Supporting Information

Tunable Multicolor Carbon Dots Prepared from Well-defined Polythiophene Derivatives and their Emission Mechanism

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1. *Chemicals and Materials*. $FeCl_3$, CaH_2, 4-Bromobenzyl bromide, N,N-dimethyldodecylamine, thiophene-3-boronic acid, tetrakis (triphenylphosphine) palladium (0), 3-thiophene-acetic acid, methoxy-PEG-OH (MW. 2000) were purchased form J&K Chemical Co. and Alfa Aesar. Other reagents were purchased from Beijing Chemical Regent Co. All chemicals and materials used were commercially available unless otherwise stated and were used without further purification. $CHCl_3$ was distilled from CaH_2 under nitrogen. Deionized water (Millipore Milli-Q grade) with resistivity of 18.2 MΩ cm^{-1} was used in all experiments.
2. *Synthesis of Polythiophenes.* All polymers in this paper were prepared via an oxidative polymerization under nitrogen in the presence of $FeCl_3$ as shown in Fig. S1. The general method for preparation of polythiophenes was carried out as follows: 4 equiv of $FeCl_3$ was dissolved in 30 mL of dry $CHCl_3$ under nitrogen, and then 1 equiv of corresponding monomers dissolved in 20 mL of $CHCl_3$ was

added dropwise. The reaction mixture was stirred at room temperature for 2 days. The resulting precipitate was collected, washed with methanol, and finally dried under vacuum to give the desired polymers. For the copolymerization, two monomers with different mole ratios (10/1, 1/1, 1/5 and 1/10) were used to give the corresponding copolythiophenes (CPT1, CPT2, CPT3 and CPT4, respectively). The polymerization of monomer gives the corresponding polythiophenes PT1 and PT2, respectively.

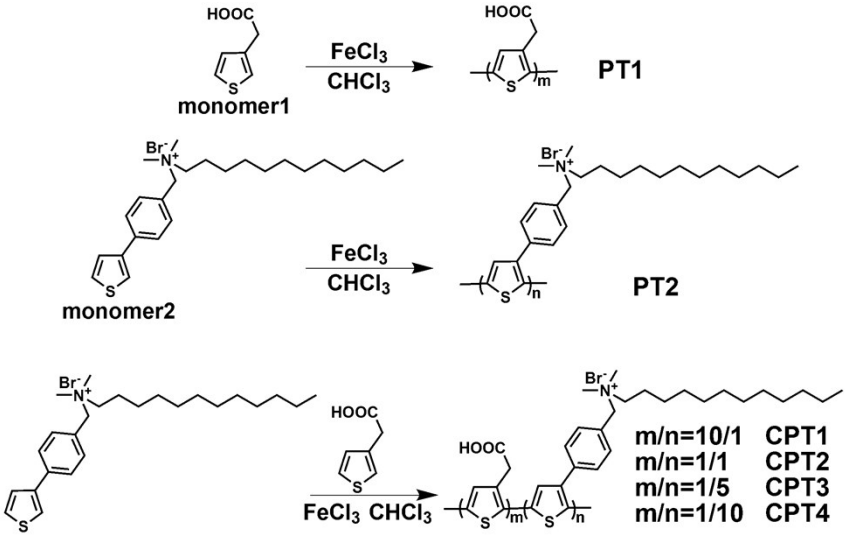

Figure S1. Synthesis of Polythiophenes.

3. *Preparation of C-dots.* The C-dots were named C-dots1, C-dots2, C-dots3, C-dots4, C-dots5, and C-dots6 and prepared by hydrothermal treatment of polythiophenes (PT) as shown in Fig. 1a. In a typical synthesis, PT was dispersed in NaOH solution. The mixture was treated ultrasonically for 30min and then transferred into an autoclave and heated at 170 ^{o}C for 24 h. After cooling to room temperature, the C-dots were collected by removing the large particles, through filtering using 0.22-μm membranes, and then dialysed against distilled water

several times to remove the residual NaOH. The C-dots were dispersed in water for further characterization and use.

