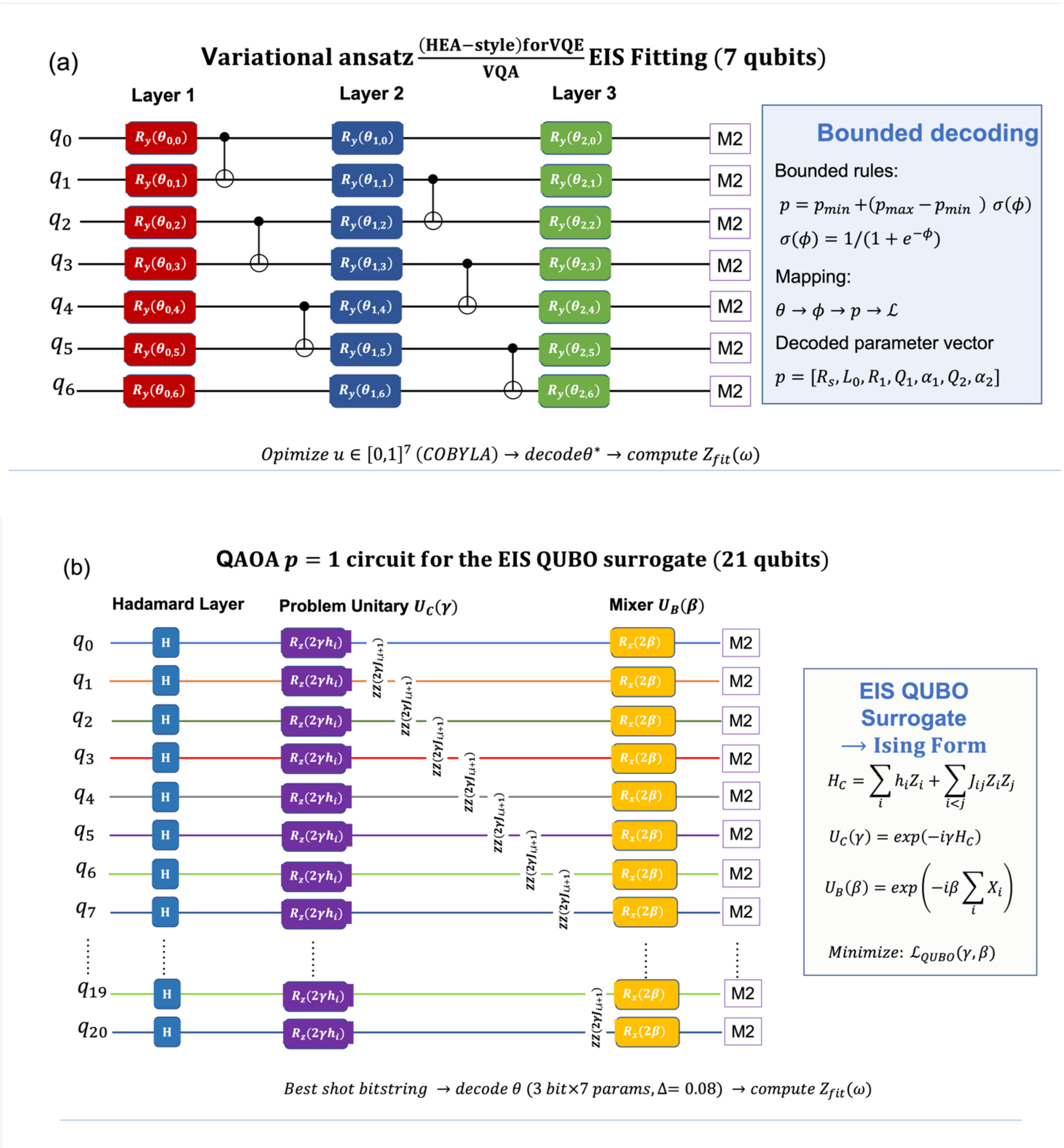
Figure 2 | Quantum inference architecture for MXene EIS parameter estimation. (a) **Continuous branch (VQE/VQA):** A 7-qubit hardware-efficient ansatz (HEA, three layers of parameterized R_y rotations with entangling links) encodes the seven circuit parameters $\theta = \{R_s, L, R_{ct}, Q_1, \alpha_1, Q_2, \alpha_2\}$. Measurement outcomes are mapped to normalized variables $u \in [0,1]^7$ and converted to physical parameters via the bounded decoding rule $p = p_{min} + (p_{max} - p_{min})\sigma(\phi)$ (and the linear/log maps defined in Table S1), ensuring feasibility ($R > 0,\ 0 < \alpha \leq 1$) throughout optimization. A derivative-free COBYLA loop updates the ansatz angles using shot-based evaluations (4096 shots) to minimize the complex-domain EIS loss, yielding a decoded θ^* used to compute $Z_{fit}(\omega)$. (b) Discrete branch (QAOA/QUBO): A local quadratic surrogate of the classical EIS objective is discretized using 3 bits per parameter (21 qubits total) and mapped to an Ising Hamiltonian $H_C = \sum_i h_i Z_i + \sum_{i<j} J_{ij} Z_i Z_j$. The $p = 1$ QAOA circuit prepares $|+\rangle^{\otimes 21}$, applies the problem unitary $U_C(\gamma) = exp\,(-i\gamma H_C)$ and mixer $U_B(\beta) = exp\,(-i\beta \sum_i X_i)$, and is sampled with 4096 shots. The most favorable measured bitstring is decoded (trust-region Δ=0.08 about the classical baseline and bounds in Table S1) to obtain θ, which is then used to generate the final EIS overlays.


