## Supplementary Information

# Facile formation of chiral nanofibers with excellent electrochemical performance via Self-assembly of carbon dots and cysteine molecules

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# Methods and Materials

## 1. Materials

All chemicals were used as received without further purification. Dimethylformamide (DMF), citric acid and urea were purchased from Beijing Chemical Works. L-cysteine (98%), and D-cysteine (98%) were purchased from Shanghai Huishi biochemical Co., Ltd. NaOH were purchased from Aladdin.

## 2. Synthesis of pristine CDs

The CDs were synthesized via a solvothermal route. Typically, 1 g citric acid and 2 g urea were dissolved in 10 ml DMF. Then the solution was sealed in a Teflon-lined stainless steel autoclave and heated at 180 °C for 24 h under static conditions and cooled to room temperature. Subsequently, the obtained brown solution was mixed with NaOH aqueous solution (50 mg $mL^{-1}$), and centrifuged. Then precipitate was washed twice with water and dissolved in 10 ml Ultra-pure water.

## 3. Synthesis of left-handed and right-handed CDs/cysteine

As-synthesized pristine CDs solution (2mL) was mixed with 72.6 mg L-cysteine and D-cysteine respectively in 10 ml Ultra-pure water under gentle stirring for 24h at room temperature ,40℃ and 60℃, respectively. Then obtained crude product was centrifuged and washed with water. After that L(D)- CDs/cysteine nanofibers were dispersed in 3.5 ml of water for further characterziations.

## 4. Characterization techniques

The surface morphologies were performed with a JEOL-7800 F field emission scanning electron microscope at an accelerating voltage of 3 kV and JEOL-6700 F field emission scanning electron microscope at an accelerating voltage of 5 kV. The transmission electron micrograph (TEM) and high-resolution transmission electron micrograph (HRTEM) images were recorded on a FEI Tecnai G2S-Twin with a field emission gun operating at 200 kV. The X-ray photoelectron spectra (XPS) was measured by ESCALab 250 Analytical XPS spectrometer with a monochromatic X-ray source (Al Kα, h = 1486.6 eV). Fourier transformed infrared (FT-IR) spectra were recorded with IFS-66V/S FT-IR spectrometer.

## 5. Optical studies

CD spectra were obtained on a Bio-Logic MOS-450 CD spectrometer. VCD spectra were measured with a ChiralIR-2X spectrometer. The pellets were prepared by adding 1-2 mg of L(D)-CDs/cysteine, CDs and L/D-cysteine powder to 100 mg of KBr. All VCD spectra were collected for 12 h at a resolution of 4 $cm^{-1}$ Photoluminescence spectra were recorded at room temperature by using FLUOROMAX-4 spectrometer, the time-resolved PL decay was carried out on Edinburgh Instrument FLS920 spectrophotometer. UV–vis absorption (UV) spectra were performed either by a Shimadzu UV-2450 spectrophotometer.

## 6. Electrochemical test

The coin cells were galvanostatically discharged/charged by Land CT2001 battery testers (Wuhan Land ElectricCo. Ltd., China)

# Supplemental figures

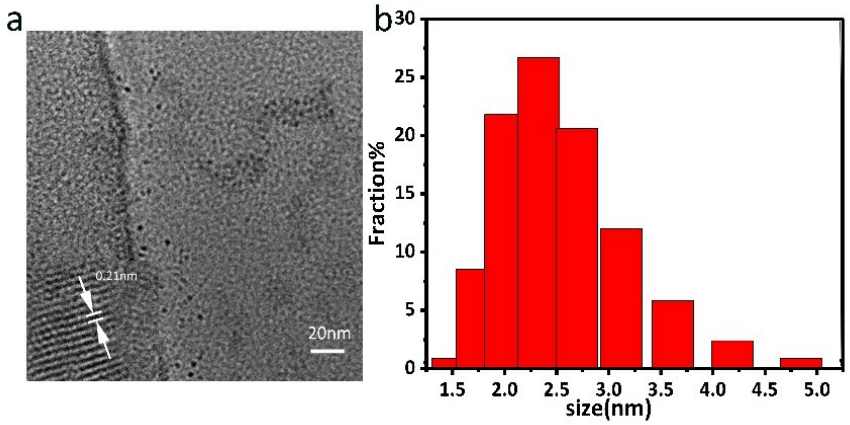


**Fig. S1** a) The TEM and HRTEM images and b) size distribution image of pristine CDs. It shows the diameter of pristine CDs with a uniform size distribution around 2 nm. The inset HRTEM image demonstrate the crystallinity of pristine CDs with a lattice parameter of 0.21 nm, which agrees with (100) lattice fringes of graphite. [1]