4. *Characterization. XRD* patterns were obtained using an X-ray diffractometer (Bruker, Germany) with Cu-Kα radiation (λ=1.5178 Å). The 2θ scanning range was from 10° to 80° with a scanning speed of 0.1°/s. TEM and HRTEM images were taken on a JEOL JEM-2100F transmission electron microscope at an acceleration voltage of 150 kV. The FTIR spectra (4000 cm^{-1} to 500 cm^{-1}) in KBr were collected on a Varian Excalibur 3100 FTIR spectrometer. UV-visible and fluorescence spectra were obtained using Hitachi U-3010 and F-4500 spectrophotometers, respectively. XPS was performed using ESCALAB 250 spectrometer with a mono X-Ray source Al Kα excitation (1486.6 eV). Binding energy calibration was based on C1s at 284.6 eV. Zeta potentials were recorded on Zetasize 3000 HS (Malvern, UK). Elemental (C, H, N and S) analyses were performed on Thermoquest Flash EA 1112 Series analyzer.

5. *Cellular Imaging and MTT Assay.* HeLa cells were obtained from the Peking Union Medical College. The HeLa cells were cultured in fresh media (DMEM/F12 supplemented with 10% fetal bovine serum, 50 unit ml^{-1} of penicillin, and 50 mg ml^{-1} of streptomycin) at 37 ^{o}C in a humidified incubator containing 5% CO_2. In the in vitro imaging experiments, HeLa cells were incubated with 100 μl of C-dots (500 μg/ml) in 1ml of culture media at 37 ^{o}C. After incubating the mixtures for 3 h, the cells were washed with PBS twice to remove non-specifically bound C-dots. Images were also acquired with a Nikon

C1si laser scanning confocal microscopy. To compare the dark toxicity the C-dots, the C-dots stock solution was diluted with fresh medium to the concentration of 500 μg/ml. The cell medium was then exchanged for C-dots medium solution. The cells were then incubated with these solutions at 37 ^{o}C in 5% CO_2 for 24 h before removing the C-dots solution and adding fresh medium. Subsequently, the plates were incubated at 37 ^{o}C in 5% CO_2 for 24 h. The cell medium solutions were exchanged for 100 μl of fresh medium, followed by the addition of 20 μl of MTT solution to each well. The culture plates were then incubated at 37 ^{o}C in 5% CO_2 for 4 h. The culture medium was discarded, and 100 μl of dimethylsulfoxide was added. The absorbance of an untreated cell population under the same experimental conditions was used as the reference point to establish 100% cell viability.

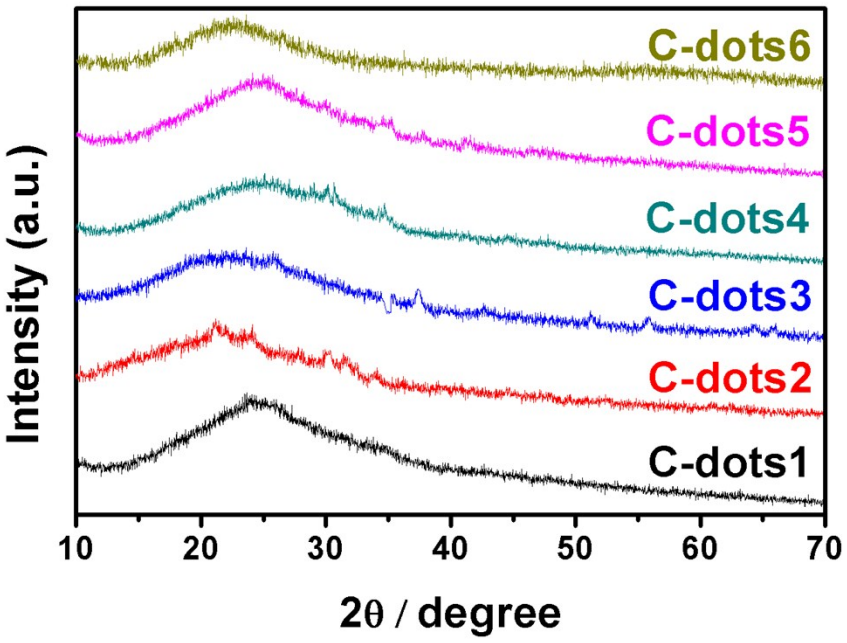

Figure S2 The XRD patterns of C-dots.

