

Platinum-based catalysts for oxygen reduction reaction simulated with a quantum computer

Portability dossier - app

agQSL portability pipeline

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Field	Value
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Paper: fetch failed, see `paper.url`

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1 Source

1.1 Domain classification

quantum chemistry (primary), with **materials** as the secondary axis. The workload is molecular active-space electronic-structure chemistry (VQE plus NEVPT2) applied to a fuel-cell electrocatalysis materials problem: the oxygen reduction reaction on pure Pt and Pt/Co surfaces. It sits on the chemistry/materials boundary, but the quantum-hardware fingerprint is chemistry (active spaces, reduced density matrices, dynamic correlation), so classify it chemistry-first.

1.2 Expert persona for Julien

A computational quantum chemist who works on transition-metal electrocatalysis and multireference embedding. They should be fluent in active-space selection (CASSCF/CASCI), strongly-contracted NEVPT2 for dynamic correlation, and periodic-DFT-to-cluster embedding for surface adsorbates. They need calibrated intuition for why a $(4e, 4o)$ / 8-qubit active space was chosen as the NISQ compromise, how n -particle RDMs measured on the QPU feed a classical NEVPT2 step (the QRDM-NEVPT2 scheme), and where the strong-correlation signal in the cobalt-bearing surface originates. Trapped-ion shot-budget and error-mitigation awareness helps, but the priority is judgement about the chemistry-modelling pipeline rather than device physics.

1.3 Related prior work (brief bibliography)

- Krompiec & Muñoz Ramo, “Strongly Contracted N-Electron Valence State Perturbation Theory Using Reduced Density Matrices from a Quantum Computer,” arXiv:2210.05702 (2022). The QRDM-NEVPT2 method (Quantinuum) that this paper applies; provenance of the exact dynamic-correlation primitive and the single most relevant prior work.
- Kandala et al., “Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets,” Nature 549, 242 (2017), arXiv:1704.05018. Same primitive (active-space VQE chemistry) on a different vendor (IBM superconducting); a portability anchor for the variational step.
- Google AI Quantum and Collaborators, “Hartree-Fock on a superconducting qubit quantum computer,” Science 369, 1084 (2020), arXiv:2004.04174. VQE-class chemistry run on superconducting hardware; a trapped-ion versus superconducting contrast for the same workload class.
- Robledo-Moreno et al., “Chemistry Beyond Exact Solutions on a Quantum-Centric Supercomputer,” Science Advances (2025), arXiv:2405.05068. Sample-based quantum diagonalisation on IBM Heron reaching far larger active spaces; the natural counterpoint to the $(4e, 4o)$ bottleneck here, and a different NISQ primitive for the same chemistry-scaling problem.
- “Quantum-centric strong and dynamical electron correlation: a resource-efficient second-order N-electron valence perturbation theory formulation for near-term quantum devices,” arXiv:2405.15422 (2024). A refined NEVPT2-on-quantum formulation; relevant to how the dynamic-correlation cost of this workflow scales across devices.

- Nørskov et al., “Origin of the Overpotential for Oxygen Reduction at a Fuel-Cell Cathode,” J. Phys. Chem. B 108, 17886 (2004), doi:10.1021/jp047349j(<https://doi.org/10.1021/jp047349j>). The canonical classical-DFT ORR thermodynamics baseline; the same application solved with classical methods, and the yardstick quantum has to beat.

1.4 Difficulty estimate

high.

- Length and SI reliance: 29-page main text plus a 10-page supplement (5 figures, 5 tables). The device-level specifics (which runs used the H1-1 hardware versus the H1-E noisy emulator, shot counts, error mitigation, the $(4e, 4o)$ active-space construction) live largely in the SI, so Julien needs it.
- Pipeline depth and an exotic primitive: the workflow stacks periodic DFT, cluster/active-space embedding, VQE on a trapped-ion QPU, and a classical QRDM-NEVPT2 post-processing step. The NEVPT2-from-quantum-RDMs primitive is non-standard and proprietary to Quantinuum, so the fingerprint extraction is more than a single-method read.
- Access: the Nature link is paywalled and currently redirects to [idp.nature.com](https://www.nature.com); the bootstrap PDF fetch already failed (see [paper.url](#)). The open-access arXiv preprint [2307.15823](https://arxiv.org/abs/2307.15823) carries the full method and supplement.

