Electronic Supplementary Material (ESI) for Lab on a Chip.

Supporting Information

Continuous Synthesis of Carbon Dots with Full Spectrum Fluorescence and the Mechanism of Multiple Color Emission

Meng Shao, Qin Yu, Nan Jing, Yu Cheng, Dong Wang, Yun-Dong Wang, Jian-Hong Xu**

Figure S1. The schematic diagram of continuous method for full-spectrum carbon dots synthesis.

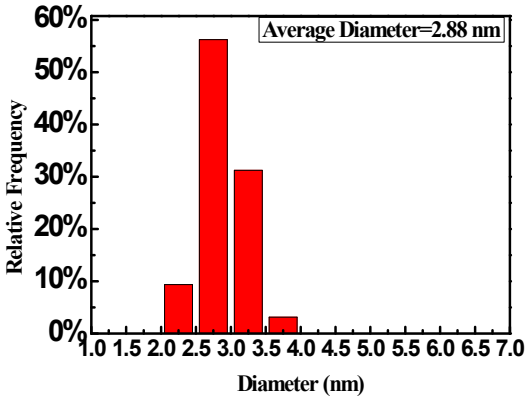


Figure. S2: The size distribution of CDs synthesized by a microreactor.

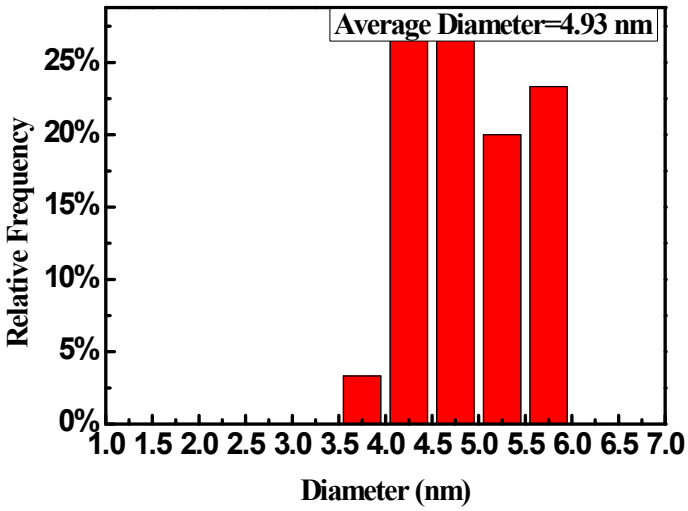


Figure. S3: The size distribution of CDs synthesized by an autoclave.

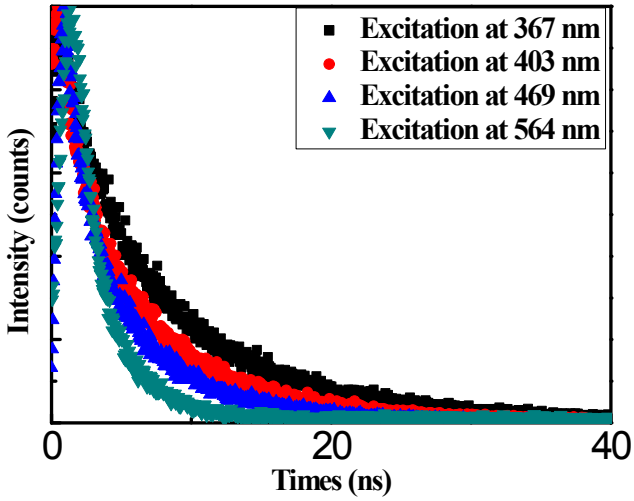


Figure. S4: Lifetime decay profiles of the carbon dots with full spectrum fluorescence under different excitation at 367, 403, 469, 564 nm.

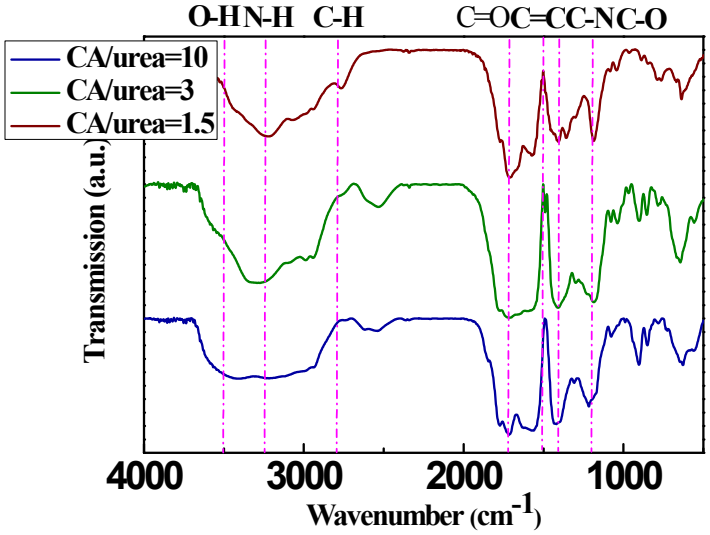


Figure. S5: The FTIR spectrum of three groups of samples.

