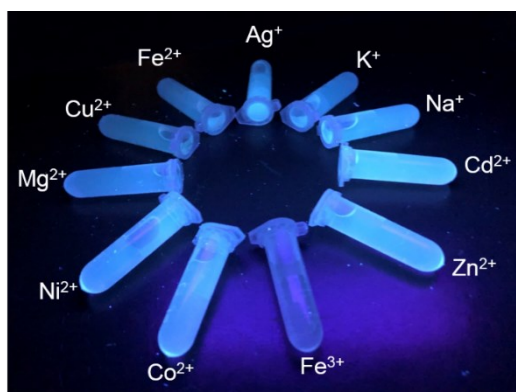
**Fig. S12** (a) Fluorescence spectra of NCQD upon the addition of various concentrations of Fe<sup>3+</sup> from 0 to 160 uM. (b) Linear relationship between  $F_0/F$  and the concentration of Fe<sup>3+</sup>, where  $F_0$  and  $F$  are the emission intensity in the absence and presence of Fe<sup>3+</sup>, respectively.



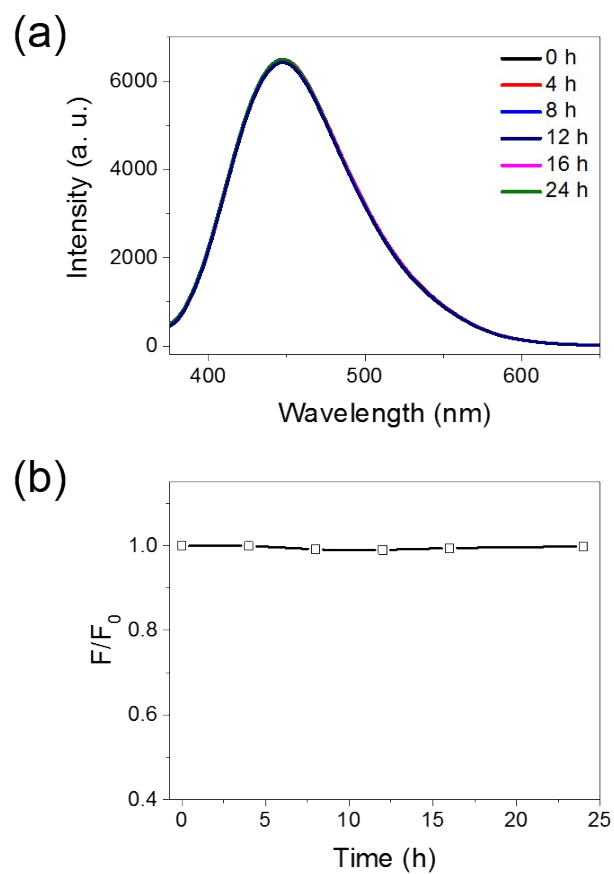
**Fig. S13** (a) Fluorescence spectra of BCQD upon the addition of various concentrations of  $\text{Fe}^{3+}$  from 0 to 160  $\mu\text{M}$ . (b) Linear relationship between  $F_0/F$  and the concentration of  $\text{Fe}^{3+}$ , where  $F_0$  and  $F$  are the emission intensity in the absence and presence of  $\text{Fe}^{3+}$ , respectively.



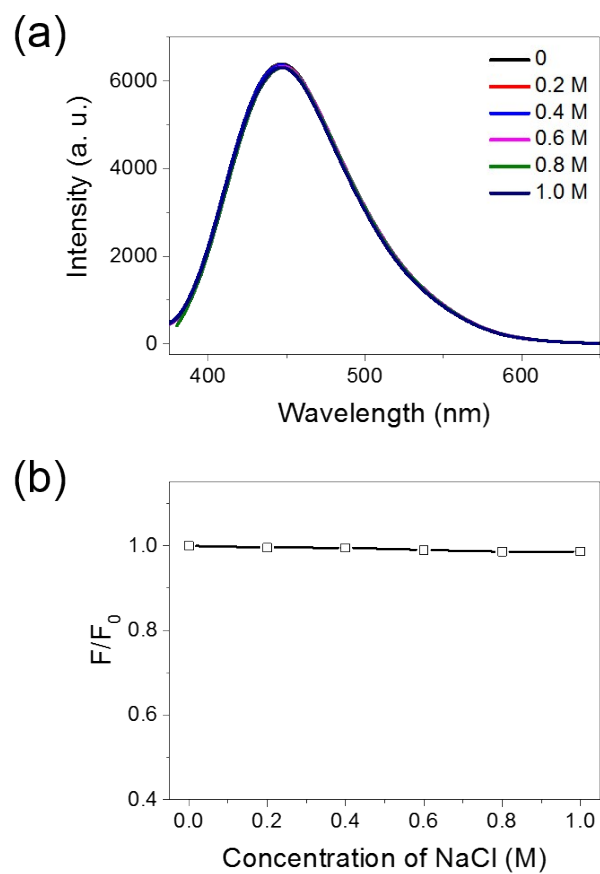
**Fig. S14** Time-resolved fluorescence decays for B<sub>1</sub>N<sub>2</sub>CQD after additions of various concentrations of Fe<sup>3+</sup>.



