Electronic Supporting Information

Long-Term Effects of Impurities on the Particle Size and Optical Emission of Carbon Dots.

Nasir Javed[a] and Deirdre M. O'Carroll* [a, b]

[a] *Department of Materials Science and Engineering, Rutgers, The State University of New Jersey, 607 Taylor Road, Piscataway, NJ 08854, United States of America. E-mail: ocarroll@rutgers.edu*

[b] *Department of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey, 123 Bevier Road, Piscataway, NJ 08854, United States of America.*

S1. Analysis of Raman Spectra

The Raman spectrum of carbon dots along with different baselines are shown in Figure S1a. Baselines were created in Origin software using two different modes: first, a user defined baseline with two points that create a straight line; and second, an Asymmetric Least Square Smoothing (ALSS). For ALSS mode the following parameters were used: asymmetric factor: 0.001; threshold: 0.05; smoothing factor: 6, 5.5, and 5; number of iterations: 100. Figure S1b shows the Raman spectrum after subtraction of the different baselines shown in Figure S1a. The relative intensities of the G-band with respect to the D-band (I_G/I_D) calculated after subtraction of the different baselines are shown in Table S1.

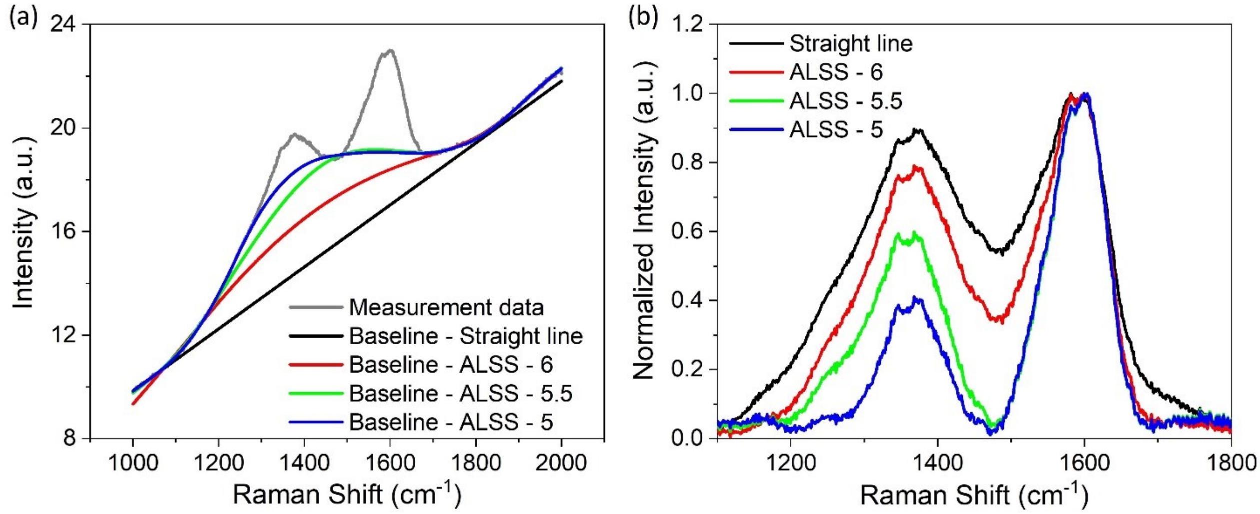

Figure S1: (a) Measured Raman signal of CDs with different baselines. Different smoothing factors, mentioned in legend, were used for baseline creation using Asymmetric Least Square Smoothing (ALSS) mode in Origin software. (b) Raman spectrum after subtraction of different baselines showing the considerable change in relative intensities of G- and D-band.

Table S1: Relative intensity I_G/I_D calculated after subtraction of different baselines

Baseline	**I_G/I_D**
Straight line	0.80
ALSS 6	0.87
ALSS 5.5	1.18
ALSS 5	2.35

S2. Change in CNP Size with Time

Figure S2 below shows average particle of size of CDs vs time after synthesis. The error bars show the standard deviation in particles size distribution. The size was measured from TEM images of CDs. The number of individual particles measured for each data point is given in Table S2 below.

