

## Supplementary materials

### $V_2CT_x$ -MXene Partially Derived Hybrid $VS_2/V_2CT_x$

### Electrode for Capacitive Deionization with Exceptional Rate and Capacity

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The salt adsorption capacity (SAC, mg·g<sup>-1</sup>) was obtained by the following equation:

$$SAC = \frac{(C_0 - C_t) \times V}{m} \quad (S1)$$

where  $C_0$  and  $C_t$  represent the concentrations of NaCl at the initial stage and  $t$  min (mg L<sup>-1</sup>), respectively;  $V$  stands for the volume of the NaCl solution (L); and  $m$  is the overall mass of the active material (g).

In addition, the salt removal rate (SRR, mg·g<sup>-1</sup>·min<sup>-1</sup>) could be determined by the following equation:

$$SRR = \frac{SAC}{t} \quad (S2)$$

among them,  $t$  (s) refers to the Charging time.

The energy consumption (EC, kw·h·kg<sup>-1</sup>-NaCl) could be calculated by the following equation:

$$EC = \frac{J \times m \times \int_{t_0}^{t_e} u dt}{3600 \times (C_0 - C_e) \times V} \quad (S3)$$

where  $J$  refers to the set current density (mA·g<sup>-1</sup>),  $m$  refers to the mass of the electrode active material (g),  $t_0$  is the time (s) at the start of a given cycle of desalination,  $t_e$  is the time (s) at the end of a given cycle of desalination,  $u$  refers to the voltage (V),  $C_e$  represents the NaCl concentration at the end of the desalination stage and  $dt$  is measured in seconds.

In the EQCM behavior, the variation of resonance width  $\Delta W_n/n$  is obtained by converting the dissipation factor:

$$\frac{\Delta W_n}{n} = f_0 \times \frac{\Delta D_n}{n} \quad (S4)$$

among them,  $f_0$  is the fundamental frequency of the quartz wafer (5 MHz) when the sample is not loaded,  $n = 1, 3, 5, 7, 9, 11, 13$ .

When the deposited film is rigid, the bandwidth of the standing wave does not increase, so the relationship between the film mass ( $\Delta m$ ) and the corresponding resonant frequency can be expressed by the classical Sauerbrey equation[1]:

$$\Delta m = -C \times \frac{\Delta f}{n} \quad (\text{S5})$$

where C is the mass sensitivity constant ( $C = \sqrt{\mu_q \times \rho_q}$ ),  $\mu_q$  and  $\rho_q$  are the elastic shear modulus and density. For a crystal with  $f_0 = 5$  MHz,  $C = 17.7 \text{ ng} \cdot \text{cm}^{-2} \cdot \text{Hz}^{-1}$ .