Action for the triager: attach the arXiv PDF (2307.15823) and its SI to this folder before Julien runs, since [paper.url](#) does not resolve to readable content. A Publisher Correction (npj Comput. Mater., [s41524-025-01513-9](#), Jan 2026) only added missing author affiliations and changes none of the science.

2 Extraction

2.1 What the paper does (one paragraph)

The paper studies the rate-determining $\text{O}_2 \longrightarrow 2\text{O}$ dissociation step of the oxygen reduction reaction (ORR) on two fuel-cell cathode catalysts: pure platinum and platinum-capped cobalt (Pt/Co). It builds a hybrid quantum-classical workflow that (i) relaxes periodic slab models with plane-wave DFT and locates transition states with the nudged elastic band method, (ii) cuts a finite cluster fragment around the adsorption site and uses an AVAS / Regional-Embedding procedure to pick a small active space, (iii) runs a variational quantum eigensolver (adaptive/ADAPT-VQE) on that active space to capture static correlation and to measure the reduced density matrices, and (iv) feeds those RDMs into a classical strongly-contracted NEVPT2 step (Quantinuum’s proprietary QRDM-NEVPT2) to recover dynamical correlation. The pure-Pt case is run on Quantinuum H1-series trapped-ion hardware; the Pt/Co case is run on the H1 noisy emulator. The headline finding is that Pt/Co is strongly correlated (large active spaces are needed), flagging it as a future quantum-advantage candidate.

2.2 Quantum hardware used

- **Vendor / machine:** Quantinuum H1-series (trapped-ion). Real-device runs are labelled “H1 quantum hardware / H1 device”; the noisy emulator is named “H1-E”, and the Methods identify it specifically as the **H1-2E** emulator (emulator of the H1-2 machine). Pure-Pt results use the physical H1 device; Pt/Co results use **only the H1-E (H1-2E) noisy emulator** (main text, “Oxygen dissociation on platinum and cobalt catalyst”, and Methods, “Multireference VQE calculations”).
- **Qubit count:** 6 qubits used for pure Pt (active space $(2e, 3o)$); 8 qubits used for Pt/Co (active space $(4e, 4o)$) (main text, “Embedding scheme” section, and Pt/Co section). Number of qubits *available* on the H1 device is not stated in the paper (H1-series machines carry 20 qubits per the vendor spec; not a paper number).
- **Connectivity:** Not stated in the paper. Substrate property of the H1-series QCCD architecture: all-to-all within the ion chain (see `vendor-notes/trapped_ion_qubits.tex`). Flagged here only as a sanity-check, not as a paper-reported value.
- **Gate set:** Not stated in the paper. Circuits were compiled through TKET / pyTKET (Methods). H1-series native basis is arbitrary-angle single-qubit rotations plus one Mølmer–Sørensen-type two-qubit entangler (arbitrary-angle $R_{ZZ}(\theta)$ / $R_{XX}(\theta)$); again from the substrate note, not from the paper.
- **Notable features leveraged:** Partition Measurement Symmetry Verification (PMSV) error mitigation applied before measurement to suppress particle-number and spin-parity symmetry breaking (main text, “Embedding scheme”; all H1/H1-E numbers in SI Tables S1–S2 include PMSV). Pauli terms grouped into mutually commuting measurement sets. Measurement of reduced density matrices up to **4th particle order** (n -particle RDMs) for the classical NEVPT2 post-step (Fig. 2 caption). The paper does **not** claim use of mid-circuit measurement or dynamic circuits.

2.3 Computational primitive

VQE, specifically adaptive VQE (Fermionic ADAPT-VQE) building on a ($k=1$)-UpCCGSD generalised unitary coupled-cluster ansatz, used both to variationally minimise the active-space energy and to measure the RDMs. A classical strongly-contracted NEVPT2 correction (QRDM-NEVPT2) is layered on top as post-processing. (The paper positions quantum phase estimation as a future fault-tolerant alternative, but QPE is **not** used here.)

