

Supporting information

Supercapacitor devices for energy storage and capacitive dye removal from aqueous solutions

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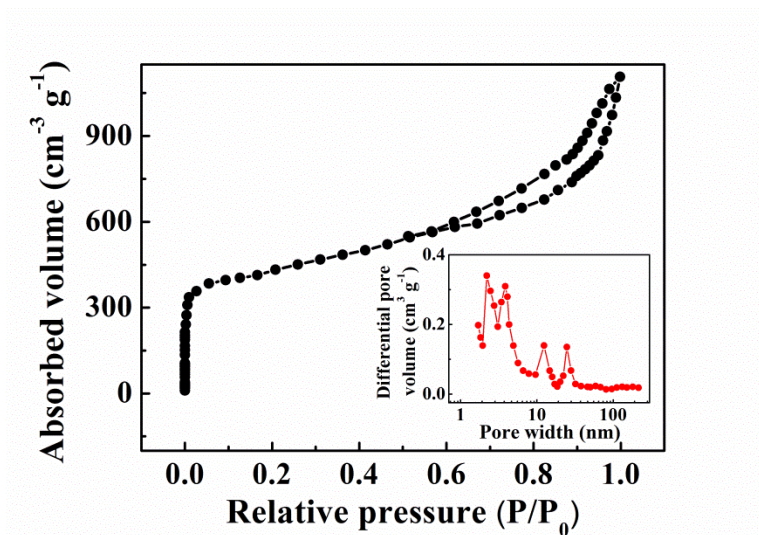


Figure S1. Nitrogen adsorption–desorption isotherms and pore size distribution of NC-MWCNT obtained by Density Functional Theory (DFT) method to the adsorption branch of N₂ isotherms. The specific surface area calculated by Brunauer-Emmett-Teller (BET) model is 1889.12 m² g⁻¹. The pore volume of 1.72 cm³ g⁻¹ was obtained using Barrett-Joyner-Halenda (BJH) model, cumulative volume of pores between 1.7 and 250.0 nm diameter.

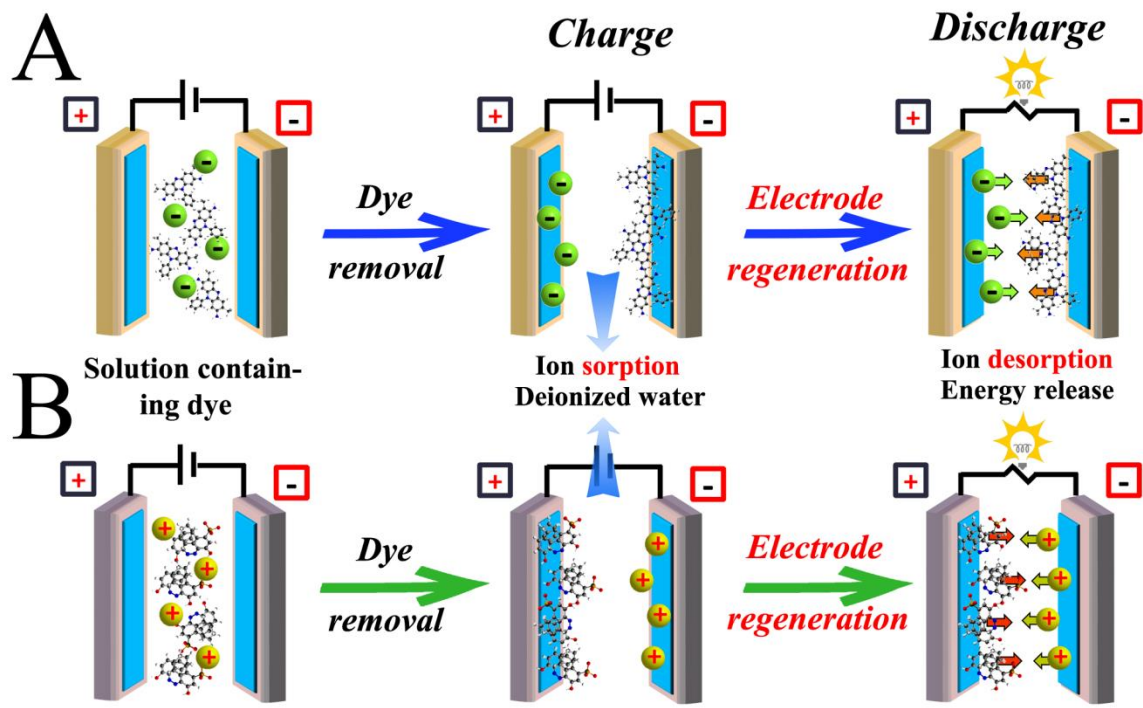


Figure S2. Charge and discharge mechanism of symmetric supercapacitor fabricated using (A) SF and (B) CL dye electrolyte. By applying voltage to the electrodes, dye ions are drawn to the surface of the electrical double layer and the supercapacitor is charged. Conversely, the ions are released from electrode when discharging the supercapacitor. The deionization and electrode regeneration were accompanied with charge-discharge process.