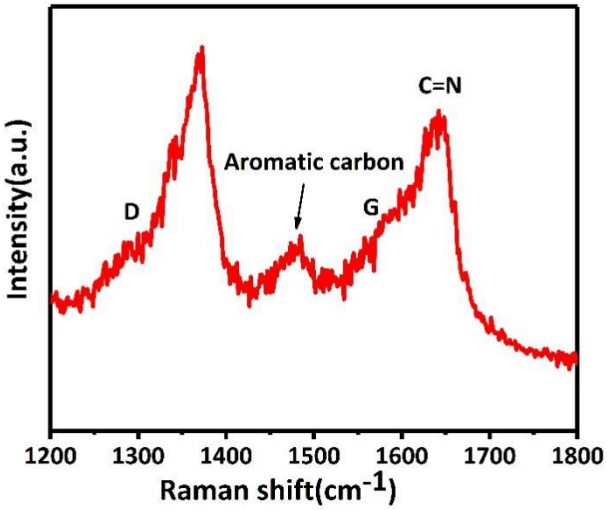


**Fig. S2** Raman spectrum of pristine CDs. Common features were observed in the 1200-1800 $cm^{-1}$ region, where the G band originates from graphitic sp2 carbon while D band indicates the existence of disorder structures or defects in the CDs. Except for the D band and G band, strong signals assigned to C=N and aromatic carbon.[2]

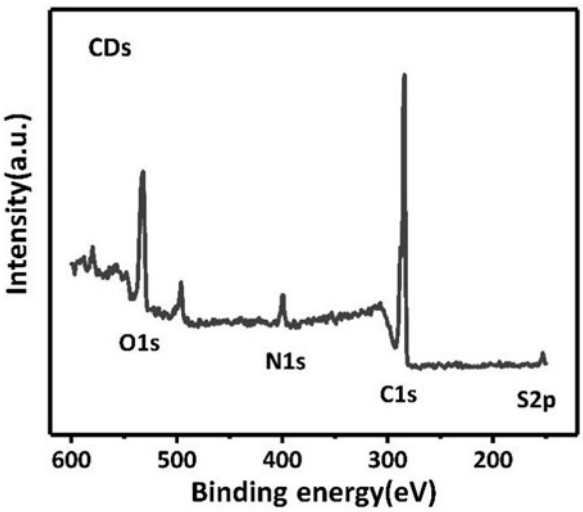


**Fig. S3** XPS spectrum of pristine CDs. From the full-scan XPS spectrum of pristine CDs, C, N, O were detected (C1s at 297.2eV, N1s at 411.2eV and O1s at 543.2 eV).

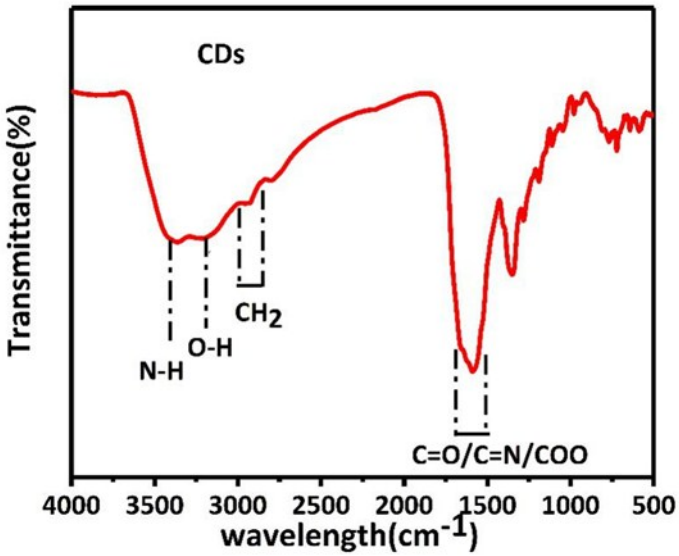


**Fig. S4** FT-IR spectrum of pristine CDs. In FT-IR spectra, broad absorption bands at 3050–3450 cm $^{-1}$ are assigned to v (O-H) and v (N-H). The strong absorption band from 1600-1700 cm $^{-1}$assigned to $v_{as}$( COO) in carboxylate groups, v (C=O) in carboxyl groups and C=N in CNH group.[3-11]