2.4 Resource fingerprint

Two distinct experiments are reported; values are given as **pure Pt** | **Pt/Co** where they differ.

Metric	Value	Source (page / equation / SI)
Qubits (logical)	6 (Pt, (2e, 3o)) 8 (Pt/Co, (4e, 4o))	Main text, “Embedding scheme” para; Pt/Co section (“required 8 qubit circuits”)
Qubits (physical)	not reported (trapped-ion; no physical-vs-logical distinction given; no device qubit budget stated)	not applicable
Circuit depth	not reported (ADAPT-VQE stated to give “moderate circuit depth”; no number)	Main text, “Embedding scheme” para
2Q-gate count (total)	not reported	not applicable
Measurement shots	Pt on H1 hardware: 10k shots \times 10 batches (bootstrap). Pt on H1-E emulator: 100k shots \times 10 batches. Pt/Co on H1-E emulator: 5 runs \times 10k shots	Fig. 3 caption (H1, 10k \times 10); SI Tab. S1/S2 captions (100k H1-E, 10k H1); main text Pt/Co section (5 runs of 10k)
Classical loop iter.	not reported (no VQE optimiser iteration count or ADAPT operator-count given)	not applicable
Wall-clock runtime	not reported	not applicable

Supporting per-run counts also reported: number of commuting-Pauli measurement circuits for the energy = **12 (pure Pt)** and **19 (Pt/Co)** (main text, “Embedding scheme” para).

2.5 Assumptions and results

- **What was claimed.** The hybrid DFT \rightarrow embedding \rightarrow VQE \rightarrow QRDM-NEVPT2 workflow is feasible end-to-end on H1-series hardware for a realistic electrocatalysis problem. For pure Pt, the $\text{O}_2 \longrightarrow 2\text{O}$ reaction is dominated by *dynamical* correlation

(recovered classically by NEVPT2), with static correlation nearly negligible; H1 hardware reproduces the statevector closely. For Pt/Co, *static* correlation is strong: relative-stability ordering only converges with large active spaces, so it is proposed as a future quantum-advantage candidate.

- **Key numbers.** Pure Pt: DFT/NEB activation $E_a = 0.69$ eV (literature 0.67 ± 0.33 eV); DFT isomer gap $E^{\text{trans}} - E^{\text{cis}} = -0.17$ eV. H1-hardware-vs-statevector deviations $\Delta(E_{TS} - E_{SV}) = 0.300$ eV and $\Delta(E^{\text{trans}} - E_{SV}) = 0.163$ eV (main text); full per-species $\Delta(E - E_{SV})$ in SI Tab. S2 (e.g. VQE on H1: O₂ 0.208, TS 0.299, 2O 0.163 eV; VQE+PT2 on H1: O₂ 0.021, TS -0.039 , 2O 0.059 eV). Pt/Co: DFT $E_a \approx 0.46$ eV, driving force $E_d = -1.30$ eV; best statevector VQE at the largest (8e, 8o) active space gives $E_a = 0.293$ eV and driving force -1.994 eV.
- **Error bars / noise.** Statistical errors are standard deviations from bootstrapping (Fig. 3 caption; SI Tab. S1). SI Tab. S1 (with PMSV) reports, for VQE: $\epsilon(E_a) = 0.039$ eV (H1-E), 0.129 eV (H1); $\epsilon(E_d) = 0.027$ eV (H1-E), 0.108 eV (H1). For VQE+PT2: $\epsilon(E_a) = 0.344$ eV (H1-E), 0.263 eV (H1); $\epsilon(E_d) = 0.031$ eV (H1-E), 0.174 eV (H1). (Note: the main text states E_a errors “not larger than $\epsilon = 0.2$ eV”, which is in tension with the larger VQE+PT2 $\epsilon(E_a)$ values in SI Tab. S1, reported as found.) Pt/Co H1-E runs: per-state std dev between 0.02 eV (reactant) and 0.1 eV (product).
- **Comparison to classical baseline.** The classical baselines are PBE-DFT (Quantum Espresso) and the statevector (Qulacs) VQE / VQE+QRDM-NEVPT2 limit; the device/emulator results are benchmarked against these, not against a large-scale classical method that the quantum run is claimed to beat. No quantum-advantage demonstration is claimed; only an argument that Pt/Co is a *future* candidate.

