Note S1 | Equivalent circuit model and impedance derivation for MXene EIS analysis

To interpret the electrochemical impedance response of the MXene electrode, we employed an equivalent circuit that captures (i) ohmic contributions from the cell and current collectors, (ii) inductive artifacts at high frequency, (iii) interfacial charge-transfer kinetics combined with non-ideal double-layer behavior, and (iv) additional distributed capacitive/pseudocapacitive storage at lower frequencies. The circuit used throughout this work is:

$$Z(\omega) = R_s + j\omega L + (R_{ct} \parallel CPE_1) + CPE_2 \tag{S1}$$

with the seven fitting parameters $\theta = \{R_s, L, R_{ct}, Q_1, \alpha_1, Q_2, \alpha_2\}$. Here, R_s represents the uncompensated series resistance (electrolyte ionic resistance, current collector/contact resistance), and L accounts for wiring/lead inductance that can dominate the phase response at the highest frequencies. The interfacial charge-transfer resistance R_{ct} is modeled in parallel with CPE_1, which describes the non-ideal electrical double layer at the MXene/electrolyte interface arising from surface heterogeneity, roughness, and a distribution of relaxation times. Finally, CPE_2 is included as an additional constant phase element to capture broader low-frequency dispersive storage and/or pseudocapacitive processes (e.g., termination-mediated surface redox and ion adsorption in a porous/lamellar network), which cannot be represented adequately by a single ideal capacitor.

A constant phase element is defined by:

$$Z_{CPE}(\omega) = \frac{1}{Q(j\omega)^{\alpha}} \tag{S2}$$

where Q is the pseudo-capacitance prefactor and $0 < \alpha \leq 1$ is the dispersion exponent. For $\alpha = 1$, the element reduces to an ideal capacitor $C = Q$ with $Z_C = 1/(j\omega C)$. Values of $\alpha < 1$ quantify deviation from ideality; smaller α indicates stronger heterogeneity and a broader distribution of relaxation times.

The impedance of the charge-transfer branch is obtained by combining R_{ct} with CPE_1 in parallel:

$$Z_{ct\|CPE_1}(\omega) = \left(\frac{1}{R_{ct}} + \frac{1}{Z_{CPE_1}}\right)^{-1} = \left(\frac{1}{R_{ct}} + Q_1(j\omega)^{\alpha_1}\right)^{-1} \tag{S3}$$

The full model thus becomes:

$$Z(\omega) = R_s + j\omega L + \frac{1}{\left(\frac{1}{R_{ct}}+Q_1(j\omega)^{\alpha_1}\right)} + \frac{1}{Q_2(j\omega)^{\alpha_2}} \tag{S4}$$

This form provides clear limiting behaviors that connect the fitted parameters to physical frequency regimes. At sufficiently high frequency, $|Z_{CPE_1}|$ and $|Z_{CPE_2}|$ decrease, and the response approaches $Z(\omega) = R_s + j\omega L$, producing a near-vertical inductive phase lead if L is appreciable. In the mid-frequency range where the interfacial branch dominates, the parallel combination yields a depressed semicircle (or arc) in the Nyquist plane; its diameter is governed primarily by R_{ct}, while the arc depression and constant phase rotation are determined by $(Q_1,\ \alpha_1)$. At lower frequencies, CPE_2 contributes a dispersive tail with phase $-\alpha_2\pi/2$, consistent with distributed capacitive/pseudocapacitive storage.

All fitting was performed in the complex domain by minimizing the total squared error between the measured and modeled impedance:

$$SSE = \sum_{k=1}^{N}|Z_{model}(\omega_k;\theta) - Z_{data}(\omega_k;\theta)|^2 \tag{S5}$$

equivalently summing squared residuals of $\Re(Z)$ and $\Im(Z)$ across all frequencies. This objective ensures that both magnitude and phase information constrain θ simultaneously and supports direct overlay comparisons in Nyquist and Bode representations.