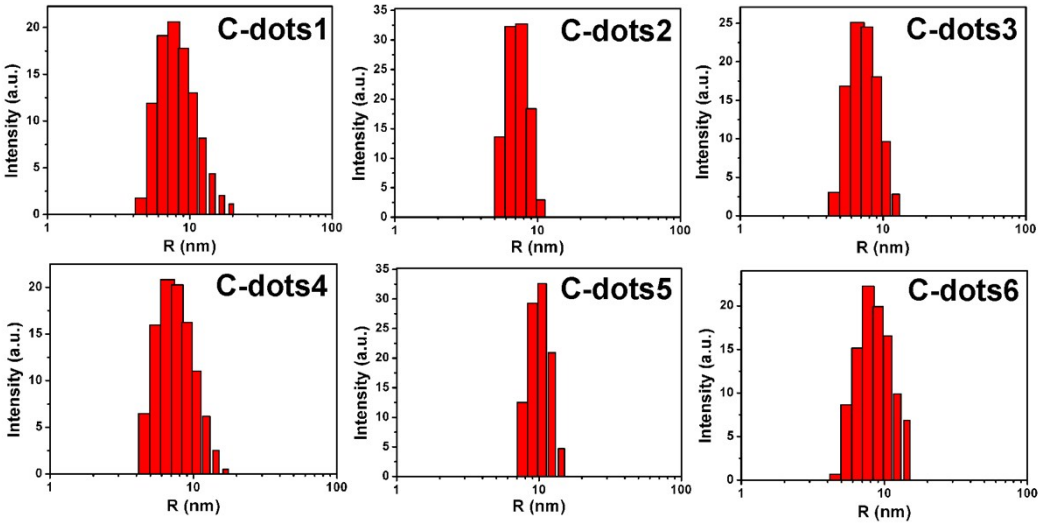

Figure S3. The DLS of various C-dots.

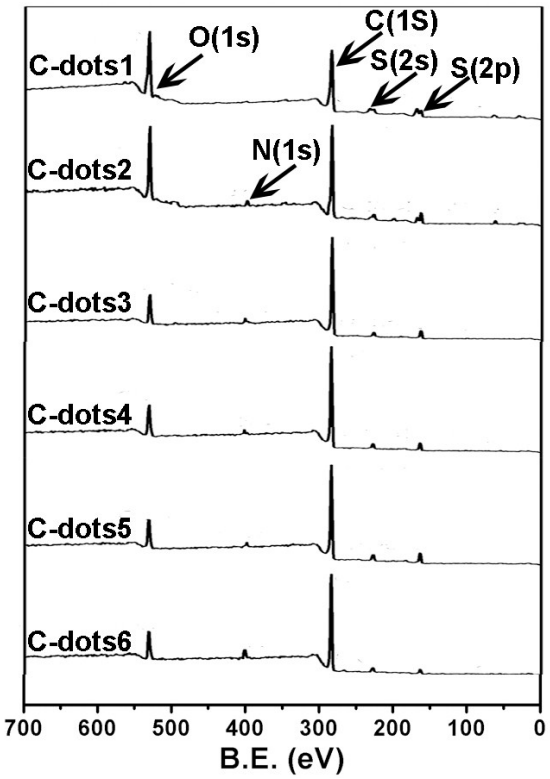

Figure S4, The XPS spectra of various C-dots.

