

Supporting Information

Surface Chemistry in Calcium Capped Carbon Quantum Dots

Shihuan Ren, Bingxu Liu, Guangting Han*, Haiguang Zhao*, Yuanming Zhang*

S.H. Ren, B.X. Liu

College of Textiles & Clothing, Qingdao University, No. 308 Ningxia Road, Qingdao 266071,

P. R. China

Dr. G. T. Han, Dr. H. G. Zhao, Dr. Y. M. Zhang

State Key Laboratory of Bio-Fibers and Eco-Textiles, College of Physics, University-Industry

Joint Center for Ocean Observation and Broadband Communication, Qingdao University,

Qingdao, 266071, China

E-mail: (kychgt@qdu.edu.cn; hgzhao@qdu.edu.cn; Zhangyuanming001@163.com)

Supporting figures and tables

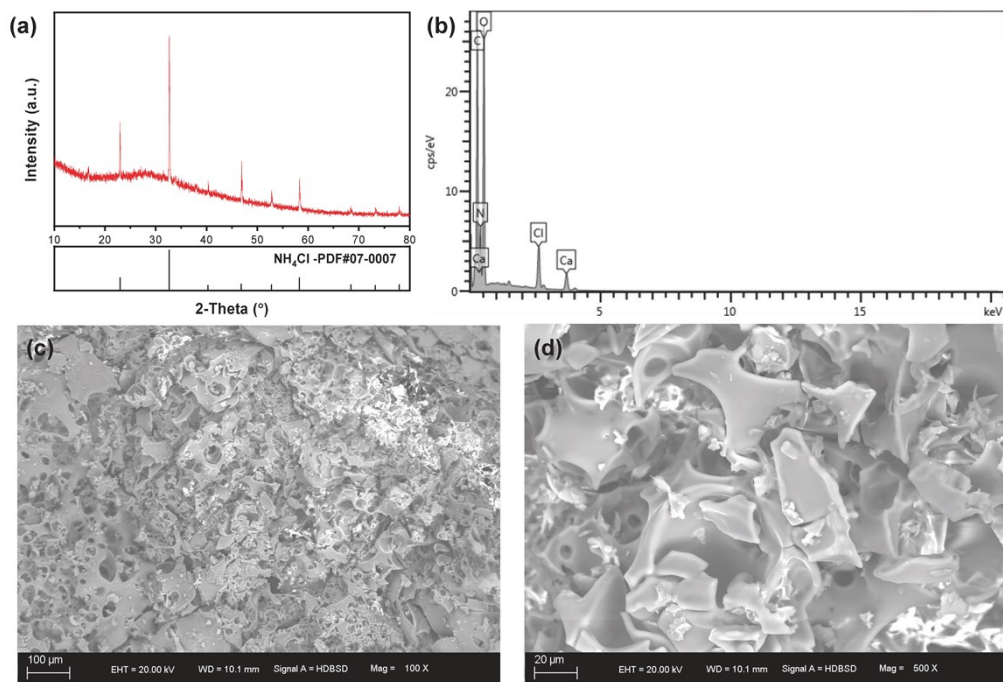


Fig. S1 (a) XRD pattern of C-dots. The C-dots is an unpurified original product prepared by space-confined vacuum heating. EDS spectra (b) of unpurified C-dots. SEM images of the C-dots with low magnification (c) and high magnification (d). A clear mesoporous network can be found based on the SEM images.

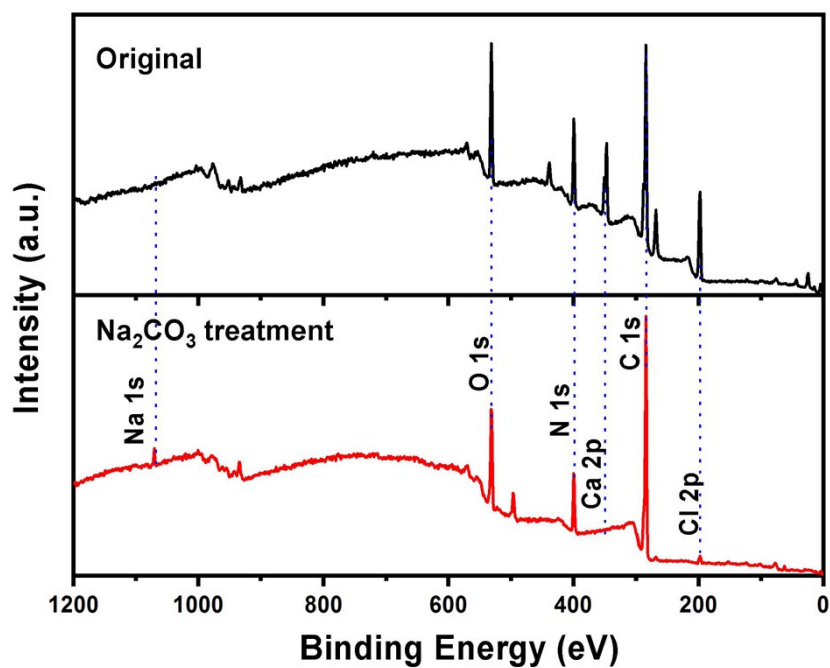


Fig. S2 The survey XPS spectra of the C-dots before (Original) and after Na₂CO₃-treatment. The Ca cations disappeared after Na₂CO₃ treatment.