TableS2: Particle size data used to plot graph shown in Figure S2

Time in weeks	1	7	14	36	47	58	64
Number of particles	383	107	252	197	610	166	624
Average size (nm)	23.50	37.86	46.65	50.75	54.69	63.24	60.07
Standard deviation	9.67	14.55	15.40	13.22	18.44	16.54	16.16

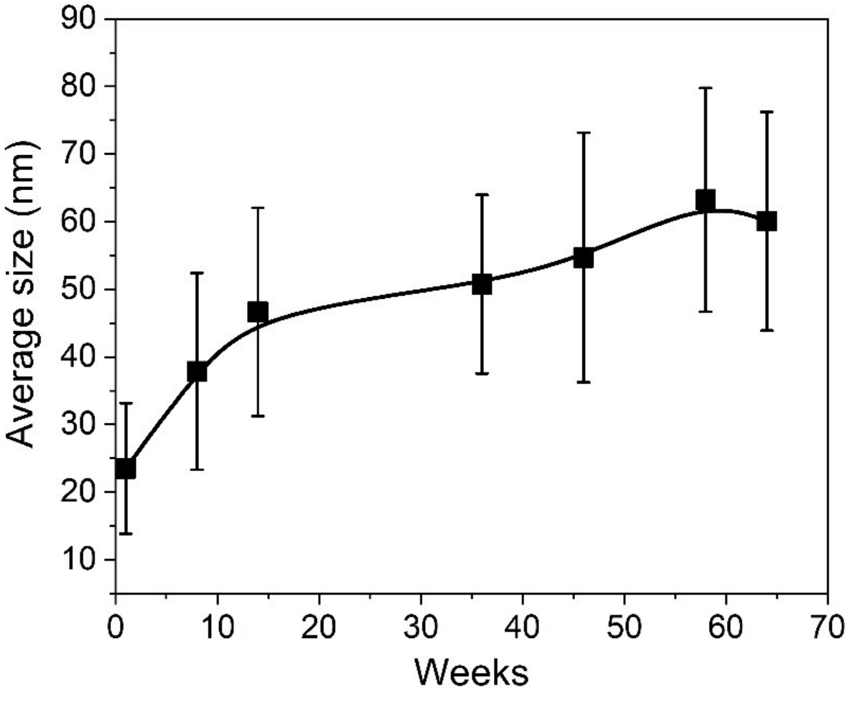

Figure S2: Average size of CDs versus time after synthesis. Error bars show the standard deviation in particle size distribution.

S3. FTIR Spectra

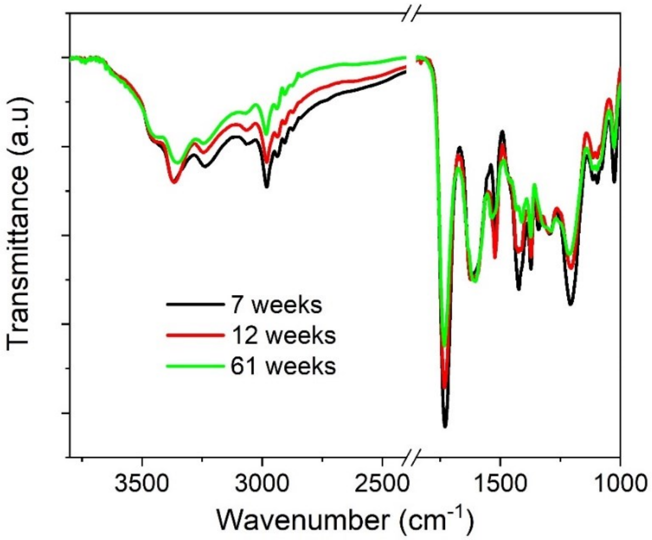

Figure S3: FTIR spectra, shown in Figure 3d of main text, plotted to show the transmittance over a wider range of wavenumbers.

S4. Dialysis progress

To check the progress of the dialysis process and to determine whether purification is complete or not, we collected samples during the dialysis process every time water was changed (after every three hours during the day), and measured their UV-visible absorbance spectra (shown in Figure S4 below). It can be seen that the absorption peak, which is attributed to C=O bonds in byproducts decrease continuously in the first 12 hours. After that there is no notable change in the intensity of the peak which shows that the purification is complete in first 12 hours. Nevertheless, the dialysis process was continued for 48 hours to maximize the purification.