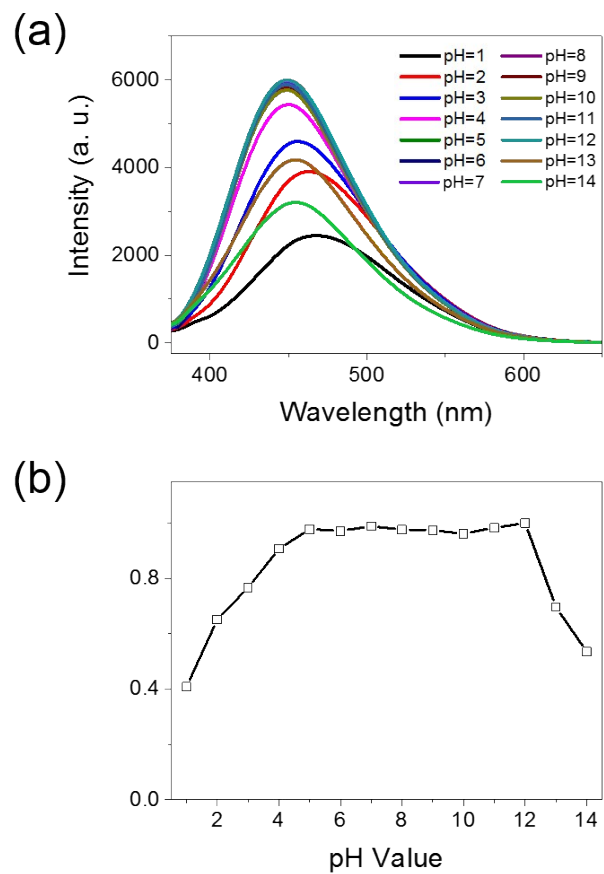
**Fig. S15** Photograph of B<sub>1</sub>N<sub>2</sub>CQD under 254 nm UV light irradiation after adding various kind of metal ions.



**Fig. S16** (a) Fluorescence spectra of B<sub>1</sub>N<sub>2</sub>CQD after 365 nm UV light irradiation. (b) Linear relationship between  $F/F_0$  and the irradiation time, where  $F_0$  and  $F$  are the emission intensity before and after UV light irradiation, respectively.



**Fig. S17** (a) Fluorescence spectra of B<sub>1</sub>N<sub>2</sub>CQD in the condition of various concentrations of NaCl from 0 to 1.0 M. (b) Linear relationship between  $F/F_0$  and the concentration of NaCl, where  $F_0$  and  $F$  are the emission intensity in the absence and presence of NaCl, respectively.



**Fig. S18** (a) Fluorescence spectra of B<sub>1</sub>N<sub>2</sub>CQD in various pH value from 1 to 14. (b) Normalized fluorescence intensity in different pH value.

**Table S2.** Comparison of CQDs-based sensors for Fe<sup>3+</sup> detection.

Entry	Fluorescent Probes	Carbon source	Linear range	LOD	Reference
1	BNCQDs	Ascorbic acid + 4-aminobenzeneboric acid	0-700 uM	7.5 uM	1
2	N-doped CDs	Alginic acid + ethanediamine	0-50 uM	10.98 uM	2
3	N-CDs	<i>Chionanthus retusus</i> fruit extract	0-2 uM	70 nM	3
4	B-CDs	Glucose + boric acid	0-16 uM	242 nM	4
5	CDs	citric acid + 1,10-phenanthroline	0-50 uM	35 nM	5
6	GN-CDs	Gallic acid + o-phenylenediamine	0-50 uM	800 nM	6
7	CDs	Folic acid	0-400 uM	2 uM	7
8	CDs	<i>Boswellia ovalifoliolata</i> bark extract	0-500 uM	0.41 uM	8
9	N-CQDs	Watermelon juice	0-300 uM	160 nM	9
10	C-QDs	Citric acid + Tris	0-50 uM	1.3 uM	10
11	B <sub>1</sub> N <sub>2</sub> CQD	citric acid + boric acid + ethylenediamine	0-160 uM	80 nM	This work

## Reference

1. L. Wang, J. S. Chung and S. H. Hur, *Dyes Pigm.*, 2019, **171**, 107752.
2. Y. Liu, Y. Liu, S.-J. Park, Y. Zhang, T. Kim, S. Chae, M. Park and H.-Y. Kim, *J. Mater. Chem. A*, 2015, **3**, 17747-17754.
3. R. Atchudan, T. N. J. I. Edison, D. Chakradhar, S. Perumal, J.-J. Shim and Y. R. Lee, *Sens. Actuators B: Chem.*, 2017, **246**, 497-509.
4. F. Wang, Q. Hao, Y. Zhang, Y. Xu and W. Lei, *Microchim. Acta*, 2016, **183**, 273-279.
5. A. Iqbal, Y. Tian, X. Wang, D. Gong, Y. Guo, K. Iqbal, Z. Wang, W. Liu and W. Qin, *Sens. Actuators B: Chem.*, 2016, **237**, 408-415.
6. S. Pang and S. Liu, *Anal. Chim. Acta*, 2020, **1105**, 155-161.
7. C. Shen, Y. Sun, J. Wang and Y. Lu, *Nanoscale*, 2014, **6**, 9139-9147.
8. G. Venkatesan, V. Rajagopalan and S. N. Chakravarthula, *J. Environ. Chem. Eng.*, 2019, **7**, 103013.
9. M. Lu, Y. Duan, Y. Song, J. Tan and L. Zhou, *J. Mol. Liq.*, 2018, **269**, 766-774.
10. M. Zhou, Z. Zhou, A. Gong, Y. Zhang and Q. Li, *Talanta*, 2015, **143**, 107-113.