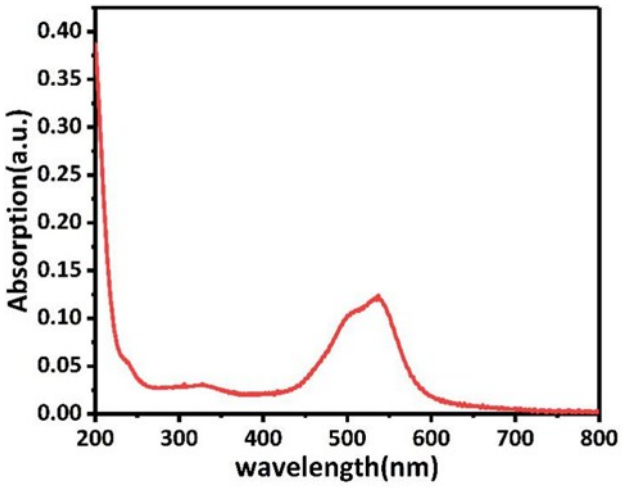


**Fig. S5** UV-vis spectra of pristine CDs aqueous solution. The absorption at 260 nm and 350 nm are the intrinsic absorption peak of carbon cores which are assigned to the π→π* transition and the n→π* transitions, respectively. The obvious visible absorption band peaked at 542 nm, indicating large sized conjugated $sp^2$ -domain in the particles. [12]

