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MoC nanoparticles-embedded carbon nanofiber aerogel as flow-through electrode for highly-efficient pseudo-capacitive deionization

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Preperation of the pure MoCs

The MoCs were prepared via a typical procedure: Firstly, 0.4 mmol ammonium molybdate and 0.4 mmol citric acid were dissolved in 100 mL of deionized water, followed by adding nitric acid dropwise until the pH reaches 1.5. Then 30 ml ethylene glycol was added into the above solution under magnetic stirring and kept at 60 °C for 8 hrs until a white gel was obtained. After that the white gel was dried at 140 °C overnight. Finally, the obtained white powder was thermally treated at 800 °C in a nitrogen atmosphere for 5 hrs with a heating rate of 5 °C/min.

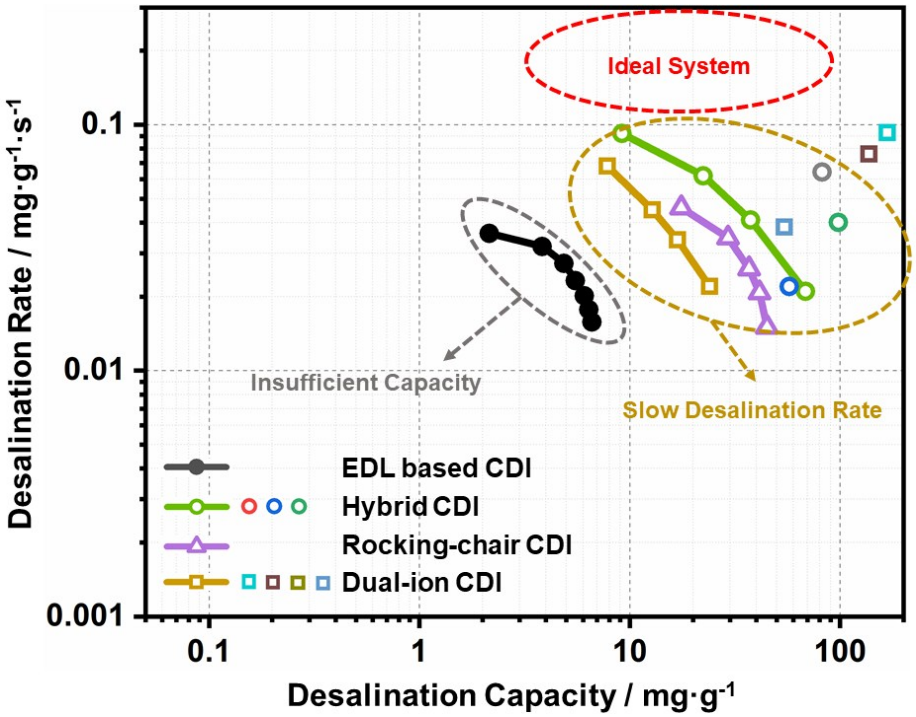

Fig. S1 Desalination capacities and rates of typical material systems from literatures (See Table S1 for detailed information).