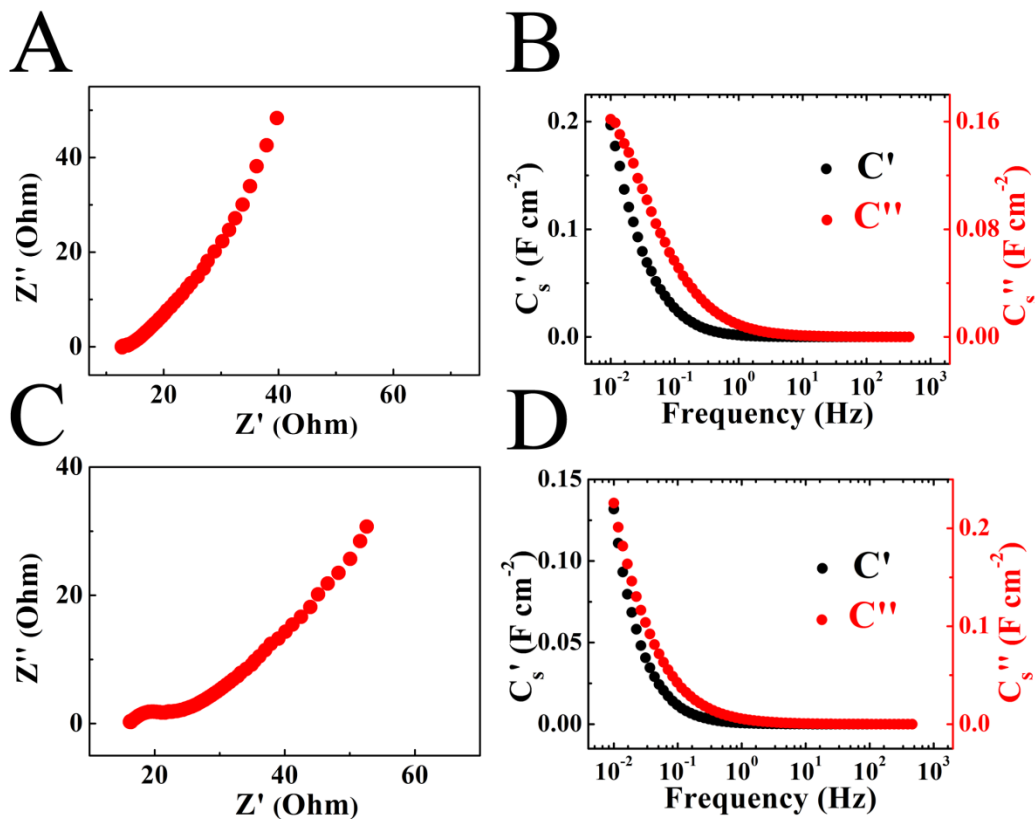


Figure S3. Impedance and AC capacitance data for supercapacitor cells, containing $400\ mg\ L^{-1}$ (A,B) SF and (C,D) CL electrolytes: (A, C) Nyquist plots and (B, D) C'_s and C''_s , calculated from the impedance data versus frequency.