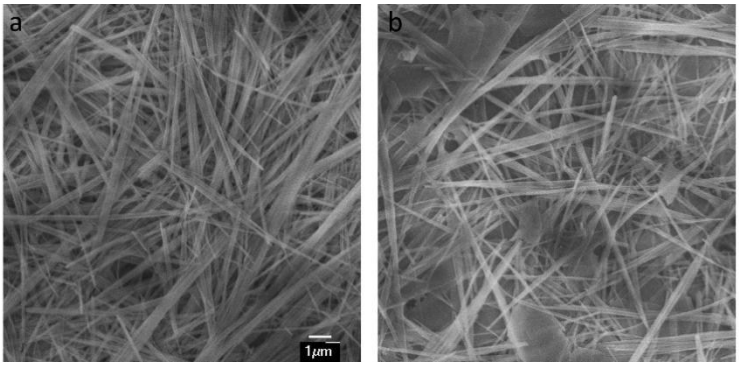


**Fig. S6** SEM images of L-CDs/cysteine nanofibers at a)room temperature and b) 60°C

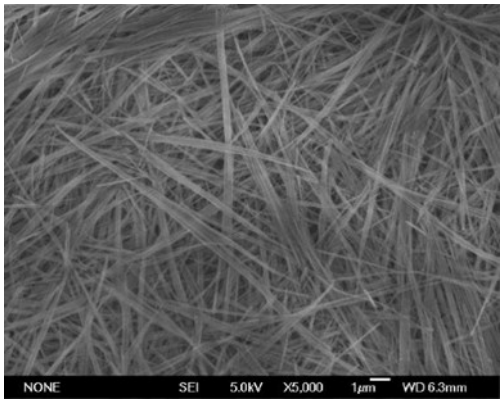


**Fig. S7** SEM images of D-CDs/cysteine nanofibers at 40°C

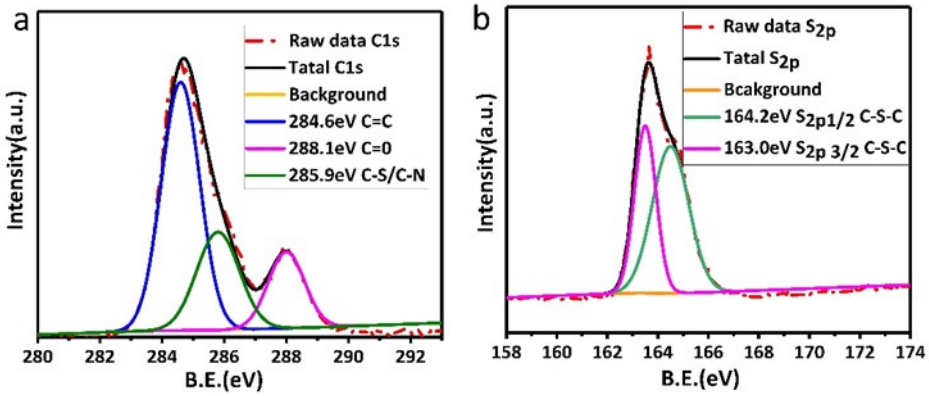


**Fig. S8** XPS survey of L-CDs/cysteine nanofibers a) deconvoluted $C_{1s}$ spectra and b) deconvoluted $S_{2p}$ spectra

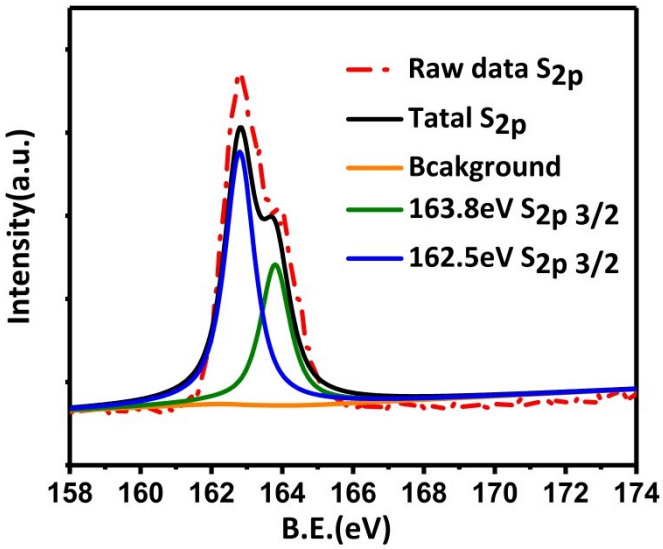


**Fig. S9** XPS survey of L- cysteinedeconvoluted $S_{2p}$ spectra. The peak deconvolution of the L-cysteine shows the presence of two S chemical sates: the first one giving rise to an $S2p_{3/2}$ signal at 162.8 eV and the second one producing a $S2p_{3/2}$ peak at 163.9 eV, which is similar to the previous report.[13]