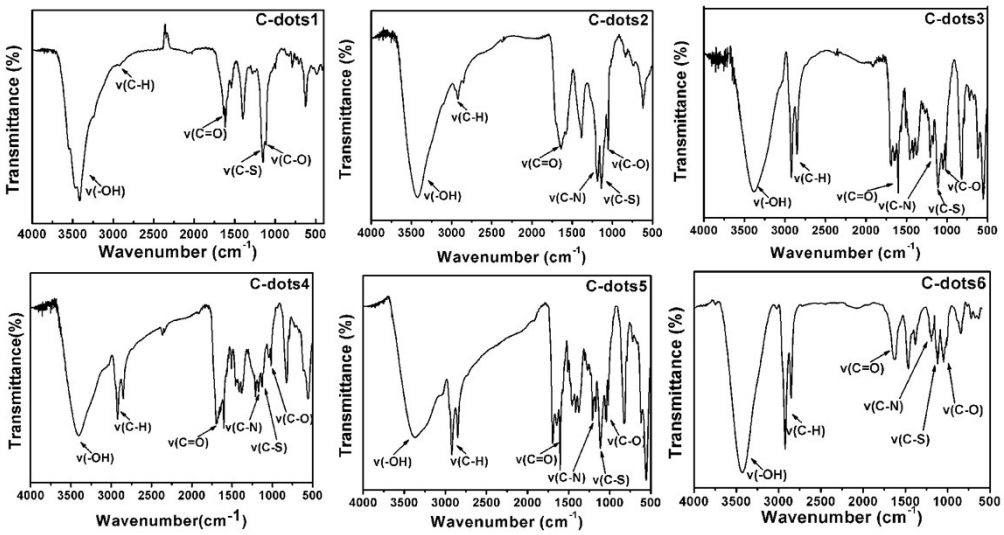

Figure S5. The FTIR analysis of C-dots.

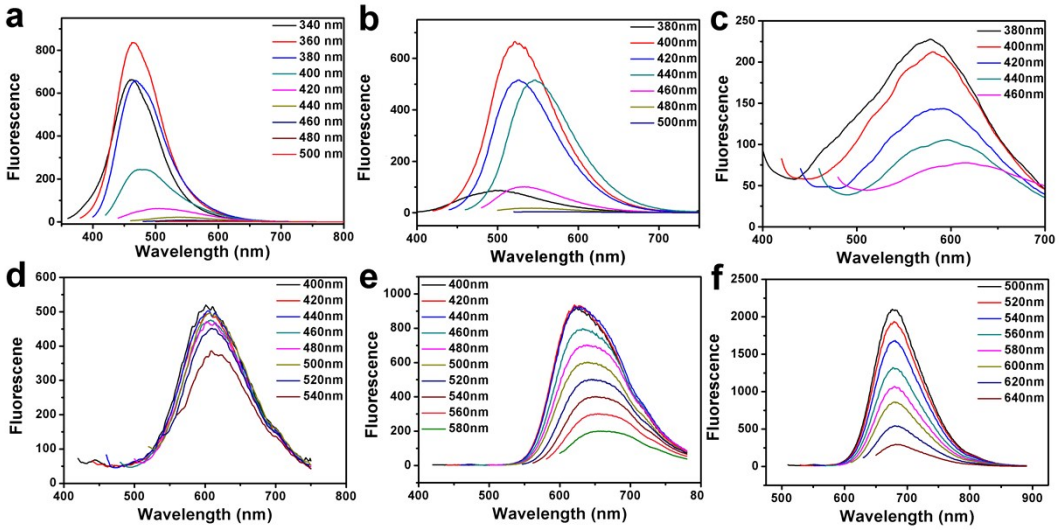

Figure S6 The fluorescence spectral of C-dots excited at different wavelength. (a: C-dots1; b: C-dots2; c: C-dots3; d: C-dots4; e: C-dots5; f: C-dots6)

