# Activated carbon aerogel as an electrode with high specific capacitance for capacitive deionization

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## Text. S1

Pseudo-first-order model：

$$\ln(q_e - q_t) = \ln q_e - k_1 t$$

Pseudo-second order kinetic model：

$$t/q_t = t/q_e + 1/(k_2 q_e^2)$$

where $q_t$ and $q_e$ are the adsorption amount at time t and equilibrium ($mg \cdot g^{-1}$), respectively. The $k_1$ is the rate constant of the pseudo-first-order adsorption ($min^{-1}$), The calculated $q_e$ ($q_{e,cal}$) and $k_1$ is obtained from the plot $\ln(q_e - q_t)$ against t. The $k_2$ is the rate constant of the pseudo-second-order adsorption ($g \cdot mg^{-1} \cdot min^{-1}$). The calculated $q_e$ ($q_{e,cal}$) and $k_2$ is obtained from the plot $t/q_t$ against t.

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The initial adsorption rate ($h_0$) is calculated by the following equation:

$h_0=k_2q_e^2$

**Text. S2**

The interaction of ion and sorbent can be evaluated by separation factor ($R_L$). $R_L$ is a dimensionless constant separation factor, an equilibrium parameter derived from the Langmuir model, and expressed as equation:

$$R_L=1/(1+bC_0)$$

Where $C_0$ is the initial concentration of ion and b is the Langmuir constant.

The $R_L$ values indicate whether the isotherm is favourable ($0 < R_L < 1$), unfavourable ($R_L > 1$), linear ($R_L = 1$) or irreversible ($R_L = 0$).

Fig S1. Schematic diagram of (a) the CDI system and (b) the CDI module.

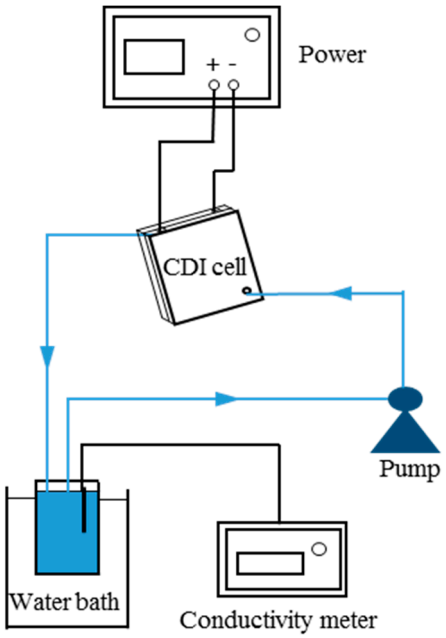
Fig S2. Relationship between concentration and conductivity of NaCl solution.

Fig S3. SEM images of CA (a) and ACA (b).

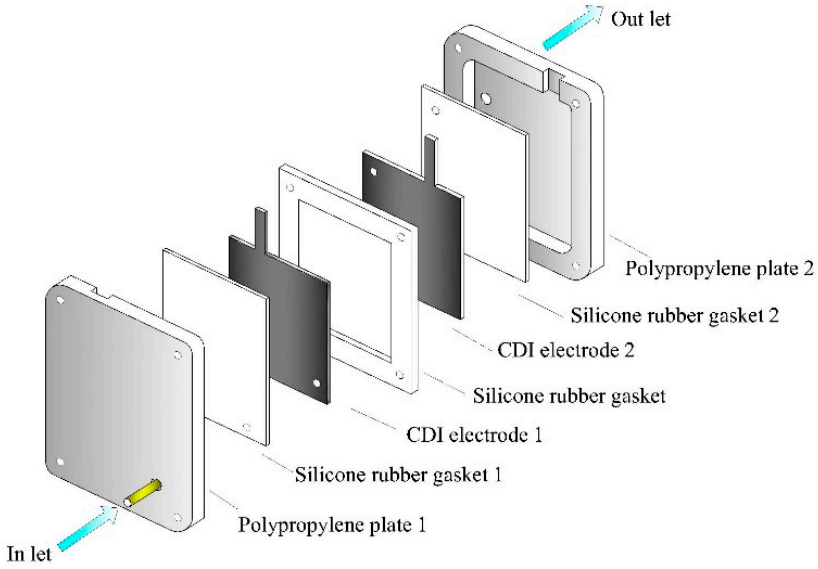
Fig S4. $N_2$ adsorption-desorption isotherms (a) and pore size distribution (b) of CA and ACA.

