Electronic Supporting Information

Pressure-triggered aggregation-induced emission enhancement in red emissive amorphous carbon dots

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Experimental Section

Preparation of CDs: CDs were synthesized through solvothermal treatment of 1,3,5-benzenetrithiol. In detail, 174 mg (1 mmol) of 1,3,5-benzenetrithiol, 10 mL of EtOH and 1 mL H_2SO_4 were added into an autoclave and heated at 200 °C for 2 h. After cooling to room temperature, large particles in the solution were removed through centrifugation and filtering. The CDs were further purified by dialyzing and then stored at 4 °C.

Characterization: Transmission electron microscopy (TEM) images were acquired by using a FEI TECNAIG2F20-S-TWIN electron microscope. The absorption and fluorescence spectra of the CDs were recorded on Persee TU-1810PC spectrophotometer and Shimadzu RF-6000 fluorescence spectrophotometer at room temperature, respectively. Fourier transform infrared spectroscopy (FTIR) was performed on a Nexus 470 (Therom Fisher) spectrometer.

Femtosecond transient absorption setup: A regeneratively amplified Ti:sapphire laser system (Coherent Libra, 50fs, 1kHz) provides the fundamental light source. The pump pulse (400 nm) is generated by focusing a portion of fundamental light into BBO crystal. In order to avoid the influence of rotational relaxation effects on dynamics, the polarization of pump pulse is randomized by depolarizing plate. The other fundamental pulse provides broadband probe pulse (white light continuum) that is produced by focusing 800 nm fundamental light into sapphire plate (3mm). The pump and probe beams are overlapped in the sample with crossing areas of 600 μm and 150 μm. After passing through the sample, the probe pulse is focused into optical fiber that is coupled to spectrometer (AvaSpec-1650F). The energy of 400 nm excitation pulse is adjusted to about 1.5 μJ/pulse by a neutral density optical filter. The pump pulse is chopped at 500 Hz to acquire pumped (signal) and un-pumped (reference) probe spectra, and the ΔOD spectrum can be obtained by processing them. The solutions are placed in 2 mm optical path length quartz cuvette. Both the instrument response function (100 fs) and temporal chirp in the probe light are determined by measuring the cross modulation of ethanol. The group velocity dispersion effect on the experiment data is corrected by home-made chirp program. For each measurement, the pump-probe delay scan is repeated three times to give the averaged experiment data.

Piezochromic Effect in CDs: To further investigate the piezochromic effect in CDs, we investigated the influence of applied pressure on the luminescence of CDs. Ethanol was used as a pressure transmitting medium (PTM). The pressure in DAC was monitored using the pressure-dependent ruby fluorescent method (ruby R1 and R2 lines). We employed IIα-type ultralow fluorescence diamonds with a culet size of 300 mm. A T301 stainless steel gasket was pre-indented by the diamonds and was drilled to generate a 100 mm diameter cavity for loading the samples. The *in-situ* PL and absorption measurements under high pressure were performed on an Ocean Optics QE65000 spectrometer. The 405 nm line of a violet diode laser and a deuterium halogen lamp were employed as the excitation source for PL and absorption, respectively. All the experiments were conducted at room temperature.

Computational details: Density functional theory (DFT) and time-dependent density function theory (TDDFT) calculations on the R-CDs were performed. The B3LYP hybrid functional and 6-31+g(d,p) basis set were used to study the ground and excited states. To simulate the pressure induced blocking of the intraparticle oscillations, "dimer" model was constructed. The monomer of R-CDs was used to represent the ambient states. We first optimized the ground states and singlet excited states. Then the emission spectrum and natural transition orbitals were obtained based on the optimized structures. The natural transition orbitals help to explain the nature of the corresponding emissive.