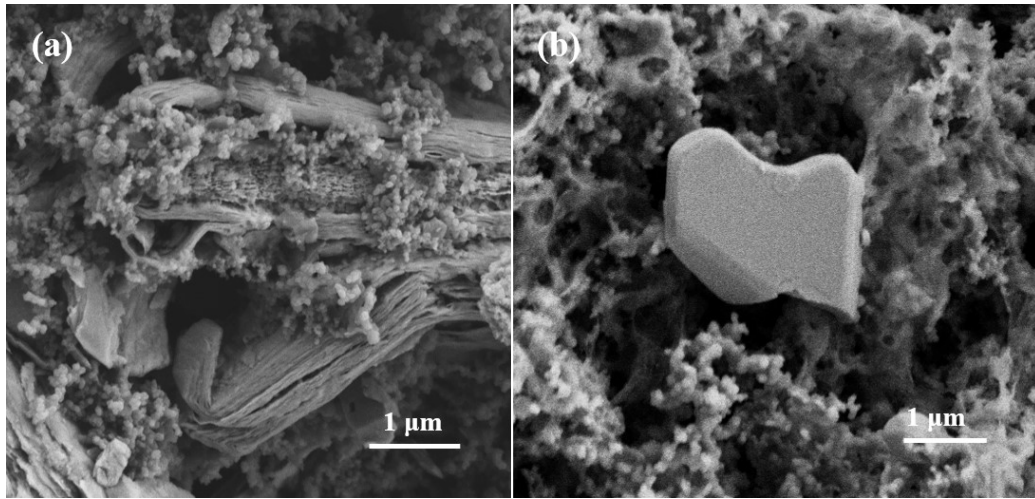


Figure S1. (a) SEM image of VS<sub>2</sub>/V<sub>2</sub>CT<sub>x</sub> film before 60-cycle of CDI desalination; (b) SEM image of VS<sub>2</sub>/V<sub>2</sub>CT<sub>x</sub> film after 60-cycle of CDI desalination.

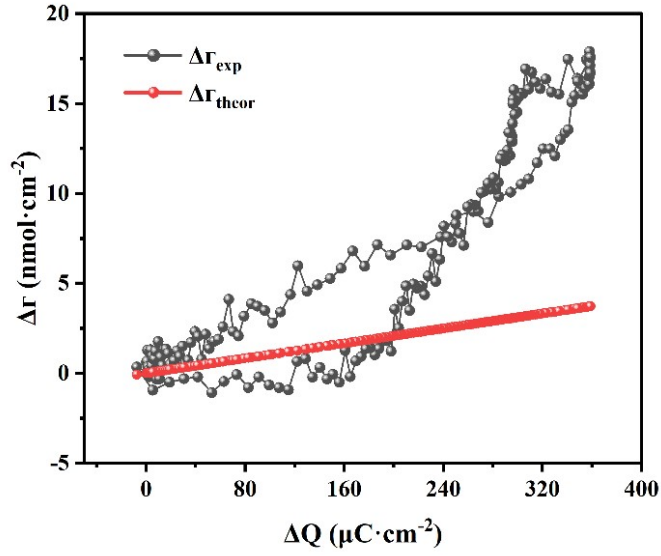


Figure S2. The theoretical and experimental ion population changes ( $\Delta\Gamma$ ) as a function of charge density ( $\Delta Q$ ) during charging and discharging process ( $n = 3$ , scan rate =  $0.03 \text{ V}\cdot\text{s}^{-1}$ ).

The experimental ion population change ( $\Delta\Gamma_{\text{exp}}$ ) can calculate by the following equation:

$$\Delta\Gamma_{\text{exp}} = \frac{\Delta m}{M_i} \quad (\text{S6})$$

where  $\Delta m$  is the mass change, and the molecular mass  $M_i$  of  $\text{Na}^+$  is  $23 \text{ g}\cdot\text{mol}^{-1}$ . The theoretical ion population change ( $\Delta\Gamma_{\text{theor}}$ ) can calculate with the adoption of Faraday's law:

$$\Delta\Gamma_{\text{theor}} = \frac{\Delta Q}{nF} \quad (\text{S7})$$

where  $\Delta Q$  is the charge passed through the electrode (C),  $n$  is the valence number of the ion ( $n=1$ ), and  $F$  is the Faraday constant ( $96485 \text{ C}\cdot\text{mol}^{-1}$ ).

Table 1. Evaluation and ranking of the operating parameters using TOPSIS-Entropy weight model

Parameters	D <sup>+</sup>	D <sup>-</sup>	Normalized score	Rank
IC-100	0.33	0	0	4
IC-300	0.01	0.33	0.5221	1
IC-500	0.24	0.12	0.1769	3
IC-700	0.15	0.19	0.3009	2
CD-40	0.12	0.15	0.2424	3
CD-50	0.06	0.22	0.3398	2
CD-60	0.05	0.20	0.3399	1
CD-70	0.24	0.003	0.0778	4
CFV-1.2	0.14	0.35	0.3895	2
CFV-1.4	0.09	0.32	0.4306	1
CFV-1.6	0.35	0.14	0.1799	3

## References

- [1] G. Sauerbrey, Use of a Quartz Vibrator for Weighing Thin Films on a Microbalance, *Eur. Phys. J. A*, 155 (2) (1959) 206–222.