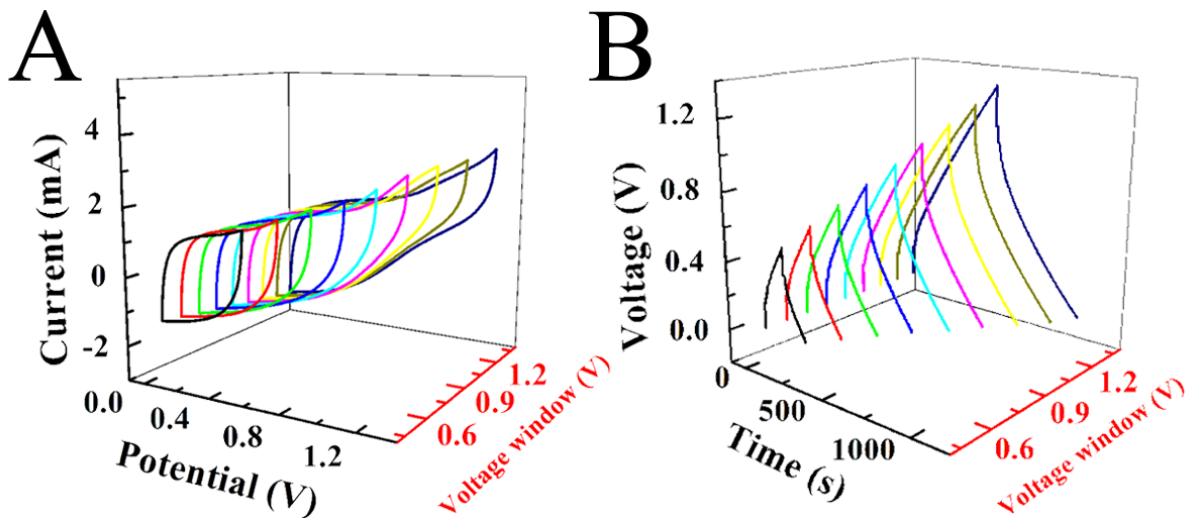


Figure S4. (A) CVs at a scan rate of 2 mV s^{-1} and (B) charge-discharge curves at a current density of 3 mA cm^{-2} at different potential windows (from 0.5 to 1.3 V) for supercapacitor cells, containing two NC-MWCNT electrodes in 400 mg L^{-1} AM as electrolyte.

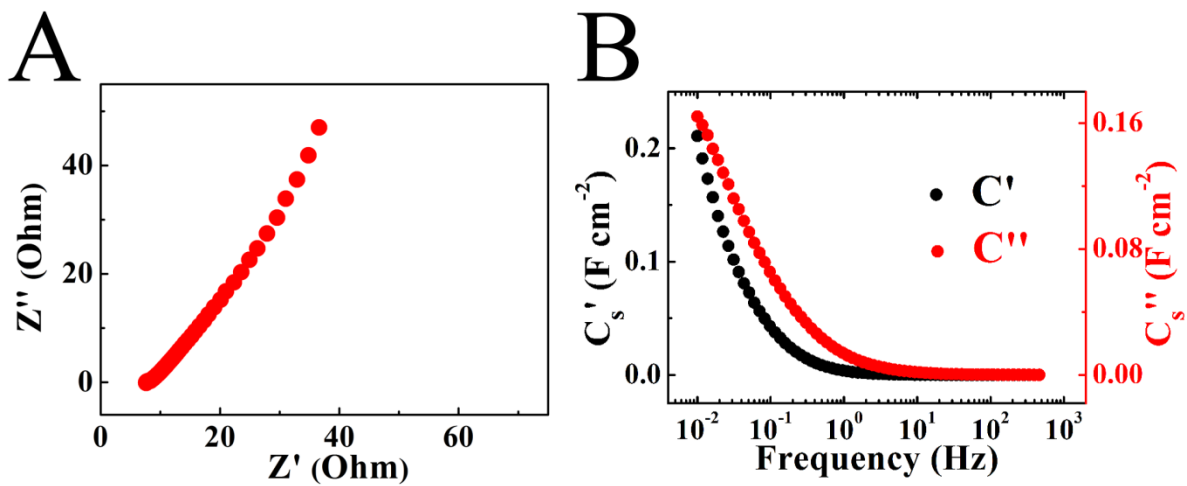


Figure S5. (A) Nyquist plot, (B) C'_s and C''_s , calculated from the impedance data, versus frequency for supercapacitor cells containing $400\ mg\ L^{-1}$ AM as electrolyte.

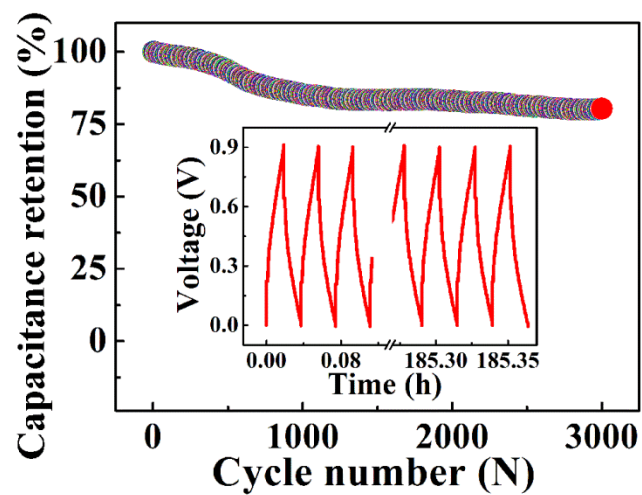


Figure S6. Capacitance retention of supercapacitor cells, containing two NC-MWCNT electrodes in 400 mg L^{-1} AM electrolyte, versus cycle number, inset shows the initial and final charge-discharge curves in the cycling performance test.