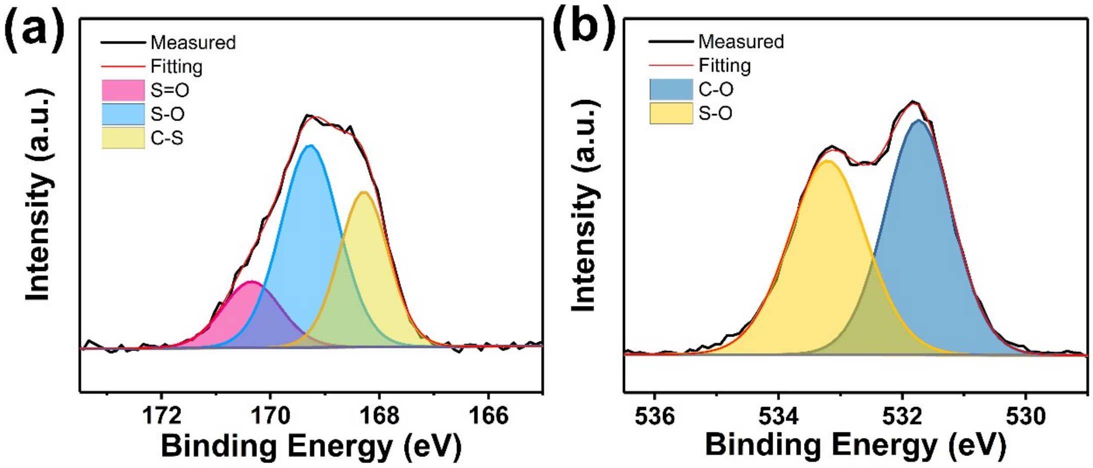

Figure S1 The high-resolution XPS of R-CDs (a) S 2p and (b) O 1s.

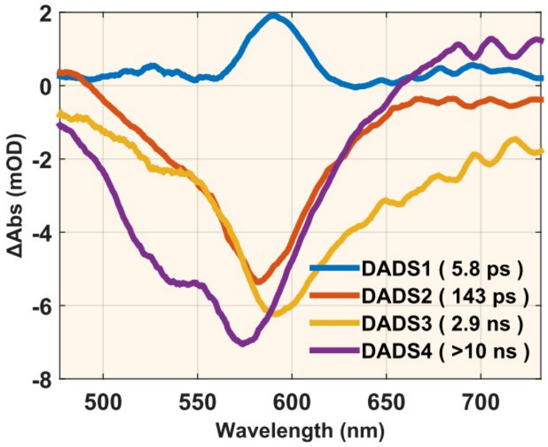

Figure S2 Results of the global fitting with four exponent decay functions showing four decay associated difference spectra (DADS) of R-CDs excited at 360 nm.

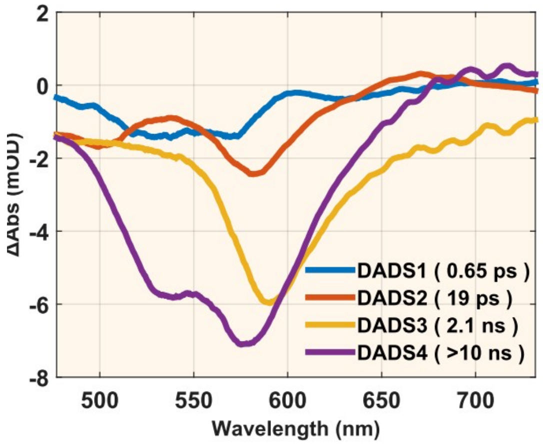

Figure S3 Results of the global fitting with four exponent decay functions showing four decay associated difference spectra (DADS) of R-CDs excited at 450 nm.

