

**Table 5 | Quantum execution settings and decoding workflow for MXene EIS fitting.** Operational settings for each branch, including circuit form and depth (HEA-style ansatz with  $reps \approx 3$  for VQE/VQA; QAOA  $p = 1$  for the discrete branch), sampling budget (4096 shots), classical outer-loop strategy (COBYLA for continuous optimization; coarse-to-refined  $(\gamma, \beta)$  grid search with best-shot selection for QAOA), and the shared bounded decoding that maps either continuous outputs  $u \in [0,1]^7$  or discrete bitstrings to physically valid  $\theta$  using the same linear/log bounds.

Branch	Circuit / depth	Shots	Classical optimizer	Angle-search	Decoding	Notes
VQE/VQA (continuous)	HEA-style ansatz, reps≈3 (Ry layers + entanglers)	4096	COBYLA (bounded in $u \in [0,1]^7$ )	—	$u \rightarrow \theta$ via bounds (linear/log). Optional logistic bounded map to enforce $[l_b, u_b]$	Direct fit against $Z(\omega)$ ; evaluates full circuit model each iteration
QAOA (discrete)	QAOA $p = 1: H - layer \rightarrow U_C(\gamma) \rightarrow U_B(\beta) \rightarrow measure$	4096	Grid search (angles) + best-shot decode	Coarse 5×5 $\gamma-\beta$ grid + refined 9×9 window (total 106 evals)	bitstring → $s = k/7 \rightarrow u = u_0 + \Delta(2s - 1) \rightarrow \theta$ via bounds (linear/log)	Ising $(h_i, J_{ij})$ from QUBO surrogate around classical baseline; final $\theta$ from best-shot