Electronic Supplementary Material (ESI) for Energy & Environmental Science.

Supplementary Information

Faradaic Electro-Swing Reactive Adsorption for CO_2 Capture

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S1. Characterization of poly(1,4-anthraquione) (P14AQ)

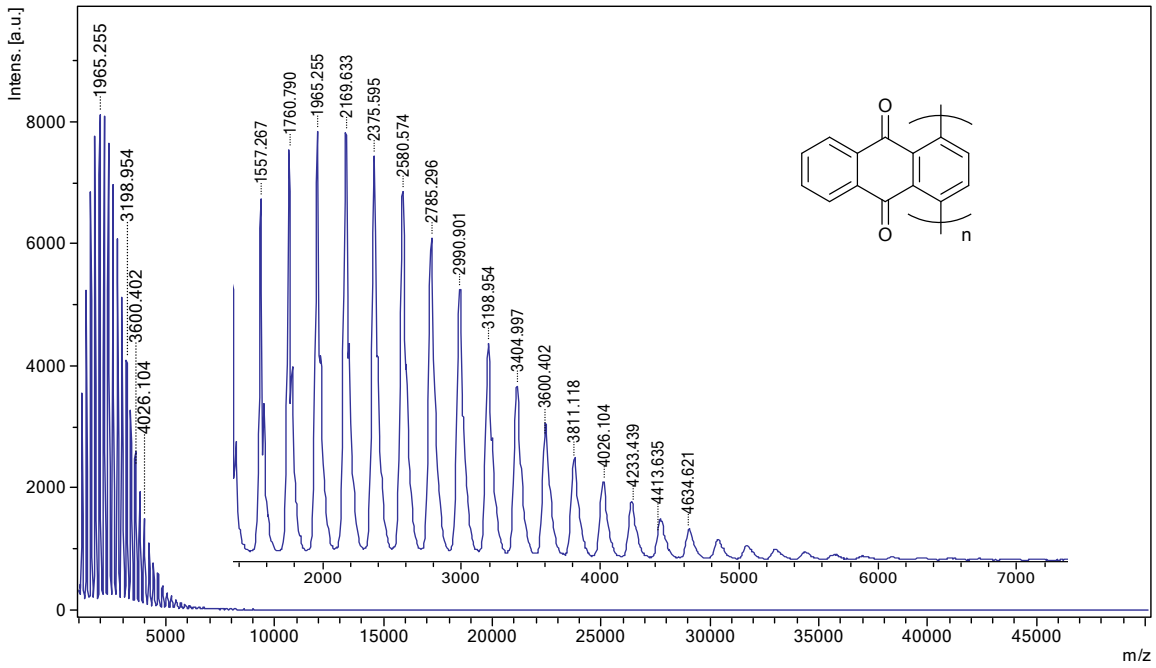

Figure S1. Matrix-assisted laser desorption/ionization (MALDI) time-of-flight (TOF) mass spectrometry of the P14AQ polymer chains after the Soxhelt extraction removal of small chains. The median chain is 10 – 11 units long and chains with as many as ~ 25 units can be seen. A sample of 1 μL at a concentration of 10 μg/mL in tetrahydrofuran with a dithranol matrix was used.

