

Figure 4 | Surrogate construction, discretization, and QAOA landscape for the discrete MXene EIS inference branch. (a) Local quadratic surrogate slice of the complex-domain objective (SSE) in the normalized parameter coordinates u for a representative two-parameter subspace (here illustrated for the $(u_{R_{ct}}, u_{Q_1})$ plane), centered about the classical baseline u^* . The colormap shows the surrogate-predicted SSE, while the overlaid 3-bit grid indicates the discrete levels used in the QUBO encoding (3 bits per parameter). The continuous VQE/VQA trajectory (smooth path) and the discrete QAOA candidate states (quantized hops) are shown to highlight how both branches explore the same bounded neighborhood but with different search granularity. (b) Coarse (γ, β) landscape for the $p = 1$ QAOA energy $\langle H \rangle$ of the Ising cost Hamiltonian derived from the surrogate QUBO, used to locate the optimal basin for angle selection. (c) Refined (γ, β) landscape (tight window centered on the best coarse cell) used to pinpoint the optimum angles (γ^*, β^*) for the final QAOA sampling (shots = 4096) and best-shot decoding. (d) Surrogate fidelity diagnostic comparing the quadratic surrogate predictions against the true complex-domain SSE evaluated from the full circuit model over the sampled neighborhood, demonstrating that the surrogate preserves the local ordering and curvature needed for reliable QUBO/QAOA optimization.