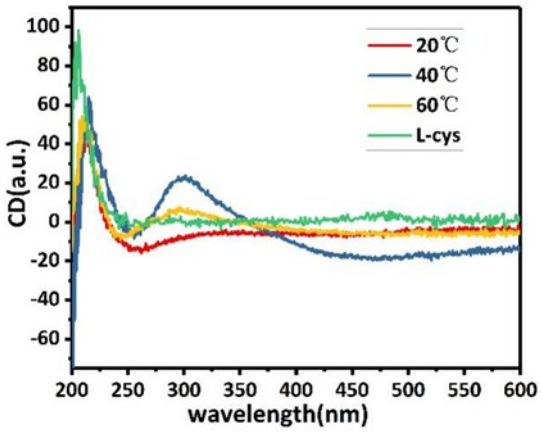


**Fig. S10** CD spectra of the aqueous solution of left-handed CDs@cysteine at different temperatures.

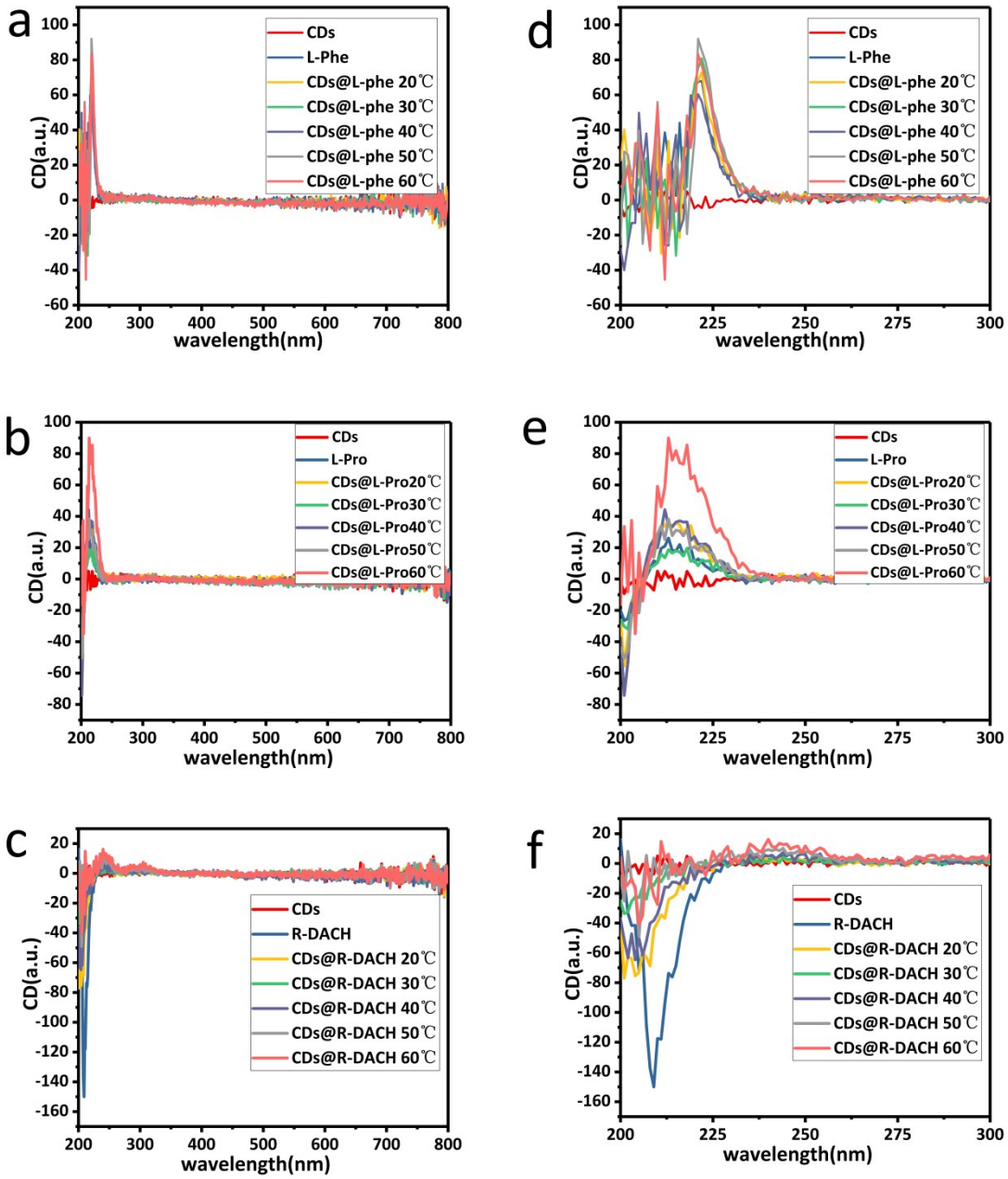


**Fig. S11** CD spectra of a) CDs@ L- phenylalanine (L-phe), b) CDs@L- proline (L-pro) and c) CDs@(R,R)- 1,2-diaminocyclohexane (R-DACH) d-f ) the CD image of the sample a-c )X-axis reduction at different temperatures, which shows that CDs and other chiral amino acids cannot produce similar chiral optical properties.

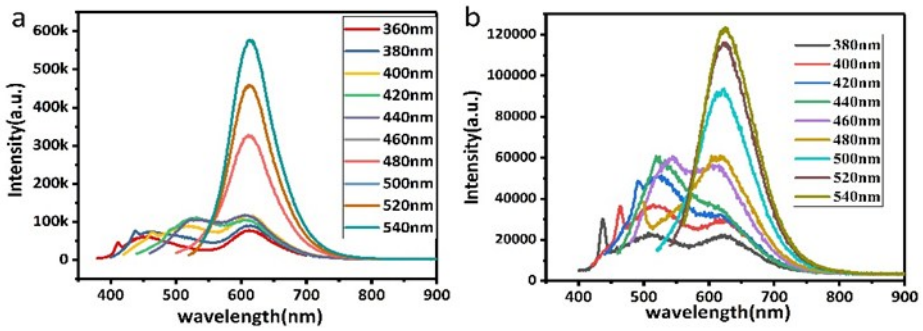


**Fig. S12** Emission spectra of the aqueous solution of a) pristine CDs after it has been present in aqueous solution for a while. b) left-handed CDs/cysteine nanofibers excited at different wavelengths.