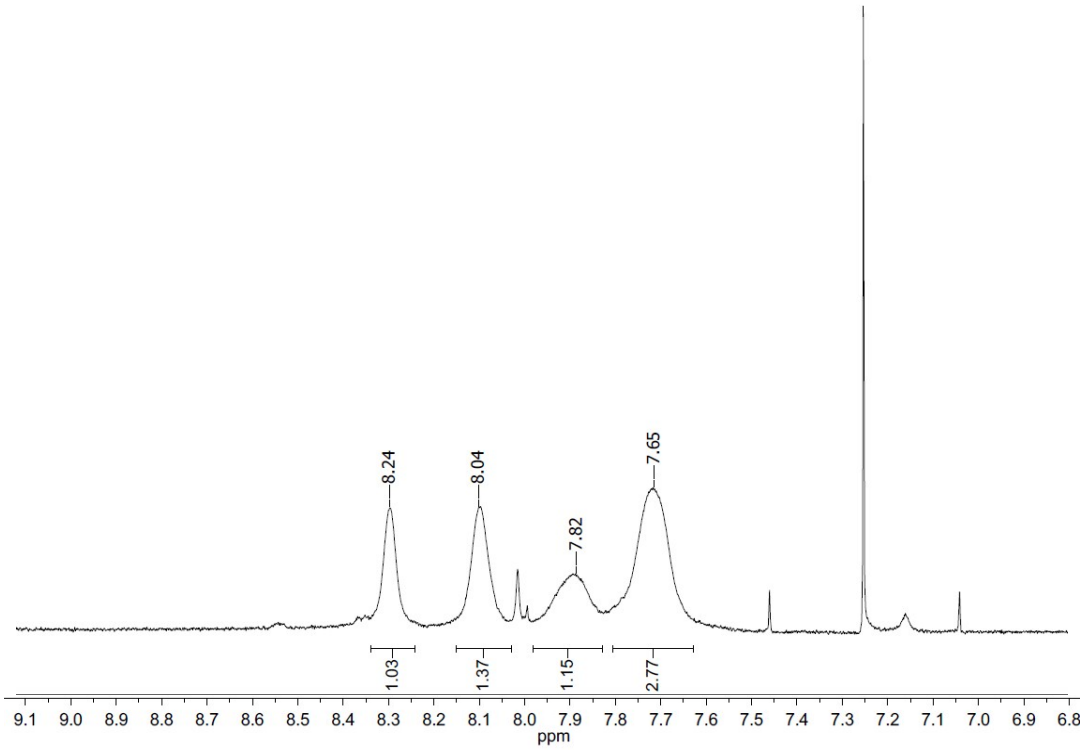

Figure S2. ^{1}H NMR of P14AQ in *d*-chloroform (600 MHz). The broadness of the peaks is a result of polymerization. The end units of the polymer chains contribute to the smaller peaks.