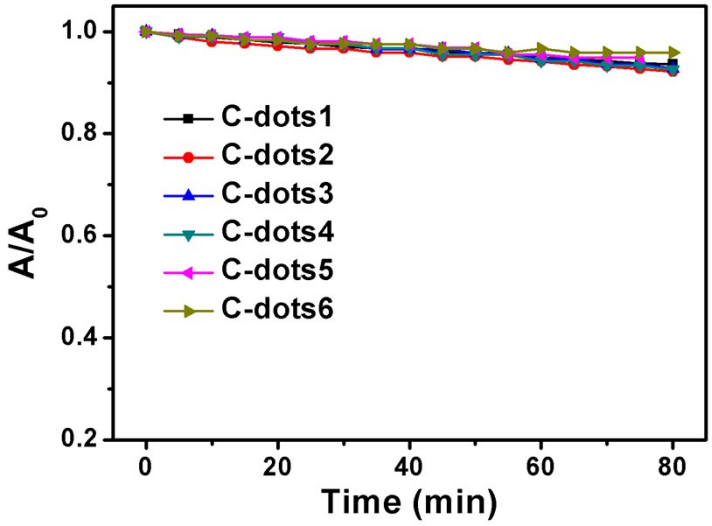

Figure S7 The photostabilities of the C-dots All of the samples were continuously irradiated using a 500-W xenon lamp. A_0 and A are the absorbance of the samples at 425 nm before and after irradiation, respectively.

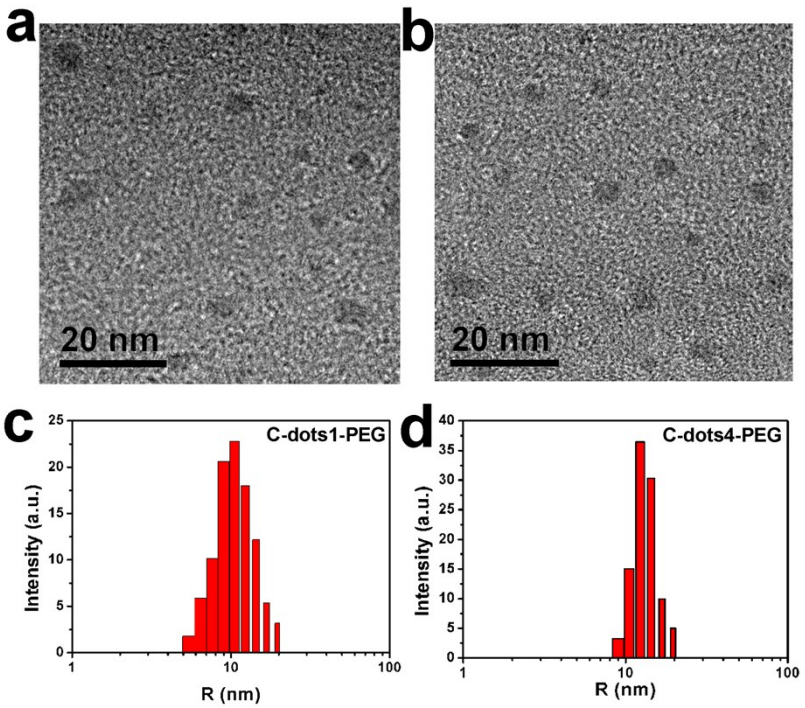

Figure S8 (a) The TEM image of C-dots1-PEG; (b) the TEM image of C-dots4-PEG; (c) the DLS analysis of C-dots1-PEG; (d) the DLS analysis of C-dots4-PEG.

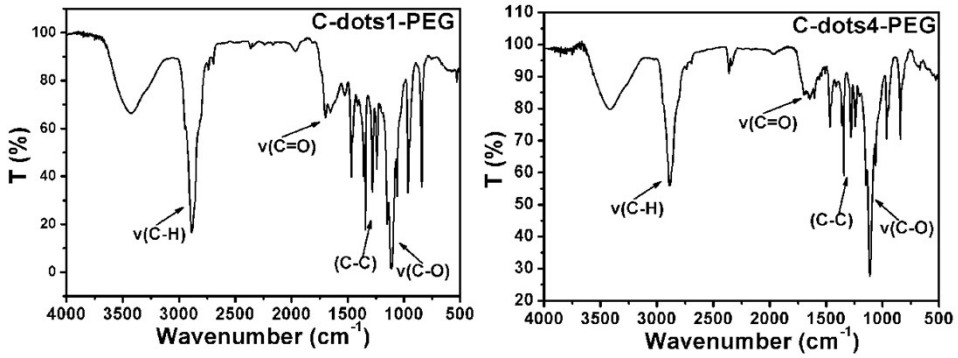

Figure S9 The FTIR analysis of C-dots1-PEG (a) and C-dots4-PEG (b).

