

**Figure 1 | Classical baseline EIS fit used as the anchor for all optimization branches.** (a) Nyquist plot ( $Z'$  vs.  $-Z''$ ) of the MXene electrode impedance, comparing the experimental data (symbols) with the best-fit response (solid line) obtained from the classical nonlinear least-squares fit of the equivalent circuit  $Z(\omega) = R_s + j\omega L + (R_{ct} \parallel CPE_1) + CPE_2$ . (b) Bode magnitude  $|Z|$  and (c) Bode phase as functions of frequency, showing that the same parameter set  $\theta = \{R_s, L, R_{ct}, Q_1, \alpha_1, Q_2, \alpha_2\}$  simultaneously reproduces both amplitude and phase across the full measurement window. This classical solution  $\theta^*$  defines the reference baseline and decoding anchor used to (i) initialize the continuous VQE/VQA branch and (ii) build the local quadratic surrogate and trust-region discretization for the QUBO/QAOA branch, enabling direct, like-for-like comparisons of quantum and classical results.