S2. UV-visible and XPS spectroscopy of P14AQ-CNT composite

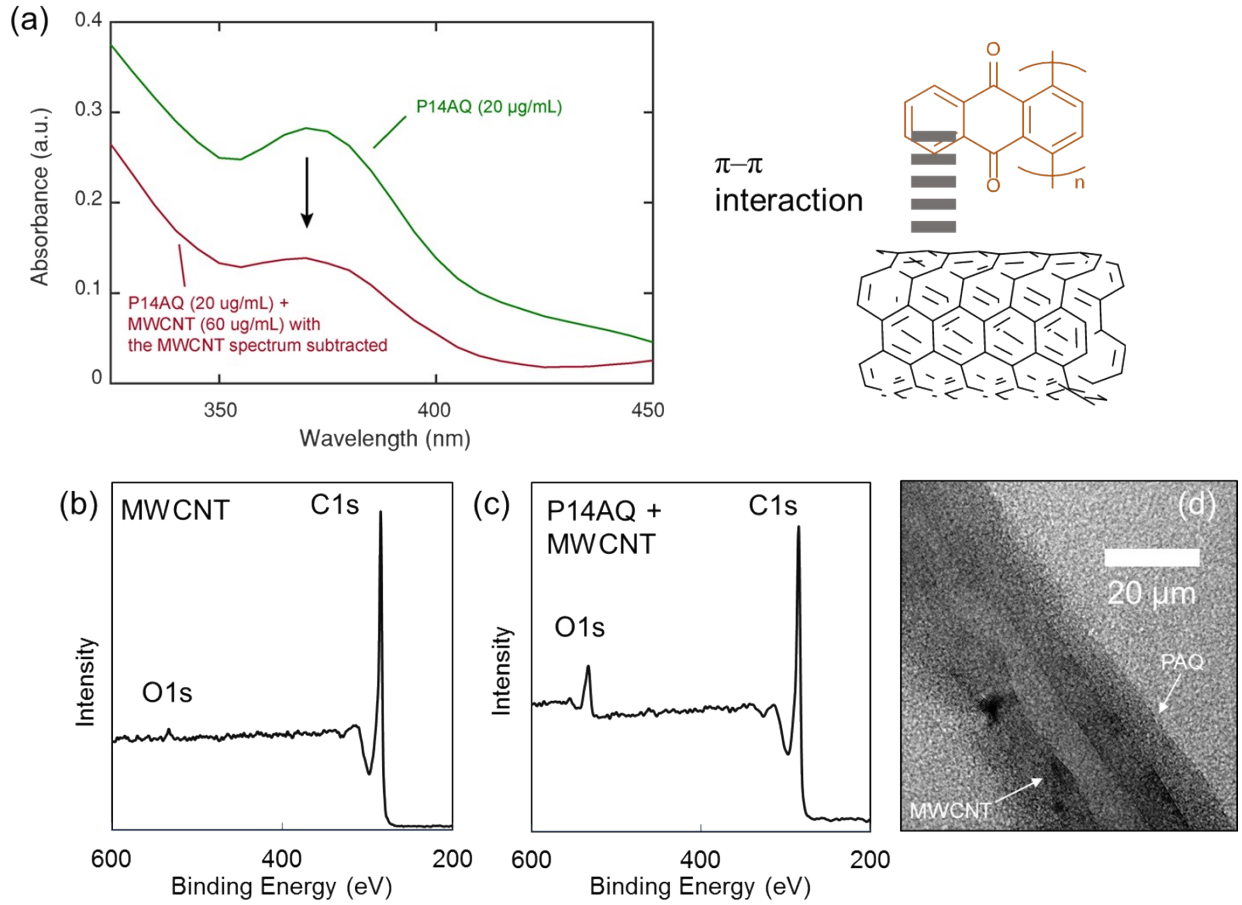

Figure S3. (a) UV-Visible spectra of P14AQ polymer in chloroform (20 µg/mL) and 1:3 P14AQ:MWCNT ink (80 µg/mL) in chloroform. This is 50-fold dilution from the actual inks. The spectrum of 60 µg/mL MWCNT was subtracted from the ink spectrum. The characteristic peak of P14AQ was diminished in the ink due to lack of $\pi \rightarrow \pi^*$, which is an indication of π- π interaction between P14AQ and MWCNT.[1] (b) XPS spectrum of MWCNT with elemental composition of C:97.6% and O:3.3%. (c) XPS spectrum of P14AQ-CNT composite with elemental composition of C:83.8% and O:16.2%. The increase in the oxygen content in (c) compared to (b) is due to the oxygens from the P14AQ polymer. (d) TEM micrograph of a single MWCNT with P14AQ coating, showing regions of layered walls of CNTs and an amorphous polymer coating.

S3. P14AQ to multi-walled carbon nanotube (MWCNT) ratio optimization

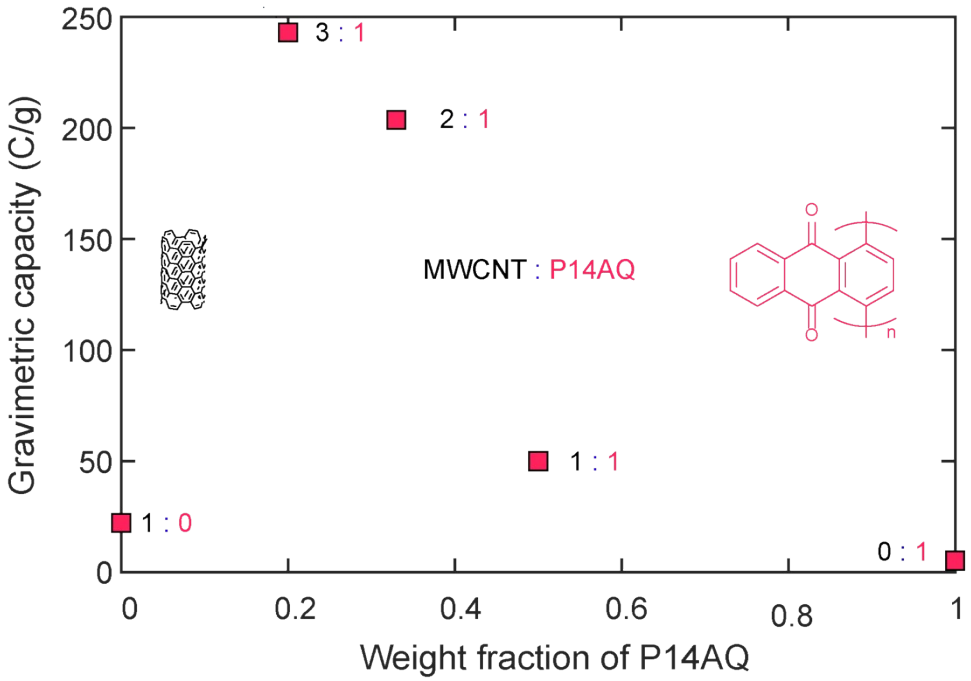

Figure S4. Weight fraction of P14AQ in the P14AQ-CNT composite was optimized for highest gravimetric capacity. This was obtained at 3:1, CNT: P13AQ by weight.[2]