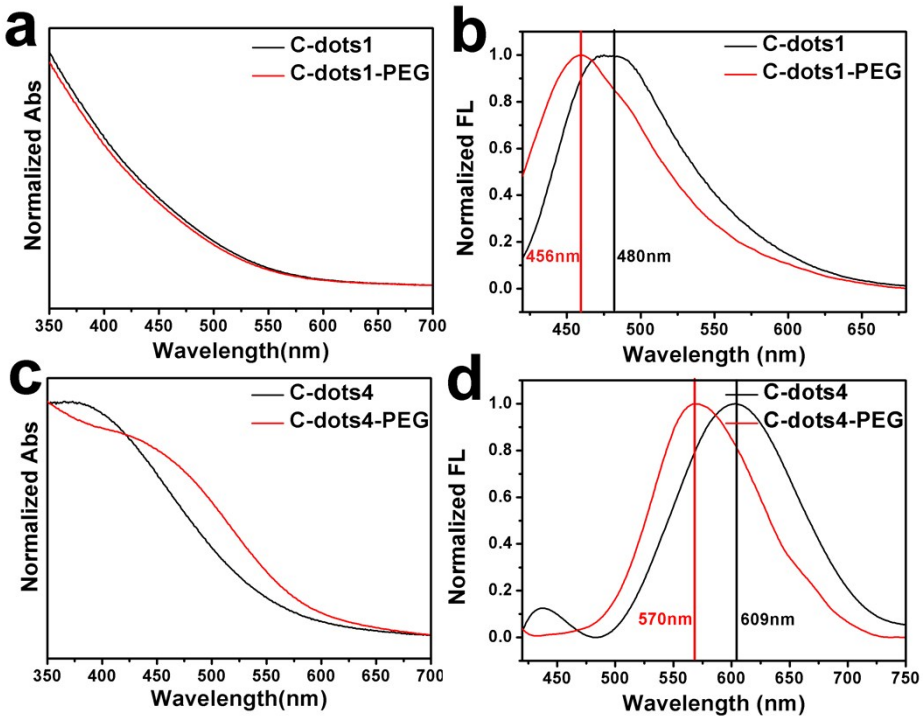

Figure S10. a) Abs spectra of C-dots1 and C-dots1-PEG; b) FL spectra of C-dots1 and C-dots1-PEG; c) Abs spectra of C-dots4 and C-dots4-PEG; d) FL spectra of C-dots4 and C-dots4-PEG.

C-dots	C[%]	H[%]	N[%]	S[%]
C-dots1	41.12	3.00	<0.3	19.23
C-dots2	45.45	3.34	0.66	17.64
C-dots3	56.71	4.17	0.88	14.36
C-dots4	56.45	4.67	1.15	12.04
C-dots5	60.60	5.34	1.27	11.59
C-dots6	62.93	8.46	3.00	8.69

Table S1 The elemental analysis of C-dots.

precursor	PT1	CPT1	CPT2	CPT3	CPT4	PT2
	- 25.1 mV	- 19.4 mV	+ 1.4 mV	+ 8.7 mV	+ 12.9 mV	+ 29.7 mV
	- 28.6 mV	- 22.2 mV	+ 1.5 mV	+ 6.7 mV	+ 9.1 mV	+ 25.1 mV
C-dots	C-dots1	C-dots2	C-dots3	C-dots4	C-dots5	C-dots6

Table S2. The Zeta potential of precursors and C-dots.

C-dots	Zeta potential[mV]
C-dots1	- 28.6
C-dots1-PEG	+ 0.66
C-dots4	+ 6.7
C-dots4-PEG	+ 14.1

Table S3. The zeta potential of C-dots1 and C-dots4 before and after coupled with mPEG-OH.