

Variational Quantum Eigensolver for Designing Metal–Organic Frameworks Optimised for Heavy Metal Sequestration in Galamsey-Polluted Waters

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Abstract

Galamsey-polluted waters remain an urgent environmental concern because artisanal and small-scale gold mining can introduce toxic heavy metals such as Hg^{2+} , Pb^{2+} and arsenic-related species into aquatic systems. Metal–organic frameworks (MOFs) are promising adsorbents for heavy metal sequestration because their metal nodes, organic linkers and pore environments can be chemically tuned for selective binding. However, the rational design of MOFs for polluted water treatment remains difficult when guided only by experimental adsorption capacity, removal efficiency or trial-and-error synthesis. This extended abstract presents a quantum-guided computational framework based on the Variational Quantum Eigensolver (VQE) for designing MOFs optimised for heavy metal sequestration in galamsey-polluted waters. The framework integrates systematic literature evidence, density functional theory (DFT) active-site screening, Hamiltonian construction, qubit mapping and VQE optimisation. UiO-66-SH- Hg^{2+} is used as the primary proof-of-concept because mercury is strongly associated with gold-mining contamination and sulfur donor sites are chemically favourable for Hg^{2+} coordination. A reduced Hg–S active-site model is formulated as a four-qubit active-space problem and benchmarked using multiple ansatz and optimiser combinations. The work positions VQE as an electronic-structure refinement tool for prioritising MOF active sites before synthesis and real-water validation.

1 Background and Motivation

Illegal and informal small-scale mining, locally referred to as galamsey, has raised serious concerns about water quality in Ghana and other mining-affected regions. Heavy metals introduced into water systems may persist, bioaccumulate and pose long-term risks to ecosystems and human health. Mercury is particularly important because of its association with gold extraction, but lead and arsenic-related species are also relevant because they represent toxic contaminants with different aqueous chemistry.

MOFs provide a versatile platform for water remediation because their structures can be modified through metal-node selection, linker functionalisation, defect engineering and composite formation. Nevertheless, adsorption performance is not governed by porosity alone. A MOF must present active sites that match the chemistry of the target contaminant. For example, Hg^{2+} is expected to favour sulfur donor sites, Pb^{2+} may interact with oxygen or nitrogen donors, and arsenic-related oxyanions may bind through Zr–OH or open Zr sites. This means that MOF design should be contaminant-specific rather than generic.

Current MOF adsorption studies often report macroscopic metrics such as adsorption capacity, removal efficiency, pH dependence and regeneration. These are essential for practical evaluation, but they do not fully explain the local electronic origin of metal selectivity. Quantum computational chemistry provides a route to study this local binding problem. VQE is particularly relevant because it is designed for estimating ground-state energies of molecular Hamiltonians using hybrid quantum–classical optimisation (Peruzzo et al., 2014; McArdle et al., 2020; Tilly et al., 2022). The challenge is that full MOF structures are too large for direct near-term VQE. Therefore, chemically meaningful active-site reduction is required.

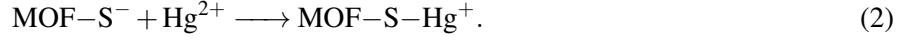
2 Proposed DFT–VQE Framework

This work proposes a DFT–VQE workflow for designing MOFs optimised for heavy metal sequestration:

SLR evidence → MOF active-site model → DFT screening → Hamiltonian construction → qubit mapping → VQE optimisation (1)

The systematic literature review component identifies target metals, candidate MOFs and likely binding motifs. The DFT component screens local metal–MOF interactions using adsorption energy, metal–donor distance, charge transfer and frontier orbital descriptors. The VQE component refines the electronic energy of selected active-space Hamiltonians.

The primary proof-of-concept is UiO-66-SH–Hg²⁺. The local binding event is represented as:



For active-space quantum simulation, this is reduced to:



The adsorption-energy descriptor is:

$$\Delta E_{\text{ads}} = E_{\text{MOF-S-Hg}^+} - (E_{\text{MOF-S}^-} + E_{\text{Hg}^{2+}}). \quad (4)$$

A favourable interaction is expected when $\Delta E_{\text{ads}} < 0$. Charge transfer is represented as:

$$\Delta q_{\text{Hg}} = q_{\text{Hg}}^{\text{adsorbed}} - q_{\text{Hg}}^{\text{isolated}}, \quad (5)$$

where $\Delta q_{\text{Hg}} < 0$ supports sulfur-to-mercury donation.