Fig S5. FTIR (a) and XPS(b) spectra of CA and ACA, C 1s (c) and O 1s (d) high-resolution XPS spectra of CA, C 1s (e) and O 1s (f) high-resolution XPS spectra of ACA.

Fig S6. Contact angles of CA (a) and ACA (b) electrodes.


Power
+ -
CDI cell
Pump
Water bath
Conductivity meter

(a)


Out let
Polypropylene plate 2
Silicone rubber gasket 2
CDI electrode 2
Silicone rubber gasket
CDI electrode 1
Silicone rubber gasket 1
Polypropylene plate 1
In let

(b)

Fig S1

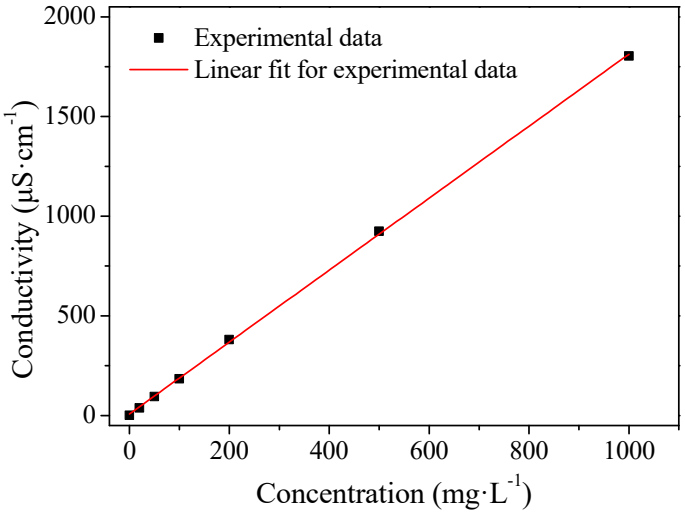
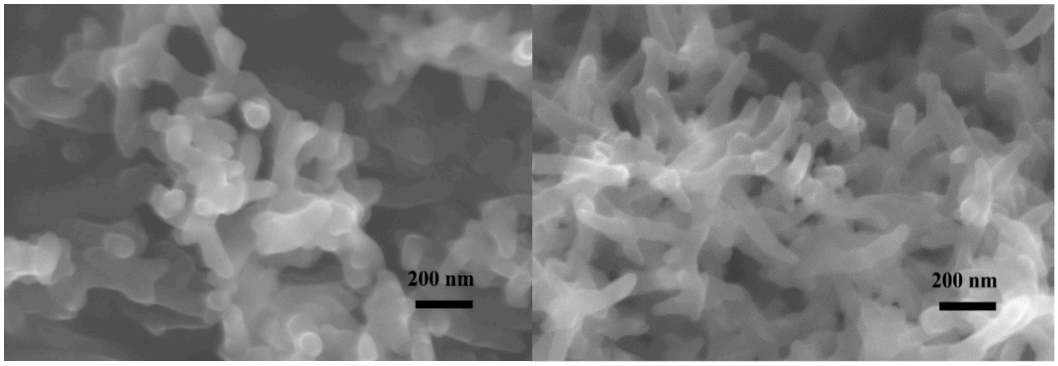

Experimental data
Linear fit for experimental data
Conductivity (μS·cm-1)
Concentration (mg·L-1)
2000
1500
1000
500
0
0
200
400
600
800
1000

Fig S2




(a) (b)

