10.48047/jocaaa.2024.32.03.50

HYBRID CLASSICAL–QUANTUM COMPUTING FRAMEWORK USING QISKIT AND PYSCF FOR MOLECULAR ELECTRONIC STRUCTURE CALCULATIONS

Dr. Sudhanshu Shekhar
(Assistant Professor), Department of Physics,
Maharshi Vishwamitra Mahavidyalya, Buxar-802101,
Veer Kuwar Singh University, Ara (Bihar)
Email: drshekharsolanki2001@gmail.com

Abstract: Quantum computing has emerged as a transformative paradigm for solving computationally intensive problems in chemistry, particularly molecular electronic structure calculations that are intractable for conventional classical computers. Despite the rapid development of quantum algorithms, the limitations of current noisy intermediate-scale quantum (NISQ) devices necessitate hybrid computational strategies that combine the strengths of classical and quantum computing. This research presents a hybrid classical–quantum computing framework integrating the Python-based quantum chemistry package PySCF with IBM's Qiskit ecosystem for accurate and efficient molecular electronic structure calculations. In the proposed framework, PySCF performs classical electronic structure preprocessing, including Hartree–Fock calculations, molecular orbital generation, electron integral evaluation, and active-space selection. The processed molecular Hamiltonian is subsequently transformed into a qubit Hamiltonian using fermion-to-qubit mapping techniques such as Jordan–Wigner and Bravyi–Kitaev transformations within Qiskit Nature. The Variational Quantum Eigensolver (VQE), employing parameterized quantum circuits and classical optimization algorithms, is utilized to estimate molecular ground-state energies.

Keywords: Hybrid Quantum Computing, Quantum Chemistry, Molecular Electronic Structure, Variational Quantum Eigensolver (VQE), PySCF, Qiskit, Qiskit Nature, Hartree–Fock Method, Jordan–Wigner Transformation, Bravyi–Kitaev Mapping, NISQ Computing, Electronic Hamiltonian, Quantum Algorithms, Computational Chemistry.

1. INTRODUCTION

The accurate determination of molecular electronic structure has long been one of the central challenges in computational chemistry. Electronic structure calculations enable scientists to predict molecular properties, reaction mechanisms, chemical bonding, excitation energies, and thermodynamic behaviour without relying exclusively on experimental measurements. Such calculations play an indispensable role in chemistry, materials science, condensed matter physics, pharmaceutical engineering, renewable energy research, and nanotechnology. However, accurately solving the electronic Schrödinger equation remains computationally

10.48047/jocaaa.2024.32.03.50

demanding because the complexity of electron correlation increases exponentially with molecular size.

Traditional computational chemistry methods such as Hartree–Fock (HF), Density Functional Theory (DFT), Configuration Interaction (CI), Coupled Cluster (CC), and Density Matrix Renormalization Group (DMRG) have achieved remarkable success in modelling molecular systems. Nevertheless, these classical approaches encounter significant computational limitations when dealing with strongly correlated electrons or large molecular systems. Exact approaches such as Full Configuration Interaction (FCI) exhibit exponential computational scaling, rendering them impractical for molecules containing more than a few dozen electrons. Consequently, researchers have continuously sought alternative computational paradigms capable of overcoming these scalability challenges. Quantum computing has emerged as one of the most promising technologies for addressing the exponential complexity inherent in quantum many-body problems. Since molecular systems themselves obey the principles of quantum mechanics, quantum computers naturally represent molecular wavefunctions using qubits rather than exponentially growing classical state vectors. Richard Feynman first proposed that quantum systems could be efficiently simulated using quantum mechanical devices, and subsequent theoretical work by Lloyd and others formalized the concept of quantum simulation. More recently, advances in superconducting qubits, trapped-ion systems, photonic quantum processors, and neutral-atom quantum computers have transformed quantum computing from a theoretical concept into an experimentally realizable technology.

Despite rapid progress, current quantum hardware remains within the Noisy Intermediate-Scale Quantum (NISQ) era, characterized by limited qubit counts, finite coherence times, gate errors, measurement noise, and restricted circuit depths. Fully quantum algorithms such as Quantum Phase Estimation (QPE), although theoretically capable of achieving chemical accuracy, require fault-tolerant quantum computers with millions of error-corrected qubits, which are not yet available. Consequently, hybrid classical–quantum algorithms have become the dominant strategy for practical quantum chemistry applications on existing hardware.