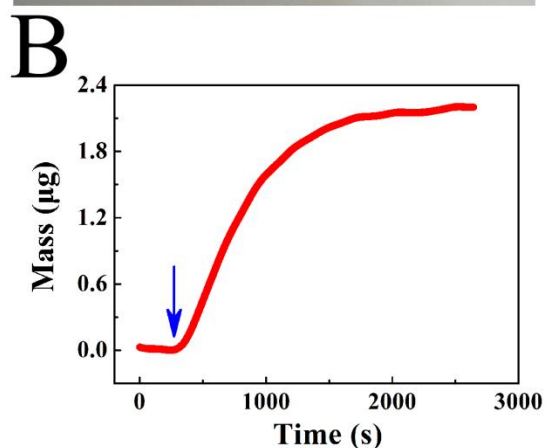
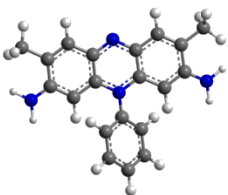
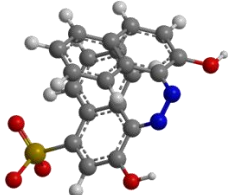
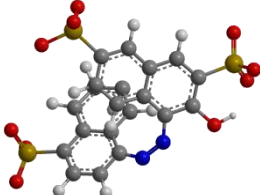


Figure S7 (A) QCM experimental setup for dye removal efficiency measurement. The working electrode was NC-MWCNT coated 9-MHz quartz crystal with mass loading of 10 μg . The counter electrode was a Pt wire. 0.3 mL of 50 mg L^{-1} AM dye solution was injected in the cell using a syringe. (B) Mass gain was measured by QCM versus time after applying a voltage of 1.0 V. Arrow shows the starting point, when voltage was applied.

The removal efficiency, measured by QCM was calculated by the maximum mass change, divided by the total amount of the dye, injected in the cell:

$$\frac{2.197 \mu\text{g}}{50 \text{ mg L}^{-1} \times 0.3 \times 10^{-3} \text{L}} = 14.65\%$$

Table 1 3D chemical structure and physical-chemical properties of dye ions.

Molecular structure			
	Safranin	Calcon	Amaranth
Molecular weight (g mol ⁻¹)	315.39	393.39	535.50
Connolly accessible area ^{1,2} (Å ²)	551.56	488.15	629.68
Connolly molecular area ^{1,2} (Å ²)	289.68	258.16	349.99
Polar surface area ^{3,4} (Å ²)	67.41	122.38	216.55
Connolly solvent excluded volume ^{1,5} (Å ³)	253.33	285.32	348.17
log P ^{6,7} (hydrophobicity)	2.43	3.58	1.32
Length (Å)	9.32	7.20	9.24
Width (Å)	6.73	5.01	6.25
Depth (Å)	1.35	4.74	5.87

*All the properties were calculated for dye ions excluding the influence of counter ions.

Molecular surface area and volume are determined using Connolly's program^{1,2,5}. In order to express hydrophobicity of the dyes, Log P was adopted^{6,7}. The chemical structures of dyes were first drawn by ChemDraw Ultra 12.0 and then the structure files were imported into Chem3D Ultra 12.0. The chemical structure of the dyes was optimized by the process Molecular

Mechanics 2 (MM2) Minimize Energy. Minimum RMS Gradient was set to 0.100. After the structure optimization, the logP of ChemPropPro and the polar surface area of Molecular Topology at the Compute Properties menu was selected and calculation was carried out. Molecular molecule size including length, width, and thickness were measured with the same software⁸⁻¹⁰.

Table S2 Capacitive adsorption performance of SF and CL dye solution under different voltage windows in the range of 0.6-1.4 V.

Voltage window	SF adsorption mass	CL adsorption mass	SF adsorption capacity	CL adsorption capacity
(V)	(μg)	(μg)	(mg/g)	(mg/g)
0.6	0.15	0.1	15	10
0.8	0.36	0.26	36	26
1	0.39	0.29	39	29
1.2	0.44	0.33	44	33
1.4	0.48	0.41	48	41

*The adsorption mass is the maximum of mass variations measured by QCM studies. The adsorption capacity was calculated by adsorption mass divided by the mass of active materials of electrode (10 μg).

References:

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