Fig. S3

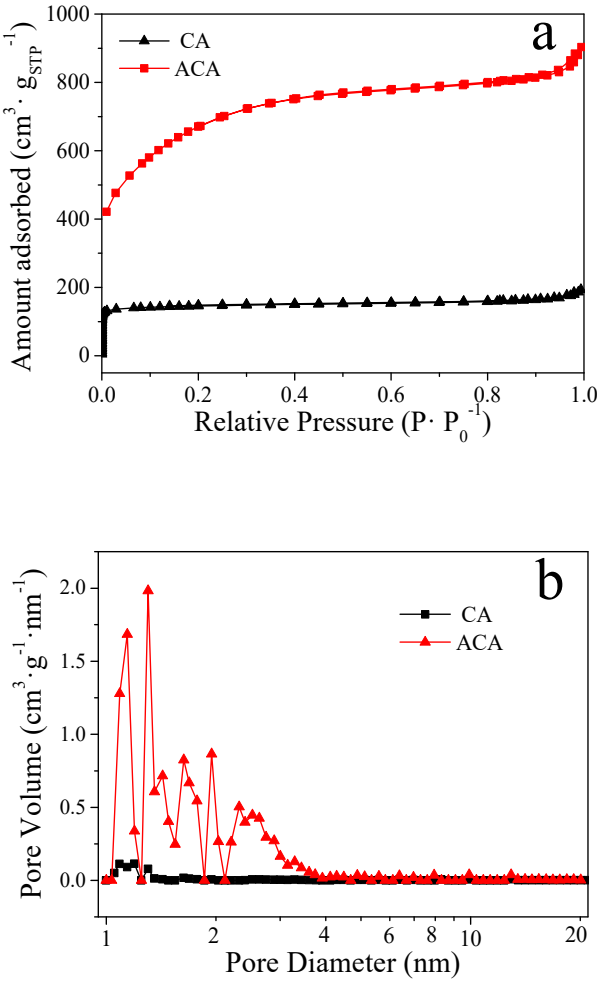

a
CA
ACA
Amount adsorbed (cm3· gSTP-1)
Relative Pressure (P· P0-1)
0
200
400
600
800
1000
0.0
0.2
0.4
0.6
0.8
1.0
b
CA
ACA
Pore Volume (cm3·g-1·nm-1)
Pore Diameter (nm)
0.0
0.5
1.0
1.5
2.0
1
2
4
6
8
10
20