S4. Calibration of P14AQ-CNT and PVFc-CNT

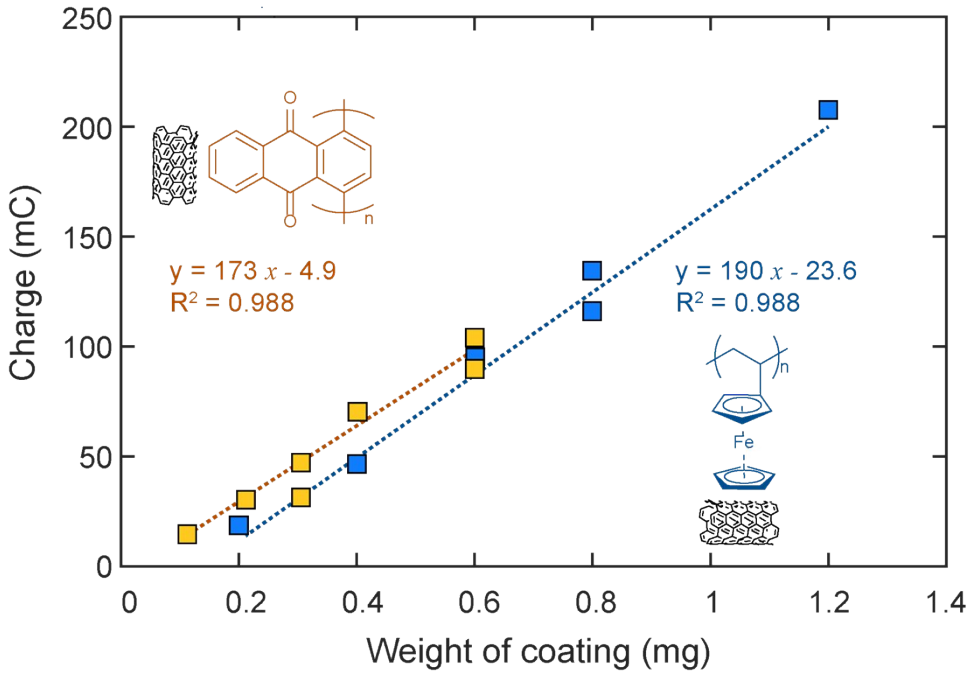

Figure S5. Calibration of charge/weight of both P14AQ-CNT and PVFC-CNT composites. Non-woven carbon fiber mat electrodes (2 cm^2) were dip-coated in the ink and dried multiple times. Each electrode was weighed and its charge was measured in potentiostatic reduction and oxidation.

S4. Electrochemical characterizations

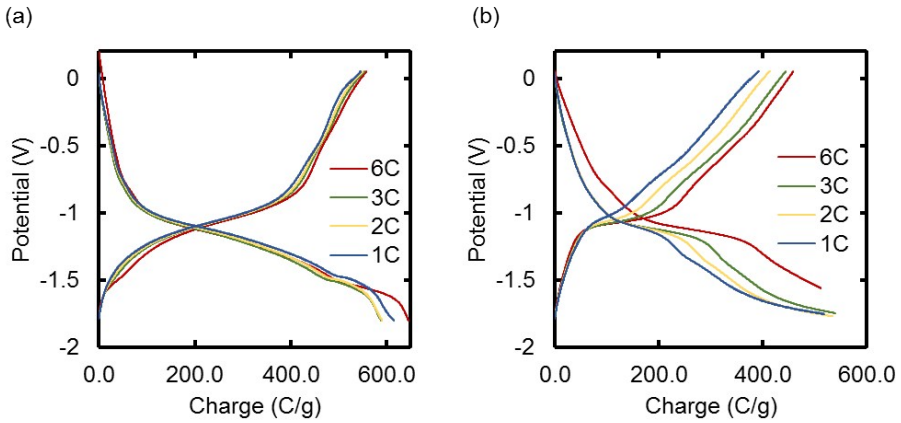

Figure S6. Galvanostatic charge-discharge cycles of the P14AQ-CNT electrode in [Bmim][Tf_2N], under (a) N_2 and (b) CO_2, vs Fc. Charge is reported as Coulombs per gram of P14AQ polymer.