3 Active-Space Hamiltonian and Qubit Mapping

The selected Hg–S interaction is converted into a reduced electronic Hamiltonian. In second quantisation:

$$\hat{H} = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s + E_{\text{core}}. \quad (6)$$

A two-electron/two-spatial-orbital active space was selected for the proof-of-concept demonstration. The spin orbitals are:

$$\{S_\alpha, S_\beta, Hg_\alpha, Hg_\beta\}.$$

Thus, the number of qubits is:

$$N_{\text{qubits}} = 2N_o = 2(2) = 4. \quad (7)$$

After qubit mapping, the Hamiltonian takes the Pauli form:

$$\hat{H}_q = \sum_i c_i P_i, \quad (8)$$

where c_i are real coefficients and P_i are Pauli strings.

Table 1: Proof-of-concept active-space VQE summary for the UiO-66-SH–Hg²⁺ model.

Component	Description
Main thesis topic	VQE for designing MOFs optimised for heavy metal sequestration in galamsey-polluted waters
Proof-of-concept system	UiO-66-SH–Hg ²⁺ active site
Reduced model	$\text{PhS}^- + \text{Hg}^{2+} \longrightarrow \text{PhS-Hg}^+$
Active space	$(N_e, N_o) = (2, 2)$
Qubit requirement	4 qubits
Mapped Hamiltonian	15 Pauli terms in the reduced proof-of-concept model
Best VQE behaviour	Problem-inspired Hg–S ansatz reached the exact active-space energy to numerical precision

4 VQE Simulation Strategy

The VQE objective is:

$$E(\theta) = \langle \psi(\theta) | \hat{H}_q | \psi(\theta) \rangle, \quad E_0 \approx \min_{\theta} E(\theta). \quad (9)$$

Three ansatz families are considered: a unitary-coupled-cluster-inspired double-excitation ansatz, a hardware-efficient ansatz and a problem-inspired Hg–S ansatz. Optimisers include COBYLA, Nelder–Mead, L-BFGS-B and Powell. The purpose of comparing ansatz–optimiser combinations is to assess convergence stability, circuit feasibility and the value of chemical structure in ansatz design.

In the reduced Hg–S demonstration, exact active-space diagonalisation gave an energy of -20.6605887134 Hartree. The problem-inspired Hg–S ansatz recovered this value to numerical precision under derivative-free optimisation. This supports the view that chemically guided ansatz construction may be more efficient for MOF–metal active-site problems than using only generic hardware-efficient circuits.

5 Significance and Expected Contribution

The proposed framework contributes to quantum machine learning and quantum chemistry by connecting environmental materials design with near-term quantum algorithms. It does not claim that VQE alone can predict full field-scale adsorption performance. Instead, VQE is positioned as a refinement layer within a broader materials discovery pipeline. The expected future pipeline is:

$$\text{computed active-site preference} \rightarrow \text{MOF synthesis} \rightarrow \text{adsorption testing} \rightarrow \text{real gamalsey water validation}. \quad (10)$$

The work also creates a pathway for future machine-learning integration. DFT descriptors, VQE energies, qubit requirements and literature-derived adsorption features can form structured datasets for learning candidate ranking functions:

$$S_{\text{candidate}} = f(\Delta E_{\text{ads}}, d_{M-D}, \Delta q_M, E_{\text{VQE}}, N_{\text{qubits}}, \dots). \quad (11)$$

Such a model could accelerate pre-screening of MOFs before expensive DFT or VQE calculations.

6 Conclusion

This extended abstract presents a VQE-based framework for designing MOFs optimised for heavy metal sequestration in gamalsey-polluted waters. UiO-66-SH-Hg²⁺ is proposed as the first proof-of-concept because it links environmental relevance, sulfur–mercury coordination chemistry and active-space feasibility for quantum simulation. The framework integrates DFT screening, Hamiltonian construction, qubit mapping and VQE optimisation. The reduced Hg–S demonstration shows that a four-qubit active-space model can be solved accurately with a chemically guided ansatz. Future work will replace the effective Hamiltonian with ab initio integrals from DFT-optimised structures, include solvation and competing ions, benchmark noisy VQE implementations and validate the predicted MOF candidates experimentally using synthetic and real gamalsey-polluted water samples.

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