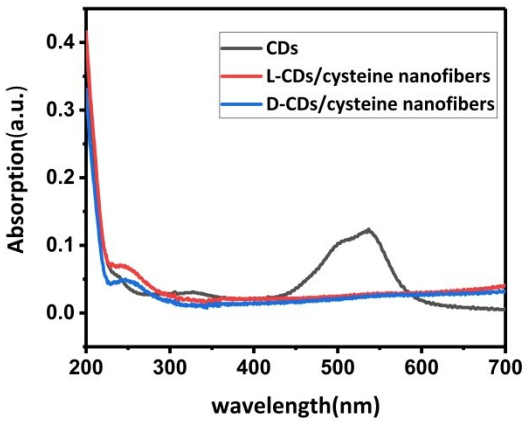


**Fig. S13** UV-vis spectra of CDs and L(D)-CDs/cysteine nanofibers aqueous solution.

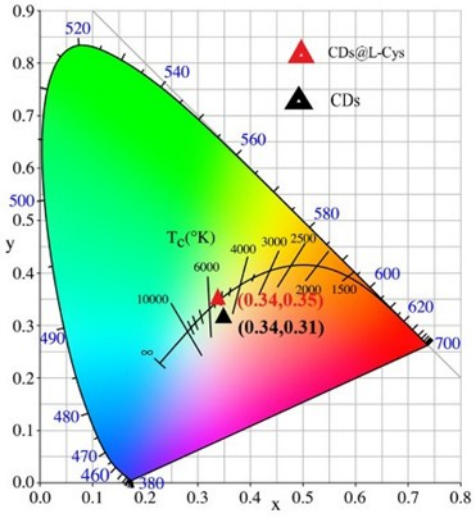


**Fig. S14** The CIE chromaticity diagram showing the coordinates of the samples presented in Fig S11. a) and b). Under excitation at 380 nm, L-CDs/cysteine nanofibers exhibits a white-light emission with CIE chromaticity coordinates of (0.34, 0.35) and a correlated color temperature (CCT) of 5300 K, and thus the emission of our L-CDs/cysteine nanofibers are called warm white-light. This warm white-light-emission is ideal applications for indoor light sources.

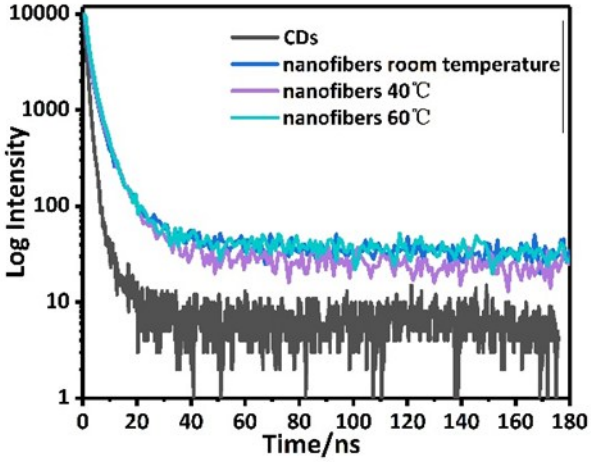


**Fig. S15** Fluorescence decay curves and fitting results of pristine CDs and L-CDs/cysteine nanofibers at different temperature recorded at emission wavelengths of 460nm in water. The PL decay of CDs and L-CDs/cysteine nanofibers curves can be well fitted into a multiexponential function with two and three lifetimes respectively. The proportion of each lifetime is shown in Table S1. The average lifetime pristine CDs and CDs@L-cysteine at room temperature, 40, 60 ° C calculated using the following Equation (1)

$\tau_{av} = (\sum \alpha_i \tau_i^2)/(\sum \alpha_i \tau_i)$ (1)

is 2.189ns, 337.3ns, 359.7ns and 294.1ns respectively. The multiple lifetimes of the phosphorescence imply various emission species, which may be a wide range of chemical environments on the surface of carbon dots for aromatic carbonyls.