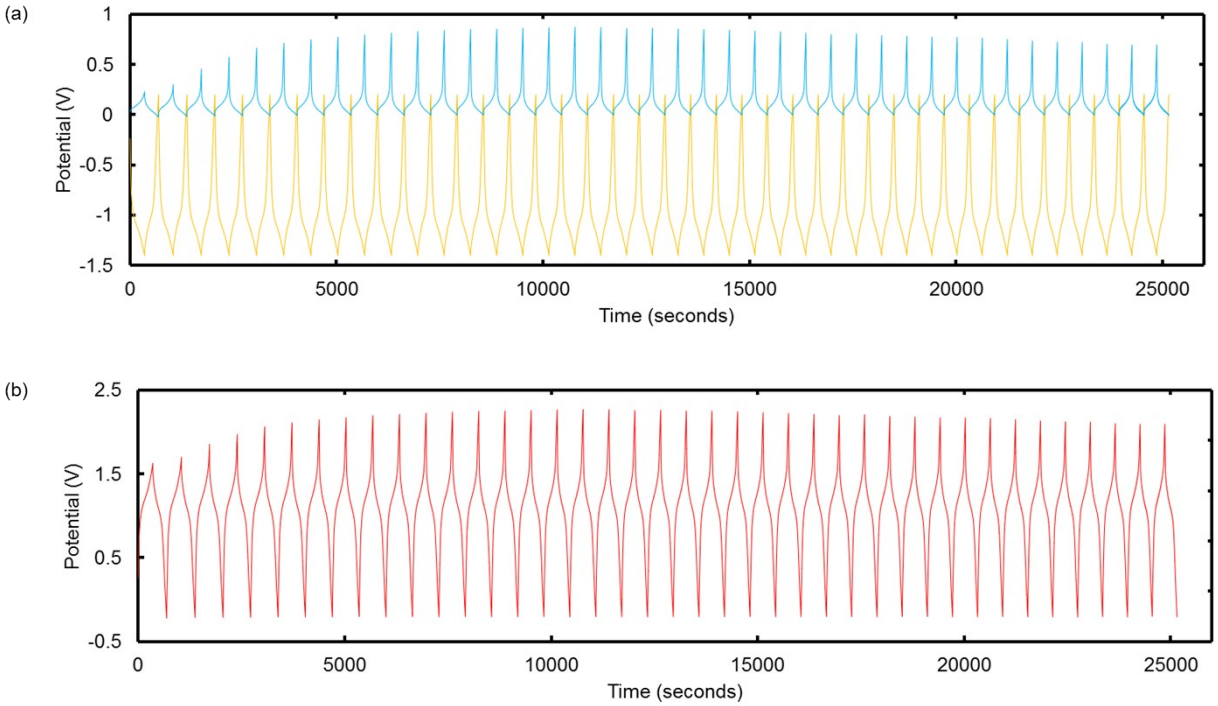

Figure S7. (a)Galvanostatic charge and discharge cycles of the electrochemical cell in [Bmim][Tf_2N], under CO_2 with PVFc-CNT (—) and P14AQ-CNT (—) being studied vs Fc. (b) The overall cell potential (—) P14AQ-CNT vs PVFc-CNT.

S5. Determination of internal volume of the sealed chamber

The internal volume of the sealed chamber was determined after loading all the cells and the insulating material via the pressure change in the cell upon increasing the internal volume. A gas-tight syringe of 50 mL was connected to the sealed loaded chamber, and the plunger was pulled in small consistent increments so that the constant number of moles of gas in the chamber expanded and its pressure dropped. In the pressure and temperature ranges of this experiment the gas was assumed to be ideal and the following equation was used:

$$P_0 V_0 = P_i V_i$$

$$\frac{P_i}{P_0} = \frac{V_i}{V_0} = \frac{V_0 + \Delta V_i}{V_0} = 1 + \frac{\Delta V_i}{V_0}$$

By plotting $\frac{P_i}{P_0}$ vs ΔV_i, the void volume can be obtained from the reciprocal of the slope.

S6. Determination of the change of moles of CO_2 in the sealed chamber

Ideal gas law was used to calculate the change in the number of moles of CO_2 in the sealed chamber Δn, from the changes in the pressure ΔP.

$$\Delta n = \frac{\Delta P V_0}{RT}$$

Where R is the gas constant and T is the temperature which was ~ 21°C.

References

1 X. Mao, G. C. Rutledge and T. A. Hatton, *Langmuir*, 2013, **29**, 9626–34.

2 X. Mao, E. H. Yan, G. C. Rutledge and T. A. Hatton, *Chem. Mater.*, 2016, **28**, 543–548.