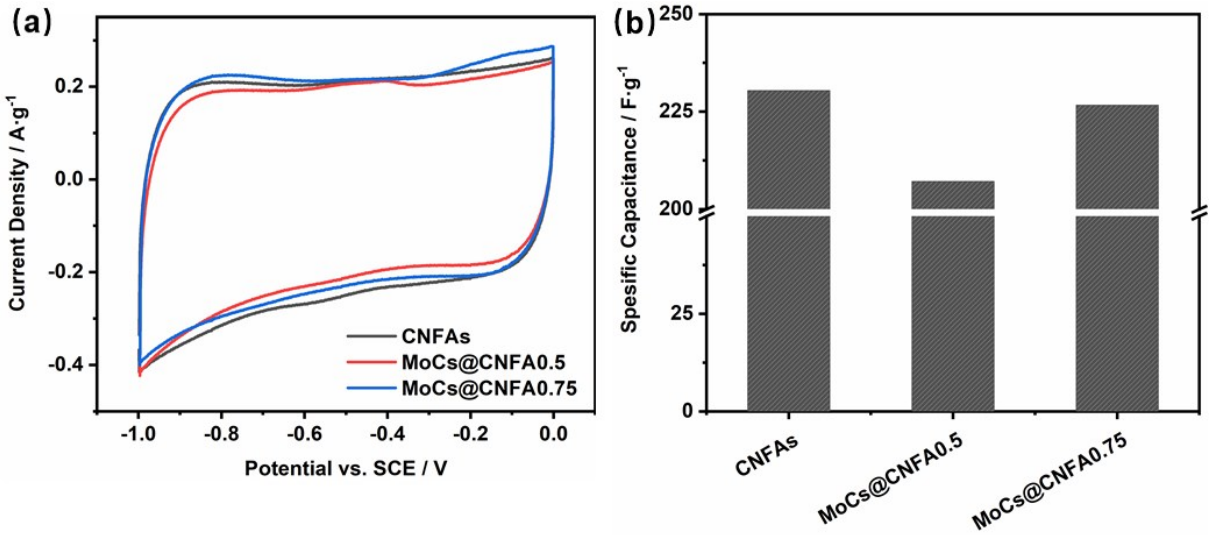

Fig. S2 (a) CV curves and (b) specific capacitance of CNFAs, MoCs@CNFA0.5, MoCs@CNFA0.75 in 1M NaCl solution;

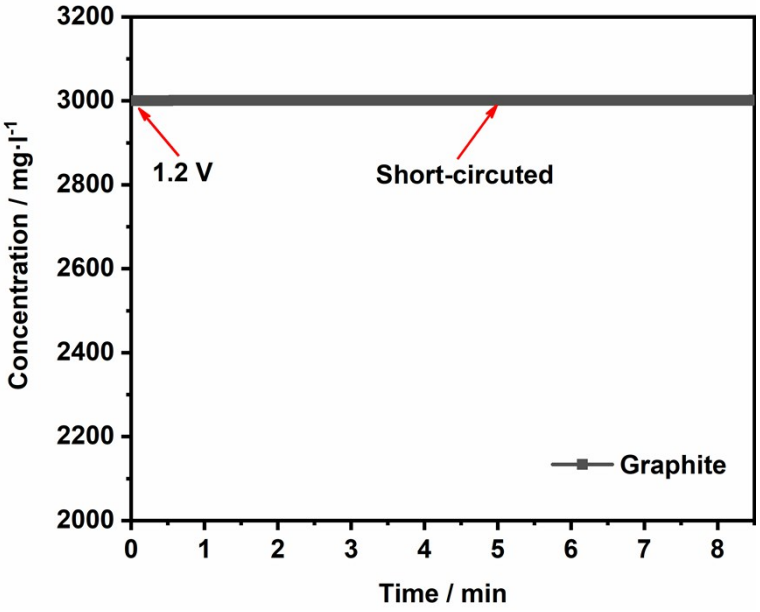

Fig. S3 Concentration transients for bare graphite electrodes at 1.2 V in NaCl solution with a feeding concentration of 3000 mg·L^{-1}.

Table S1 Comparison of the desalination capacities and rates performance among various carbon, pseudo-capacitive, and faradic electrode materials reported in the literature.

Electrode Material	Cell design	Cycling Mode	Power Mode	Voltage/Current	C_0 ($mg \cdot l^{-1}$)	SDC ($mg \cdot g^{-1}$)	ADR ($mg \cdot g^{-1} \cdot s^{-1}$)	Ref.
Porous carbon	CDI	B.M.	C.V.	1.2 V/-	50	2.2	0.0360	[1]
		B.M.	C.V.	1.2 V/-	50	6.6	0.0160	
$Na_2FeP_2O_7$	HCDI	B.M.	C.V.	1.2 V/-	584.4	30.2	0.0810	[2]
		B.M.	C.V.	1.2 V/-	5844.0	32.6	0.1430	
		B.M.	C.C.	1.2 V/3.0 $mA \cdot cm^{-2}$	584.4	7.8	0.0680	
		B.M.	C.C.	1.2 V/2.0 $mA \cdot cm^{-2}$	584.4	12.8	0.0450	
		B.M.	C.C.	1.2 V/1.5 $mA \cdot cm^{-2}$	584.4	16.9	0.0340	
		B.M.	C.C.	1.2 V/1.0 $mA \cdot cm^{-2}$	584.4	24.0	0.0220	
		B.M.	C.C.	1.2 V/3.0 $mA \cdot cm^{-2}$	5844.0	20.6	0.0688	
		B.M.	C.C.	1.2 V/2.0 $mA \cdot cm^{-2}$	5844.0	26.2	0.0458	
		B.M.	C.C.	1.2 V/1.5 $mA \cdot cm^{-2}$	5844.0	29.0	0.0344	
		B.M.	C.C.	1.2 V/1.0 $mA \cdot cm^{-2}$	5844.0	34.0	0.0230	
$Na_3V_2(PO_4)_3$@C	HCDI	B.M.	C.V.	1.0 V/-	5844.0	137.2	0.0760	[3]
PNDIE	HCDI	B.M.	C.V.	1.8 V /-	1000.0	54.20	0.0383	[4]
MOFs-derived $NaTi_2(PO_4)_3$/C	HCDI	B.M.	C.V.	1.8 V /-	1000.0	167.40	0.0930	[5]
Nafion-coated activated carbon	RCDI	B.M.	C.C.	1.2 V/1.0 $mA \cdot cm^{-2}$	584.4	23.30	0.0294	[6]
		B.M.	C.C.	1.2 V/1.25 $mA \cdot cm^{-2}$	584.4	29.90	0.0251	
		B.M.	C.C.	1.2 V/1.5 $mA \cdot cm^{-2}$	584.4	35.00	0.0200	
		B.M.	C.C.	1.2 V/1.0 $mA \cdot cm^{-2}$	1168.8	19.10	0.0378	
		B.M.	C.C.	1.2 V/1.25 $mA \cdot cm^{-2}$	1168.8	25.90	0.0313	
		B.M.	C.C.	1.2 V/1.5 $mA \cdot cm^{-2}$	1168.8	30.40	0.0270	
		B.M.	C.C.	1.2 V/2.0 $mA \cdot cm^{-2}$	1168.8	35.60	0.0216	
		B.M.	C.C.	1.2 V/1.0 $mA \cdot cm^{-2}$	2922.0	17.50	0.0462	
		B.M.	C.C.	1.2 V/1.25 $mA \cdot cm^{-2}$	2922.0	29.10	0.0345	
		B.M.	C.C.	1.2 V/1.5 $mA \cdot cm^{-2}$	2922.0	36.70	0.0262	
		B.M.	C.C.	1.2 V/2.0 $mA \cdot cm^{-2}$	2922.0	41.10	0.0207	
		B.M.	C.C.	1.2 V/3.0 $mA \cdot cm^{-2}$	2922.0	44.50	0.0151	

