

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 (γ, β) 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 θ using the same linear/log bounds.

Branch	Circuit / depth	Shots	Classical optimizer	Angle-search	Decoding	Notes
VQE/VQA (continuous)	HEA-style ansatz, $reps \approx 3$ (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 γ - β grid + refined 9×9 window (total 106 evals)	bitstring $\rightarrow s = k/7 \rightarrow u = u_0 + \Delta(2s - 1) \rightarrow \theta$ via bounds (linear/log)	Ising (h_i, J_{ij}) from QUBO surrogate around classical baseline; final θ from best-shot