(a)
Variational ansatz (HEA−style)forVQE / VQA EIS Fitting (7 qubits)
Layer 1
Layer 2
Layer 3
q_0 q_1 q_2 q_3 q_4 q_5 q_6
$R_y(\theta_{0,0})$ $R_y(\theta_{0,1})$ $R_y(\theta_{0,2})$ $R_y(\theta_{0,3})$ $R_y(\theta_{0,4})$ $R_y(\theta_{0,5})$ $R_y(\theta_{0,6})$
$R_y(\theta_{1,0})$ $R_y(\theta_{1,1})$ $R_y(\theta_{1,2})$ $R_y(\theta_{1,3})$ $R_y(\theta_{1,4})$ $R_y(\theta_{1,5})$ $R_y(\theta_{1,6})$
$R_y(\theta_{2,0})$ $R_y(\theta_{2,1})$ $R_y(\theta_{2,2})$ $R_y(\theta_{2,3})$ $R_y(\theta_{2,4})$ $R_y(\theta_{2,5})$ $R_y(\theta_{2,6})$
M2
Bounded decoding
Bounded rules:
$p = p_{min} + (p_{max} - p_{min})\ \sigma(\phi)$
$\sigma(\phi) = 1/(1+e^{-\phi})$
Mapping:
$\theta \to \phi \to p \to \mathcal{L}$
Decoded parameter vector
$p = [R_s, L_0, R_1, Q_1, \alpha_1, Q_2, \alpha_2]$
$Opimize\ u \in [0,1]^7\ (COBYLA) \to decode\theta^* \to compute\ Z_{fit}(\omega)$
(b)
QAOA $p = 1$ circuit for the EIS QUBO surrogate (21 qubits)
Hadamard Layer
Problem Unitary $U_C(\gamma)$
Mixer $U_B(\beta)$
q_0 q_1 q_2 q_3 q_4 q_5 q_6 q_7 q_{19} q_{20}
H
$R_z(2\gamma h_i)$
$ZZ(2\gamma J_{i,i+1})$
$R_x(2\beta)$
M2
EIS QUBO Surrogate ⟶ Ising Form
$H_C = \sum_i h_i Z_i + \sum_{i<j} J_{ij} Z_i Z_j$
$U_C(\gamma) = exp(-i\gamma H_C)$
$U_B(\beta) = exp\left(-i\beta \sum_i X_i\right)$
$Minimize:\ \mathcal{L}_{QUBO}(\gamma, \beta)$
$Best\ shot\ bitstring \to decode\ \theta\ (3\ bit{\times}7\ params, \Delta = 0.08) \to compute\ Z_{fit}(\omega)$