AgCl-$Na_{0.44}MnO_2$	DEDI	B.M.	C.C.	1.5 V /100 mA g^{-1}	890.0	57.40	0.0220	[7]
		B.M.	C.C.	1.5 V /200 mA g^{-1}	890.0	34.70	—	
		B.M.	C.C.	1.5 V /300 mA g^{-1}	890.0	27.20	—	
		B.M.	C.C.	1.5 V /500 mA g^{-1}	890.0	24.80	—	
		B.M.	C.C.	1.5 V /1000 mA g^{-1}	890.0	18.80	0.2090	
BiOCl-$Na_{0.44}MnO_2$	DEDI	B.M.	C.C.	1.5 V /100 mA g^{-1}	760.0	68.50	0.0210	[8]
		B.M.	C.C.	1.5 V /200 mA g^{-1}	760.0	37.5	0.0410	
		B.M.	C.C.	1.5 V /300 mA g^{-1}	760.0	22.40	0.0620	
		B.M.	C.C.	1.5 V /500 mA g^{-1}	760.0	9.20	0.0920	
$NaTi_2(PO_4)_3$-Ag nano-particles	DEDI	B.M.	C.C.	1.4 V /100 mA g^{-1}	2500.0	105.00	—	[9]
		B.M.	C.C.	1.4 V /200 mA g^{-1}	2500.0	77.00	—	
		B.M.	C.C.	1.4 V /300 mA g^{-1}	2500.0	50.00	—	
		B.M.	C.C.	1.4 V /500 mA g^{-1}	2500.0	26.00	—	
		B.M.	C.C.	1.4 V /1000 mA g^{-1}	2500.0	15.00	—	
Na3V2(PO4)3@C-AgCl	DEDI	B.M.	C.C.	1.4 V /100 mA g^{-1}	1000.0	98.00	0.0400	[10]
		B.M.	C.C.	1.4 V /500 mA g^{-1}	1000.0	34.0	0.3140	
$Na_3V_2(PO_4)_3$-rGO aerogel	DEDI	B.M.	C.C.	1.4 V /100 mA g^{-1}	1000.0	103.75	—	[11]
		B.M.	C.C.	1.4 V /150 mA g^{-1}	1000.0	79.17	—	
		B.M.	C.C.	1.4 V /200 mA g^{-1}	1000.0	63.33	—	
		B.M.	C.C.	1.4 V /300 mA g^{-1}	1000.0	39.17	0.0940	

*The abbreviations in Table S1 are listed as follow:

SDC: specific desalination capacity; C_0: initial concentration; ADR: average desalination rate; B.M.: batch mode; S.P.: single-pass mode; C.C.: constant current; C.V.: constant voltage; RCDI: rocking-chair CDI; DEDI: dual-ion electrochemical desalination.

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