Fig. S4

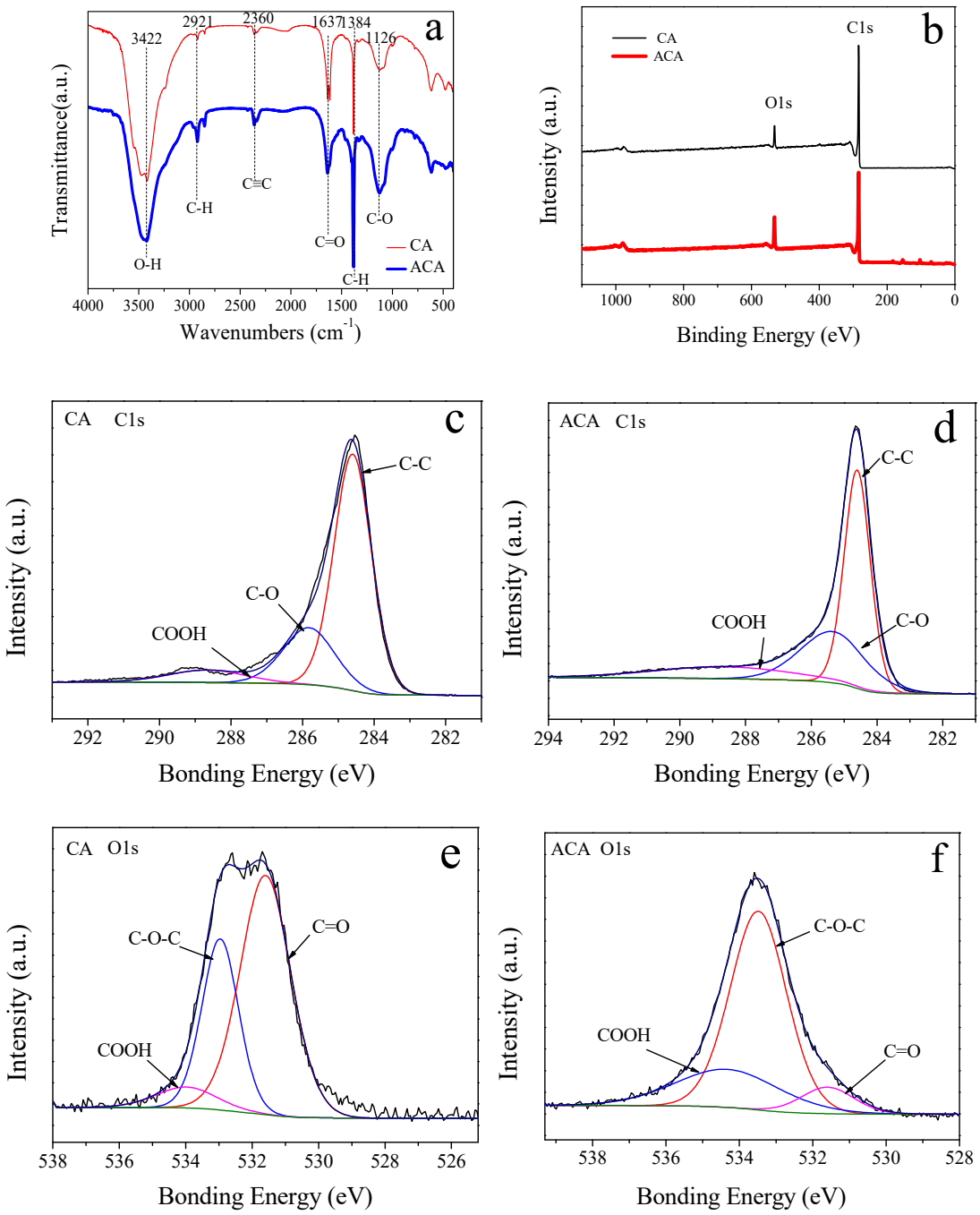
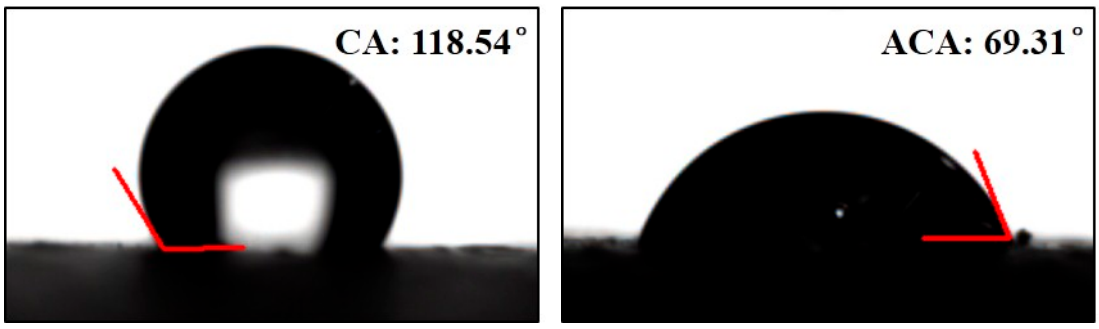

a
Transmittance(a.u.)
3422
2921
2360
1637
1384
1126
C≡C
C-H
C=O
C-O
O-H
C-H
CA
ACA
Wavenumbers (cm-1)
b
CA
ACA
C1s
O1s
Intensity (a.u.)
Binding Energy (eV)
c
CA C1s
C-C
C-O
COOH
Intensity (a.u.)
Bonding Energy (eV)
d
ACA C1s
C-C
COOH
C-O
Intensity (a.u.)
Bonding Energy (eV)
e
CA O1s
C-O-C
C=O
COOH
Intensity (a.u.)
Bonding Energy (eV)
f
ACA O1s
C-O-C
COOH
C=O
Intensity (a.u.)
Bonding Energy (eV)

Fig. S5




(a) (b)

Fig. S6