2.6 Portability flags

- **Trapped-ion, modest qubit count, modest depth.** Only 6 (Pt) / 8 (Pt/Co) active qubits and “moderate” ADAPT-VQE depth; nothing here intrinsically requires trapped-ion hardware. The workload is a generic small-active-space VQE and should port to any platform with comparable two-qubit fidelity. The binding constraint is *gate/measurement fidelity for chemical accuracy*, not connectivity or qubit count.
- **PMSV error mitigation is part of the result.** Every reported H1/H1-E number includes Partition Measurement Symmetry Verification post-selection. A port must supply an equivalent symmetry-verification / mitigation layer or the energies will degrade; the raw (unmitigated) device numbers are not reported.
- **4-particle RDM measurement.** The QRDM-NEVPT2 step needs RDMs up to 4th particle order measured on the device, i.e. many additional measurement bases (12 commuting circuits for Pt, 19 for Pt/Co for the energy alone, plus the RDM bases). Measurement-overhead scaling, not gate depth, is the dominant cost and will scale steeply with active-space size on any platform.
- **All-to-all connectivity used implicitly.** The UpCCGSD/ADAPT ansatz has generalised (all-pairs) excitations; on H1 these map onto an all-to-all chain with no routing overhead. On a fixed-coupling lattice (heavy-hex / linear) the same ansatz incurs SWAP overhead, relevant for Brillant’s analysis, but the paper does not quantify it.
- **Proprietary software/method coupling.** The pipeline is tied to Quantinuum’s InQuanto + QRDM-NEVPT2 (Krompiec & Muñoz Ramo, arXiv:2210.05702) and TKET. The QRDM-NEVPT2 dynamical-correlation primitive is non-standard; reproducing

the workflow elsewhere requires re-implementing the RDM-to-NEVPT2 step.

- **Native gate decomposition.** Circuits are compiled to the H1 native Mølmer–Sørensen $R_{ZZ}(\theta)$ basis via TKET; a port to a CZ/CNOT or \sqrt{i} SWAP basis must recompile. The paper gives no gate-count budget, so the decomposition cost is unquantified here.

2.7 Caveats

- **Paper not attached by the triager.** The dossier shipped with only `dossier.md` and a failed-fetch `paper.url` (the Nature link `s41524-024-01460-x` is paywalled and redirects to `idp.nature.com`). I retrieved the open-access arXiv preprint **2307.15823** (PDF + LaTeX source, now saved under `paper.pdf`, `paper-source.tar.gz`, and `paper-source/`) per Romain’s sourcing note, and extracted from the arXiv main text (`sn-article.tex`) and Supplementary Information (`sn-si.tex`). Equation and table values above are copied from that TeX source. I did not have the published Nature/npj typeset version; per the dossier note the Jan-2026 Publisher Correction (`s41524-025-01513-9`) only fixed author affiliations and changes none of the science, so the arXiv numbers should match.
- **Hardware vs emulator split is easy to misread.** The title and abstract say “simulated with a quantum computer”, but only the **pure-Pt** ($(2e, 3o)$, 6 qubits) experiment ran on the **physical H1 device**. The strongly-correlated **Pt/Co** case (the paper’s headline quantum-relevance result) ran on the $(4e, 4o)$ NISQ active space using the **H1-E (H1-2E) noisy emulator only**, not on hardware. Treat any “ran on a quantum computer” framing of the Pt/Co result with care.
- **Several device resource numbers are genuinely absent.** Circuit depth, total two-qubit-gate count, VQE optimiser iteration counts, ADAPT operator counts, and wall-clock runtimes are not reported anywhere in the main text or SI; these are marked “not reported” rather than estimated.

3 Portability matrix