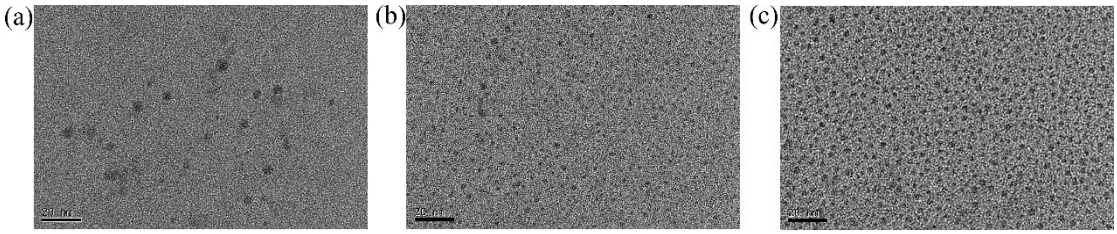


Figure. S6: The TEM image of sample A, B and C respectively. The scale bar of all the pictures is 20 nm.

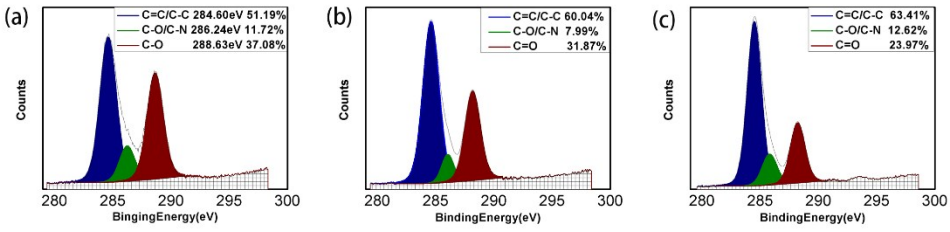


Figure. S7: (a) The XPS analysis of C1s at sample A. (b) The XPS analysis of C1s at sample B. (c) The XPS analysis of C1s at sample C.

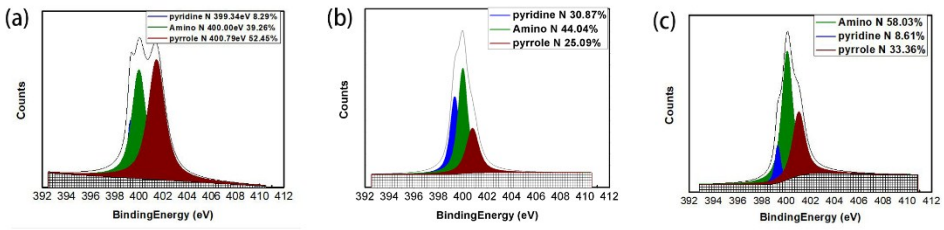


Figure. S8: (a) The XPS analysis of N1s at sample A. (b) The XPS analysis of N1s at sample B. (c) The XPS analysis of N1s at sample C.

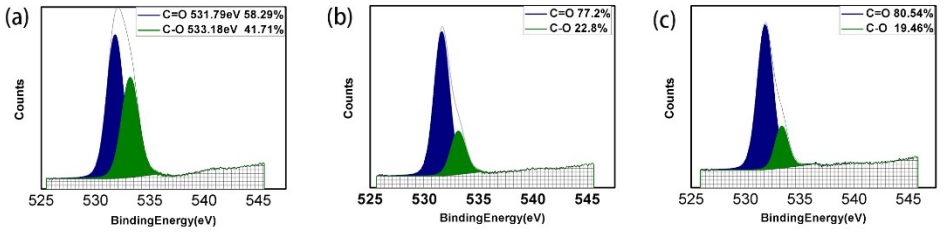


Figure. S9: (a) The XPS analysis of O1s at sample A. (b) The XPS analysis of O1s at sample B. (c) The XPS analysis of O1s at sample C.