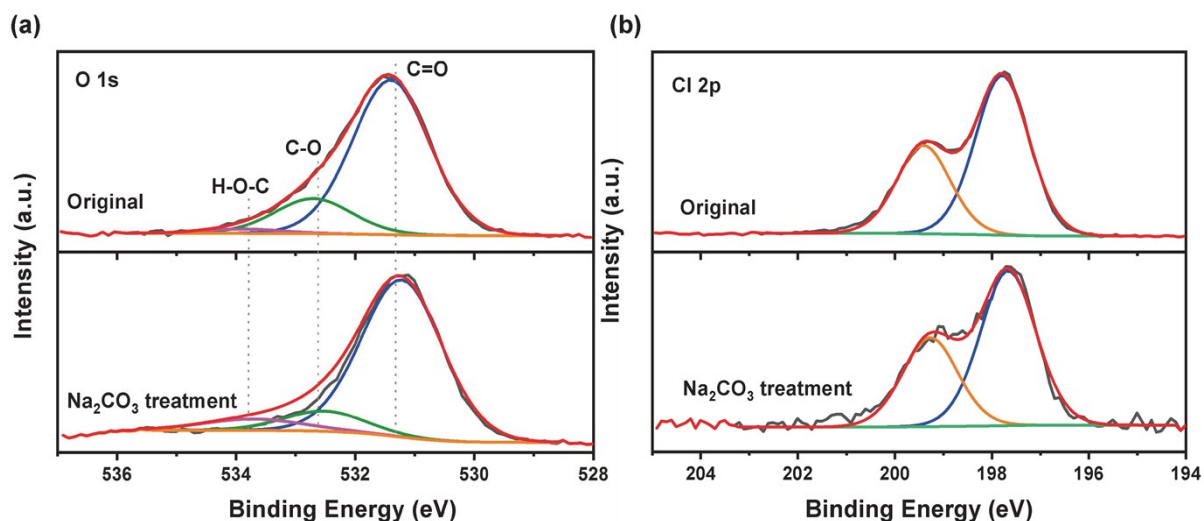


Fig. S3 (a) High resolution XPS O 1s (a) and (b) Cl 2p spectra of the C-dots before (Original) and after Na₂CO₃-treatment.

