Note S3 | Parameter bounds and bounded decoding (Table S1)

To ensure physically meaningful impedance fits and to stabilize both the classical and quantum optimization branches, all circuit parameters were constrained to predefined bounds and accessed through a *bounded decoding* map. The MXene EIS model uses seven parameters: $\theta = \{R_s, L, R_{ct}, Q_1, \alpha_1, Q_2, \alpha_2\}$ in the equivalent circuit $Z(\omega)$ (**Note S1**). Each parameter has a clear physical interpretation and admissible range. The purpose of **Table S1** is therefore twofold: (i) to define *physically plausible* ranges that prevent non-sense solutions (e.g., negative resistances, $\alpha > 1$), and (ii) to provide a single, consistent decoding rule used by all solvers (classical NLLS, VQE/VQA, and QAOA).

S3.1 Motivation for bounded domains.

EIS fitting for heterogeneous electrodes is often ill-conditioned because multiple parameter combinations can produce nearly indistinguishable spectra, particularly when constant phase elements are used. Unbounded optimization can drift into extreme values (e.g., $Q \to 0$ with compensatory shifts in α and R_{ct}), which yields good numerical SSE but violates electrochemical meaning. Bounding controls such degeneracies, improves convergence, and makes solver outputs comparable. We therefore enforce $R_s > 0$, $R_{ct} > 0$, $L \geq 0$, $Q_{1,2} > 0$, and $0 < \alpha_{1,2} \leq 1$. For parameters spanning orders of magnitude (L, Q_1, Q_2), bounds are specified on a log scale to avoid biasing the search toward large values.

S3.2 Normalized solver coordinates and decoding.

All optimizers operate on a normalized coordinate vector $u \in [0,1]^7$, which is mapped into physical parameters θ through a deterministic decoding:

1. Linear decoding (for $R_s, R_{ct}, \alpha_1, \alpha_2$)

$$p(u) = p_{min} + u\,(p_{max} - p_{min}) \tag{S10}$$

2. Log decoding (for L, Q_1, Q_2)

$$p(u) = 10^{log_{10}(p_{min})+u[log_{10}(p_{max})-log_{10}(p_{min})]} \quad \text{(S11)}$$

This mixed linear/log strategy makes the normalized space approximately "balanced" across parameters with different natural scales and ensures that a uniform step in u corresponds to a comparable *relative* change for log-scale parameters.

In the VQE/VQA continuous branch, each qubit encodes a continuous latent variable that is decoded into u (and then into θ). Practically, the VQA optimizer updates a real-valued parameter vector that is clipped to $[0,1]$ at every iteration, ensuring feasibility by construction. (When desired, the same feasibility can be enforced smoothly via a logistic map $u = \sigma(\phi) = 1/(1 + e^{-\phi})$, which avoids hard clipping while guaranteeing $u \in (0,1)$.)

S3.3 Discrete (QAOA/QUBO) encoding with local trust region.

In the QAOA branch, each parameter is discretized with **3 bits** (8 levels), giving 21 binary variables total. The bitstring is first converted to a level $s_i \in \{0,1/7, \dots,1\}$ for each parameter. To avoid global discretization artifacts and to keep the QUBO surrogate valid, we apply a local trust-region decoding around a classical baseline u_o:

$$u_i = clip(u_{0,i} + \Delta\,(2s_i - 1) \quad \text{(S12)}$$

with $\Delta = 0.08$ used in this study. This rule restricts the discrete search to a controlled hypercube around the baseline (i.e., a local surrogate neighborhood), improving both interpretability and identifiability while keeping decoded parameters strictly within Table S1 bounds. After decoding u, the same linear/log maps above are applied to obtain θ.

S3.4 Practical implications.

Because all solvers share the *same* bound set and decoding rules (**Table S1**), differences among (classical / VQE–VQA / QAOA) results reflect algorithmic behavior rather than inconsistent parameter domains. Moreover, bounded decoding supports robust uncertainty analyses: noise refits, basin-of-attraction tests, and identifiability metrics are all computed within the same feasible region, making comparisons and SI reproducibility straightforward.