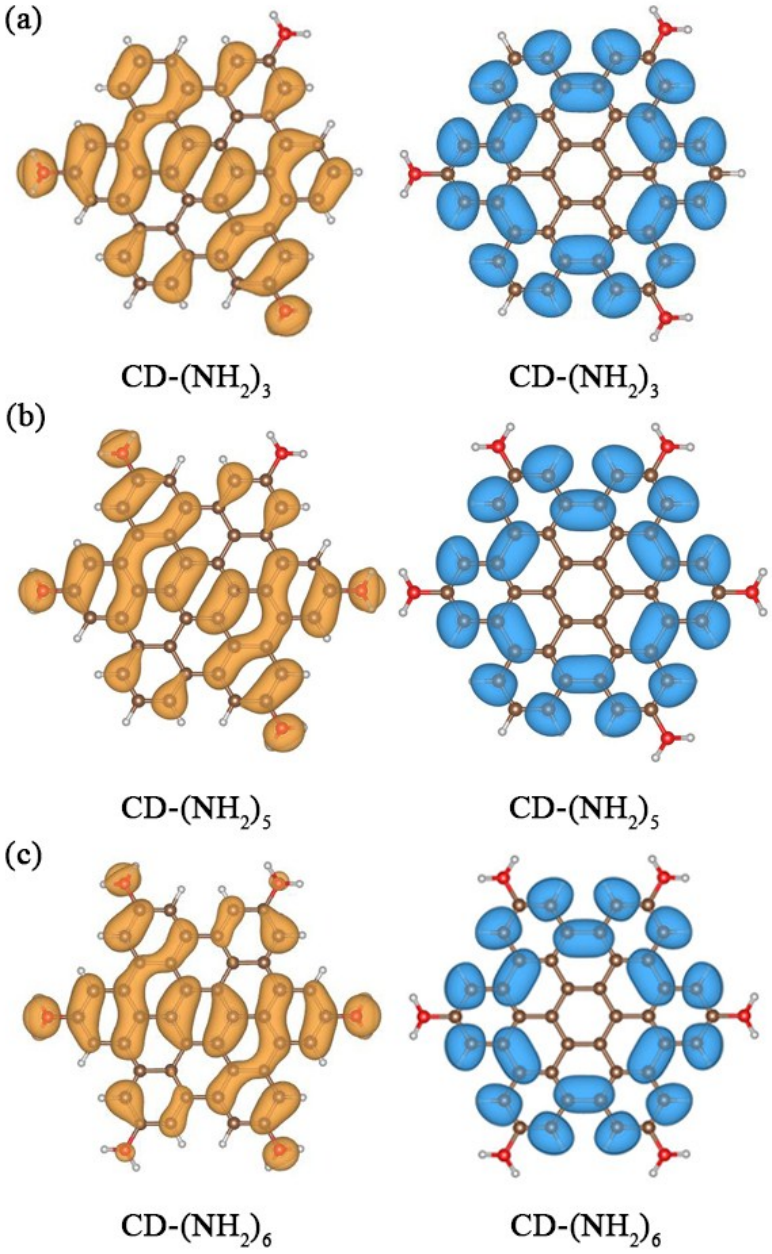


Figure. S10: HOMO and LUMO charge densities of CD-$(NH_2)_5$ and CD-$(NH_2)_6$ with same isosurface value, and the brown, red and gray spheres represent C, N and H atoms, respectively.

Table S1 Experimental conditions of three groups of experiments.

	Mole fow rate of CA ($mol/10^3min$)	Mole fow rate of urea ($mol/10^3min$)	The mole ratio of CA to urea	The reaction time (min)	Temperature (℃)
Compound		**HOMO**			**LUMO**
		C p_z		**N p_z**	**C p_z**
Sample A	3.64	0.36	10	20	250
Sample B	3.00	1.00	3	20	250
Sample C	2.20	1.80	1.5	20	250

Table S2 The element compositions of CDs.

	C (Atomic%)	N (Atomic%)	O (Atomic%)
Sample A	53.13	1.2	45.67
Sample B	58.91	7.22	33.87
Sample C	64.24	9.52	26.24

Table S3 Different substitution configurations of CD-$(NH_2)_3$ and their relative energy

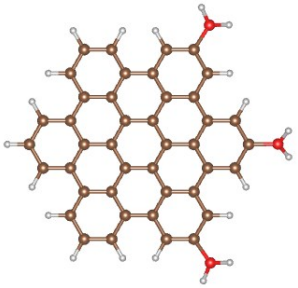
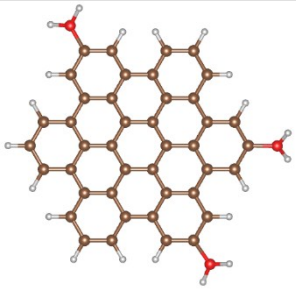
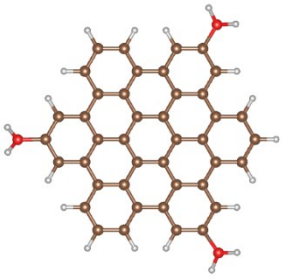
CD-$(NH_2)_3$	**a**	**b**	**c**
Optimized structure			
Relative energy (eV)	0.00981	0.00838	0

Table S4 Contributions of C p_z and N p_z orbitals in HOMO and LUMO of CD and CD-$(NH_2)_n$ (n= 1, 5, 6)

CD	100%	0	100%
CD-$(NH_2)_1$	87.2%	12.8%	100%
CD-$(NH_2)_3$	86.8%	13.2%	100%
CD-$(NH_2)_5$	82.1%	17.9%	100%
CD-$(NH_2)_6$	82.3%	17.7%	100%