Disclaimer

Challenge 1: Characterizing Candidate Materials for Electrolysis Catalysts for Water Splitting

1. Context and Relevance

The global push toward green hydrogen production, for instance to power trucks and buses, has positioned water splitting via electrolysis as a cornerstone technology for decarbonizing energy systems. Efficient electrolysis relies on catalysts that accelerate the two half-reactions making up water splitting, namely, hydrogen evolution reaction (HER) at the cathode and oxygen evolution reaction (OER) at the anode, while minimizing energy losses. Despite significant progress, identifying and optimizing candidate materials for these reactions remains a key challenge, as current catalysts often rely on scarce and expensive metals such as platinum, iridium, and ruthenium. In addition, the extraction of many of these materials is environmentally unfriendly and scaling up production of these catalysts for industrial electrolyzers is difficult. Furthermore, even high-performance catalysts can suffer from limited long-term stability or suboptimal efficiency under real operating conditions.

Traditionally, the search for new catalysts combines experimental synthesis and characterization with trial-and-error testing in electrochemical cells. This approach is time- and resource-intensive, often requiring months of iterative lab work for each candidate material. Computational screening methods, including density functional theory (DFT) simulation and molecular dynamics (MD) simulations, have accelerated the process, but they are constrained by computational cost, accuracy limitations, and the challenge of predicting behavior under realistic electrolyzer conditions. These bottlenecks create a critical need for approaches that can systematically evaluate, rank, and optimize candidate materials, taking into account not only catalytic activity but also abundance, manufacturability, and

operational durability.

2. Challenge Overview

In this hackathon challenge, participants are tasked with developing a quantum computing solution – such as Variational Quantum Eigensolvers (VQE), quantum subspace diagonalization or other hybrid quantum-classical approaches – to explore the modeling of candidate catalyst materials for water splitting. The solution should explore how quantum algorithms can be applied to simulate and benchmark the properties of candidate catalysts for water splitting. The key focus of the challenge is to demonstrate a computational pipeline that provides insight into catalytic activity and stability, and that can be benchmarked against well-known reference catalysts like platinum or iridium oxide, for example.
Participants are encouraged to:

- Start with a simple model that outputs one relevant property of candidate catalysts, e.g. ground-state energy, stability, overpotential estimates, or adsorption energy of intermediates (H*, O*, OH*), before moving on to a more complicated model.
- Incorporate classical pre- or post-processing steps (e.g., geometry optimization, data visualization)
- Benchmark their results against known reference catalysts or reaction intermediates
- Clearly document their workflow to ensure reproducibility and extensibility
- Demonstrate a compelling path toward a potential quantum advantage, with a clear articulation of the challenges that must be overcome.

3. Detailed Problem Description

a. Mathematical Problem / Model Description

The central goal of the challenge is to compute properties of candidate catalyst systems using a quantum computing approach. At the core, each candidate material can be modeled as a molecular Hamiltonian (written in second quantization):

$$\hat{H} = \sum_i h_i \hat{c}_i^\dagger \hat{c}_i + \sum_{i<j} h_{ij} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_j \hat{c}_i$$

Here, h_i represents one-electron terms (kinetic energy and nuclear attraction), h_{ij} represents two-electron Coulomb interaction terms, and c_i are fermionic creation and annihilation operators for orbital i. The terms h_i and h_{ij} are sometimes also called “one- and two-electron integrals”, respectively.

The ground-state energy E_0 of this Hamiltonian is an indicator for the stability of the catalytic site:

$$E_0 = \min_{|\psi(\vec{\theta})\rangle} \langle \psi(\vec{\theta}) | \hat{H} | \psi(\vec{\theta}) \rangle$$

where $|\psi(\theta)\rangle$ is a parameterized quantum state (ansatz), and θ are variational parameters. Teams are encouraged to explore VQE, related hybrid quantum-classical algorithms or quantum subspace diagonalization to minimize this expectation value efficiently.

Other quantities of interest for benchmarking may include:

- Adsorption energies of intermediates (H*, O*, OH*):

$$E_{\text{ads}} = E_{\text{system+adsorbate}} - E_{\text{system}} - E_{\text{adsorbate}}$$

- Reaction energetics along HER/OER steps, which can be derived from combinations of ground-state and intermediate energies.

The challenge encourages participants to build a computational pipeline that can compute some or all of these energies, and/or other relevant quantities of the materials, for multiple candidate materials and compare them against known reference catalysts, providing insight into activity, stability, and potential efficiency of each candidate system.

