

**Figure 3 | Spectral overlays comparing classical and quantum-derived EIS fits for the same MXene circuit model.** (a) Nyquist representation ( $Z'$  vs.  $-Z''$ ) and (b) Bode magnitude  $|Z|$  and (c) Bode phase versus frequency for the MXene electrode, showing the experimental data (symbols) overlaid with impedance predictions from three parameter-estimation routes using an identical circuit topology  $Z(\omega) = R_s + j\omega L + (R_{ct} \parallel CPE_1) + CPE_2$ . The classical nonlinear least-squares baseline (orange) provides the reference  $\theta^*$ . The VQE/VQA continuous branch (green) uses a 7-qubit HEA ansatz with bounded decoding to infer  $\theta$  directly by minimizing the complex-domain loss. The QAOA discrete branch (red) solves a 21-qubit (3-bit  $\times$  7-parameter) surrogate QUBO/Ising instance with  $p=1$  QAOA and decodes the best-shot bitstring (trust-region  $\Delta=0.08$ ) to obtain  $\theta$ . Across Nyquist,  $|Z|$ , and phase spectra, the quantum branches reproduce the measured response with comparable fidelity to the classical fit, demonstrating that both continuous and discrete quantum inference pipelines can recover physically consistent MXene EIS parameters within the same model class.