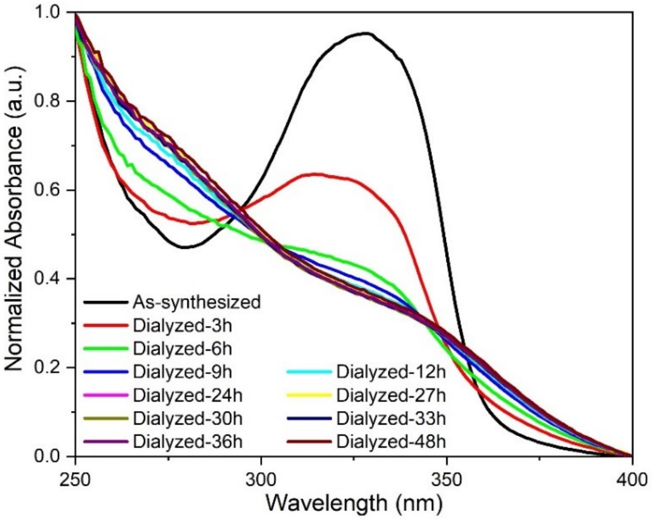

Figure S4: UV-Visible absorption spectra of as-synthesized product and dialyzed samples collected after regular intervals during the dialysis

S5. Photoluminescence of Dialysate:

Photoluminescence spectra of the dialysate was measured at the same conditions at which photoluminescence of the impure CD dispersion was measured. Spectra are shown in Figure S5 below. Photoluminescence quantum yield of the dialysate (measured with excitation wavelength of 340 nm and emission integrated from 350 nm to 550 nm) is 39.2%.

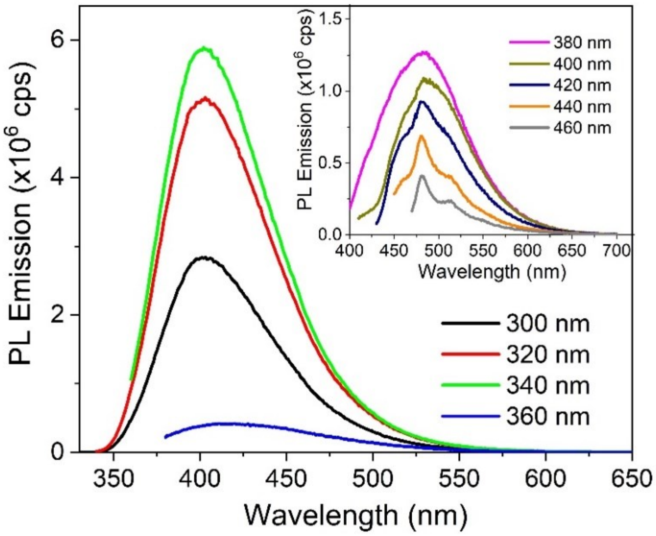

Figure S5: Photoluminescence emission of the dialysate measured at different excitation wavelengths. Excitation and emission slit width was set to 1 nm for spectra shown in main panel. Spectra shown in the inset were recorded with excitation and emission slit width of 2 nm.

S6. Solvent Dependence of Photoluminescence of impure CDs:

Figure S6 below shows the PL emission spectra of CDs without purification (when size is increasing) dispersed in ethanol (left) and in water (right) for comparison. PL emission intensity around 550 nm (where solvent dependent emission was observed in purified CDs) is found to be a slightly higher in ethanol as compared to that in water.

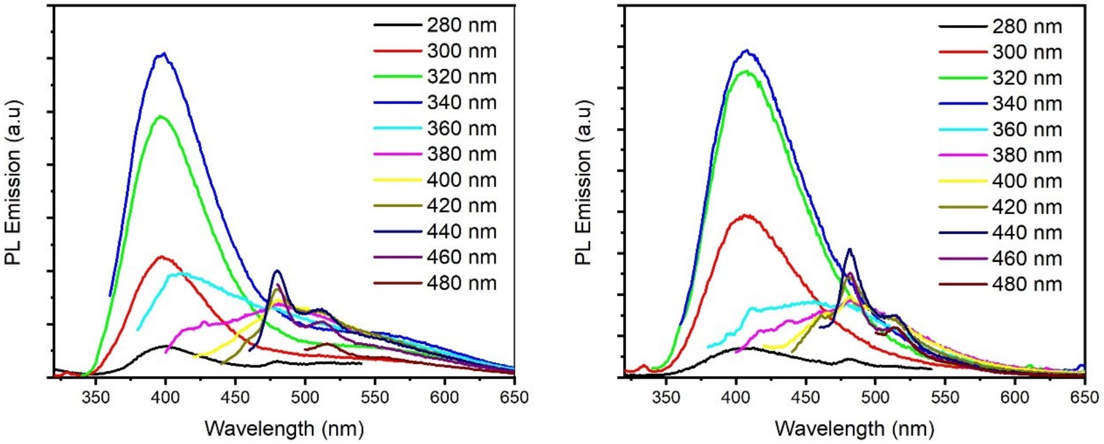

Figure S6: PL emission of CDs without purification obtained 65 weeks after synthesis and dispersed in ethanol (left) and in water (right) measured at different excitation wavelengths.