**Table S1.** The photoluminescence QYs of CDs and L-CDs/cysteine nanofibers at different temperature aqueous solution under excitation of 420 nm.

| Sample | CDs | 20 °C | 40 °C | 60 °C |
|---|---|---|---|---|
| QYs | 6.19% | 1.33% | 1.23% | 0.04% |

**Table S2.** Fluorescence decay value of pristine CDs and CDs@ L-cysteine nanofibers

| Sample | $\tau_1$ | $A_1$% | $\tau_2$ | $A_2$% | $\tau_3$ | $A_3$% | $\tau_{av}$ |
|---|---|---|---|---|---|---|---|
| CDs | 1.178ns | 93.9 | 5.515ns | 6.10 | | | 2.189ns |
| CDs@L-cysteine at 20 °C | 1.414 ns | 45.69 | 5.704ns | 30.68 | 347.0ns | 23.63 | 337.3ns |
| CDs@L-cysteine at 40 °C | 1.320 ns | 45.92 | 5.431ns | 30.68 | 373.1ns | 23.63 | 359.7ns |
| CDs@L-cysteine at 60 °C | 1.461 ns | 43.89 | 4.916ns | 36.53 | 305.9ns | 19.58 | 294.1ns |

**Table S3.** The zeta potentials of CDs and CDs@L-cysteine nanofibers at different temperature aqueous solution.

| Sample | CDs | room temperature | 40°C | 60°C |
|---|---|---|---|---|
| Zeta potential | -11.8mV | 9.77mV | -5.97mV | -3.33mV |

## Supplementary References


[1] H. F. Liu, Z. H. Li, Y. Q. Sun, X. Geng, Y. L. Hu, H.M. Meng, J. Ge and L. B. Qu, *Scientific Reports* , 2018, **8**, 1086.
[2] M.J. Matthews, M.A. Pimenta, G. Dresselhaus, M.S. Dresselhaus, M. Endo, *Physical Review B*, 1999, **59**, R6585-R6588.
[3] C. J. Reckmeier, J. Schneider, A. S. Susha and A. L. Rogach, Opt. Express, 2016, 24, A312;
[4] D. Chen, W. Wu, Y. Yuan, Y. Zhou, Z. Wan and P. Huang, *J. Mater. Chem. C*, 2016, **4**, 9027
[5] Y. Chen, M. Zheng, Y. Xiao, H. Dong, H. Zhang, J. Zhuang, H. Hu, B. Lei and Y. Liu, *Adv. Mater*, 2016, **28**, 312;
[6] S. Zhu, J. Shao, Y. Song, X. Zhao, J. Du, L. Wang, H. Wang, K, Zhang, J. Zhang and B. Yang, *Nanoscale*, 2015, **7**, 7927.
[7] Y. Wang, S. Kalytchuk, L. Wang, O. Zhovtiuk, K. Cepe, R. Zboril and A. L. Rogach, *Chem. Commun*, 2015, **51**, 2950.
[8] S. Sun, L. Zhang, K. Jiang, A. Wu and H. Lin, *Chem. Mater*, 2016, **28**, 8659.
[9] H. Li, X. He, Z. Kang, H. Huang, Y. Liu, J. Liu, S. Lian, C. A. Tsang, X. Yang and S. T. Lee, *Angew. Chem. Int. Ed*, 2010, **49**, 4430.
[10] C. J. Reckmeier, J. Schneider, A. S. Susha and A. L. Rogach, *Opt. Express*, 2016, **24**, A312.
[11] D. Chen, W. Wu, Y. Yuan, Y. Zhou, Z. Wan and P. Huang, *J. Mater. Chem. C*, 2016, **4**. 9027.
[12] C. J. Reckmeier, J. Schneider, A. S. Susha and A. L. Rogach, *Opt. Express*, 2016, **24**, A312.
[13] O. Cavalleri, L. Oliveri, A. Dacca, R. Parodi and R. Rolandi, *Applied Surface Science*,2001, **175**, 357