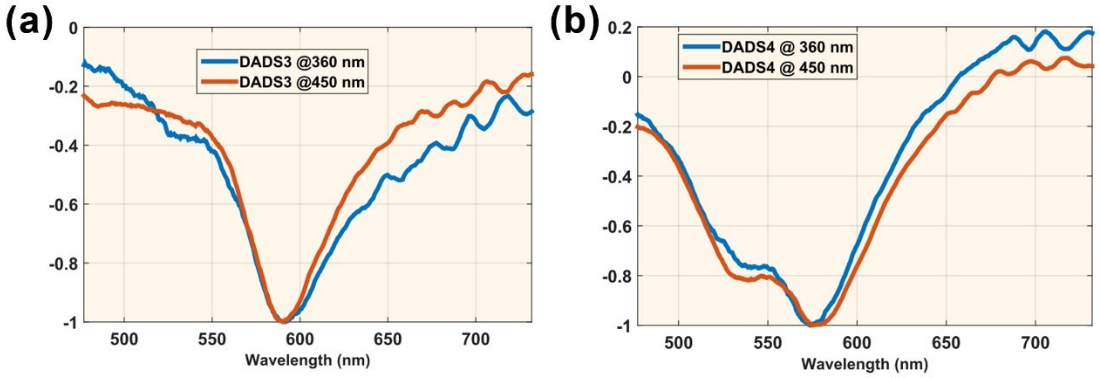

Figure S4 The normalized spectra of the third DADS3 and the fourth DADS4 excited at (a) 360 nm and (b) 450 nm.

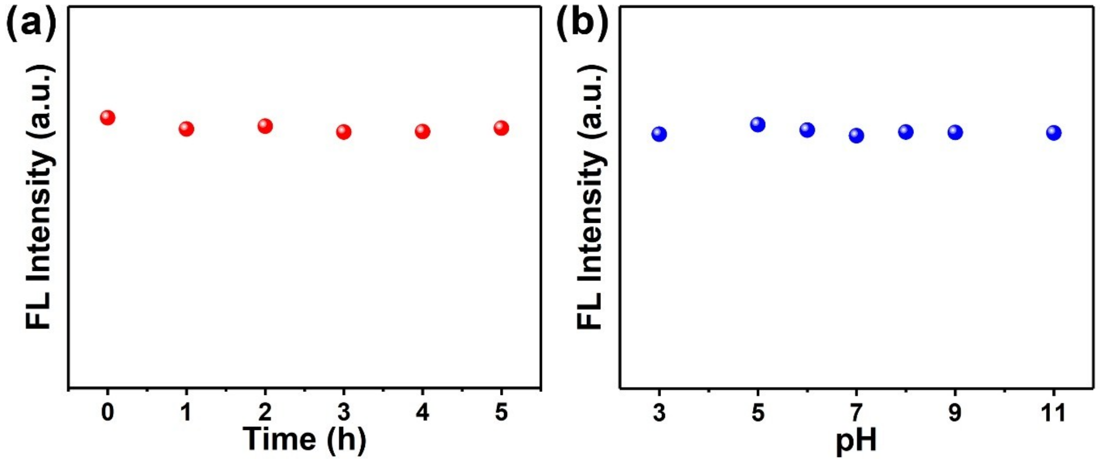

Figure S5 The stability of R-CDs (a) under 365 nm light, (b) under different pH conditions.

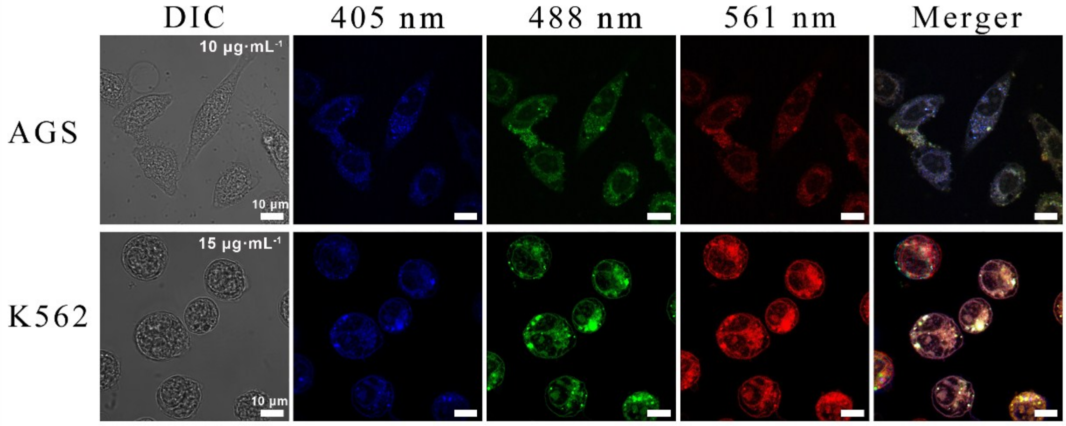

Figure S6 Bright-field photomicrograph of the AGS and K562 cells incubated with R-CDs.