Fermion-qubit mapping:

For this, the fermionic creation and annihilation operators in the Hamiltonian H (above) need to be mapped to qubit systems, which are not fermionic by design. Common fermion-qubit mappings are the Jordan-Wigner, Bravyi-Kitaev or the Parity Mapping (see links in Resources).

After the mapping, the qubit Hamiltonian is typically a sum of Pauli strings, that is,

$$\hat{H}_{\text{qubit}} = \sum_k \alpha_k P_k$$

where each P_k is a tensor product of Pauli operators (I,X,Y,Z) acting on the qubits, and α_k are real coefficients. The formulation of the energies as minimization problems now carries over to this Hamiltonian, which can directly be implemented on quantum computing hardware.

b. Proposed Quantum Approaches

Quantum computing approaches for this challenge should enhance the computational capabilities of the analysis of candidate catalysts in order to determine their fit with respect to key metrics such as energetic efficiency, abundance of needed resources, cost, durability and stability under operating conditions, or fabrication. Suggested approaches include:

- VQE for estimating energies such as the ground state energy of molecules, adsorption energies of intermediates, potentials.
- Other hybrid quantum-classical approaches or
- Quantum subspace diagonalization.
- Another option could be to focus on data-driven workflows to screen and rank candidate catalysts and make use of quantum-enhanced machine learning techniques by combining material descriptors, computational predictions, and experimental data.

The participants are encouraged to also think about fault-tolerant quantum algorithms that may further enhance the computational pipeline. However, when it comes to the working prototype, a key deliverable of this hackathon challenge, NISQ algorithms will likely be the only viable option.

4. Expected Deliverables (Course Project)

1) Working Prototype
A functioning implementation (classical, quantum, or hybrid) tested on at least a simplified instance of the chosen problem.

2) Technical Report
A concise report (≈ 6–10 pages) including:

- problem description and assumptions,
- chosen approach and justification,
- implementation outline,
- results and comparison with a classical baseline,
- limitations and future directions.

3) Justification for Quantum Use
A short section explaining classical bottlenecks and why a quantum or hybrid method could be beneficial in principle.

4) Broader Impact (Short)
A brief note on the practical or societal relevance of solving this problem.

5) Final Presentation — 20 minutes
A **20-minute in-class presentation** summarizing the work, followed by Q&A.

6) Code Submission
Submit all scripts/notebooks used to generate results, with short instructions to run them.

Notes:

- Depth is preferred over breadth: it is better to develop one approach carefully than to list many without depth.
- The goal is not to prove a current quantum speedup, but to demonstrate understanding and a credible rationale for future advantage.

5. Resources

[Context] SDG 7: https://sdgs.un.org/goals/goal7

[Context] Intro to computational chemistry for non-polluting fuels: https://kids.frontiersin.org/articles/10.3389/frym.2021.648750?utm_source=chatgpt.com

[SDK, Intro] Qiskit's Chemistry Module, also contains links to implemented Jordan-Wigner, Bravyi-Kitaev and Parity mappings: https://quantum.cloud.ibm.com/docs/de/api/qiskit/0.32/qiskit_chemistry

[SDK, Intro] Qiskit Nature Workflow: https://qiskit-community.github.io/qiskit-nature/#

[SDK] Jordan Wigner Mapping on Qiskit: https://qiskit-community.github.io/qiskit-nature/stubs/qiskit_nature.second_q.mappers.JordanWignerMapper.html

[SDK, Data] PySCF, classical chemistry simulations, including an API to extract one- and two-electron integrals, i.e. h_i and h_{ij}: https://pyscf.org/

[SDK] Psi4 for chemistry simulations including export capabilities for integrals h_i and h_{ij}: https://psicode.org/

[SDK, Data] OpenFermion for chemistry simulations, interfaces with PySCF and Psi4 to obtain the integrals h_i and h_{ij}: github.com/quantumlib/OpenFermion

[Method] Quantum subspace diagonalization https://quantum.cloud.ibm.com/learning/fr/courses/quantum-diagonalization-algorithms/krylov

[Tutorial] OpenFermion Tutorial by Google QuantumAI:
https://quantumai.google/openfermion/tutorials/intro_workshop_exercises

[Further Literature] Seminal paper showing how chemistry simulations can hopefully once be enhanced through quantum algorithms on fault-tolerant quantum computers:
https://arxiv.org/abs/1605.03590