Note S7 | Code + data availability

To support full reproducibility of the MXene EIS fitting workflow, we provide (i) the raw impedance dataset, (ii) processed fit outputs, and (iii) the analysis scripts required to regenerate all main-text and Supporting Information figures/tables. The dataset includes the measured frequency vector f and complex impedance $Z(\omega) = Z'(\omega) + jZ''(\omega)$, together with the fitted impedance curves, residuals, and derived artifacts used for the quantum branch (QUBO/Ising coefficients and decoding maps). All numerical outputs are stored in non-proprietary formats (CSV/TXT) to facilitate reuse across platforms.

S7.1 Data availability. The raw EIS data for the MXene electrode are provided as a single CSV file containing frequency (Hz), real impedance $Z'(\Omega)$, and imaginary impedance $Z''(\Omega)$. Processed data products include: (i) classical NLLS fitted parameters and fitted $Z_{fit}(\omega)$, (ii) complex-domain residuals and normalized residuals, (iii) bounded parameter ranges and decoding map (**Table S1**), (iv) QUBO and Ising coefficient lists (h_i, J_{ij}) for QAOA, (v) $\gamma-\beta$ energy landscape grids (coarse and refined), and (vi) robustness/identifiability replicate outputs (noise refits, parameter clouds, and correlation matrices). These files are deposited in a public repository (e.g., Figshare/Zenodo) under a DOI at publication time: **DOI: [to be inserted upon acceptance]**. The repository also contains a "manifest" file listing each artifact, its format, and the figure/table it reproduces.

S7.2 Code availability. All scripts used for EIS fitting, quantum encoding, and figure/table generation are released under an open-source license (MIT/BSD-3 recommended for broad reuse) in a public version-controlled repository (e.g., GitHub) with a permanent archive snapshot (Zenodo DOI) at publication time. The release includes: (i) a requirements.txt or environment.yml specifying package versions, (ii) a single-entry run_all.py pipeline that reproduces all figures/tables from raw data, and (iii) modular functions for the circuit model, bounded decoding, and QAOA utilities. A commit hash and tagged release (e.g., v1.0.0) will be referenced in the paper to guarantee exact provenance: **Code version: [tag + commit hash]**.

S7.3 Reproducibility notes. All random procedures (noise injection, random starts, QAOA sampling) are seeded and logged. Figures are generated at publication quality (vector PDF + 600 dpi PNG) with consistent axis formatting suitable for **Nano Energy**. The scripts are hardware-agnostic: they run on CPU-only environments, and quantum routines are implemented in a simulator-style form (p=1 QAOA via efficient transforms). Users may optionally replace the simulator with an actual quantum backend while keeping the same decoding and objective definitions.