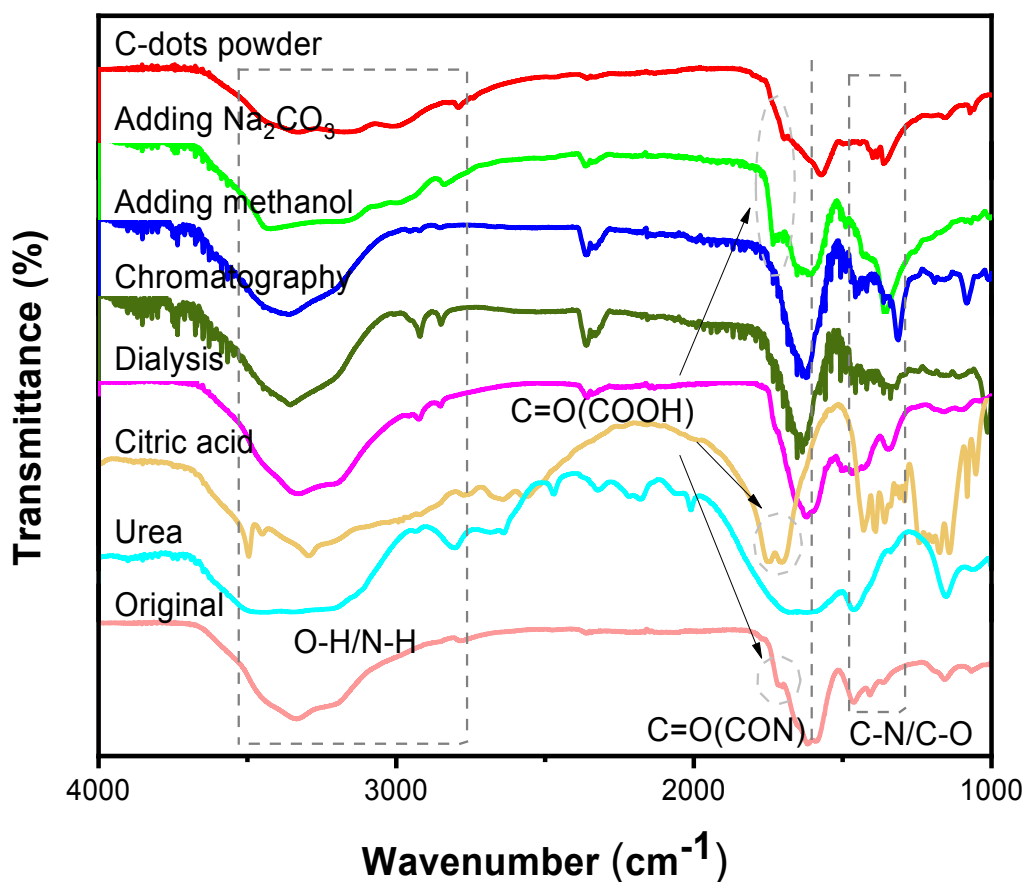


Fig. S4 FT-IR spectra of the Na₂CO₃-treatment C-dots during the different purification procedures. For comparison, the Citric acid, Urea, and the “Original” C-dots (without Na₂CO₃ treatment) were also included.

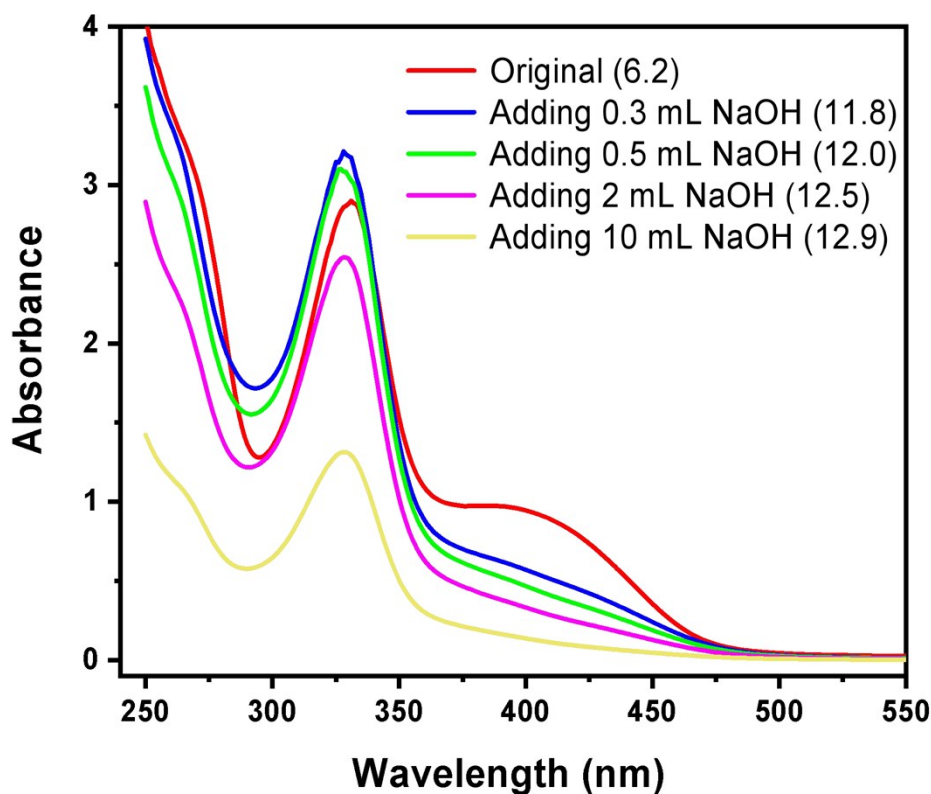


Fig. S5 Absorption spectra of C-dots after NaOH treatment.

Table S1. The atomic percentage of the elements of the Original and Na_2CO_3 -treatment samples. The ratios were estimated based on the XPS spectra as shown in Figure S2. The molar ratio of the Ca/Cl is close to 2, indicating that CaCl_2 was presented in the Original C-dots.

Element	Atomic percentage, Original (%)	Atomic percentage, Na_2CO_3 treatment (%)
C	58.9	75.93
N	12.59	10.54
O	12.38	12.12
Cl	10.86	0.95
Ca	5.44	0
Na	0	0.46

Table S2. Molar percentage of different carbon components under different treatment conditions.

Component	Molar percentage of Original (%)	Molar percentage of Na_2CO_3 treatment (%)
C=C/C-C	62.69	72.68
C-N	12.81	11.55

C-O	4.81	7.41
-C=O	19.69	8.36

Table S3. Molar percentage of different nitrogen composition under different treatment conditions.

Component	Molar percentage of Original (%)	Molar percentage of Na₂CO₃ treatment (%)
Pyridinic N	89.76	95.94
NH groups	10.24	4.06

Table S4. Mass evolution of the C-dots product during the purification process. **Stage I** : 1 g of C-dots was treated with 2.6 g (excess) of Na₂CO₃ aqueous solution after precipitation by ethanol; **Stage II** : gel chromatography; **Stage III**: dialysis (dialysis tube, 500 Da). The powder was obtained by using 0.33g citric acid, 0.66g urea and 0.33 g CaCl₂.

Purification	Stage I	Stage II	Stage III
Obtained powder (g)	2.57	2.4	0.3