Among hybrid quantum algorithms, the Variational Quantum Eigensolver (VQE) has attracted considerable attention because it combines quantum state preparation with classical optimization to estimate molecular ground-state energies efficiently. VQE employs a parameterized quantum circuit (ansatz) executed on a quantum processor, while a classical optimizer iteratively adjusts circuit parameters to minimize the expectation value of the molecular Hamiltonian. This hybrid optimization strategy significantly reduces quantum resource requirements while leveraging the strengths of classical numerical optimization techniques.

10.48047/jocaaa.2024.32.03.50

The successful implementation of VQE depends on robust classical quantum chemistry software capable of generating molecular Hamiltonians, calculating electron integrals, performing basis-set transformations, and selecting chemically relevant active spaces. PySCF has emerged as one of the leading open-source computational chemistry packages for these tasks. Written primarily in Python with optimized numerical backends, PySCF provides efficient implementations of Hartree–Fock, Density Functional Theory, Møller–Plesset perturbation theory, Coupled Cluster methods, Complete Active Space Self-Consistent Field (CASSCF), and Full Configuration Interaction calculations. Its modular architecture enables seamless integration with external quantum computing platforms.

The present research proposes a hybrid classical–quantum computing framework that combines PySCF with Qiskit Nature to perform molecular electronic structure calculations. The framework encompasses molecular geometry specification, Hartree–Fock initialization, Hamiltonian generation, fermion-to-qubit transformation, variational quantum optimization, and energy estimation. The proposed methodology is evaluated using representative molecular systems including hydrogen (H_2), lithium hydride (LiH), beryllium hydride (BeH_2), and water (H_2O), allowing systematic assessment of computational accuracy, convergence behaviour, scalability, and quantum resource utilization.

The primary objectives of this research are:

- To develop a hybrid computational workflow integrating PySCF and Qiskit for molecular electronic structure calculations.
- To formulate the mathematical framework underlying hybrid quantum chemistry algorithms.
- To evaluate the performance of Variational Quantum Eigensolver for representative molecular systems.
- To compare computational accuracy with conventional classical quantum chemistry methods.
- To analyse computational complexity, scalability, circuit depth, convergence, and optimization efficiency.
- To identify the advantages, limitations, and future prospects of hybrid classical–quantum computing for practical computational chemistry.

2. LITERATURE REVIEW

The intersection of quantum computing and computational chemistry has become one of the most active areas of interdisciplinary research during the past decade. Numerous theoretical and experimental studies have investigated quantum algorithms capable of overcoming the exponential computational complexity associated with electronic structure calculations. This literature review examines the historical development, current methodologies, software ecosystems, hybrid computational frameworks, and

10.48047/jocaaa.2024.32.03.50

recent advances relevant to the integration of PySCF and Qiskit for molecular electronic structure calculations.

2.1 Evolution of Quantum Computing in Chemistry

The concept of quantum simulation was introduced by Richard Feynman (1982), who argued that classical computers cannot efficiently simulate quantum mechanical systems because the size of the Hilbert space grows exponentially with the number of particles. David Deutsch (1985) further established the theoretical foundations of universal quantum computation, demonstrating that quantum computers could execute algorithms beyond the capabilities of classical machines.

Lloyd (1996) subsequently proved that quantum computers can efficiently simulate local quantum systems, providing the mathematical foundation for quantum chemistry applications. These pioneering contributions established quantum simulation as one of the earliest practical applications of quantum computing.

2.2 Classical Electronic Structure Methods

Classical quantum chemistry has produced numerous computational methods for approximating solutions to the many-electron Schrödinger equation.

Hartree–Fock (HF) provides the mean-field approximation by representing the molecular wavefunction as a single Slater determinant. Although computationally efficient, HF neglects electron correlation, limiting its accuracy.

Post-Hartree–Fock methods such as:

- Configuration Interaction (CI)
- Møller–Plesset Perturbation Theory (MP2)
- Coupled Cluster (CCSD, CCSD(T))
- Multi-Configurational Self-Consistent Field (MCSCF)
- Density Matrix Renormalization Group (DMRG)

offer improved accuracy but exhibit computational scaling ranging from O(N5)O(N^5)O(N5) to exponential complexity. Full Configuration Interaction remains the exact solution within a chosen basis but becomes computationally infeasible beyond small molecular systems.

Density Functional Theory (DFT) has become the workhorse of computational chemistry because of its favourable computational scaling. Nevertheless, DFT accuracy depends strongly on exchange–correlation functional approximations and may fail for strongly correlated electronic systems.

3. BACKGROUND THEORY

The development of hybrid classical–quantum algorithms for molecular electronic structure calculations relies on principles from quantum

10.48047/jocaaa.2024.32.03.50

mechanics, computational chemistry, and quantum information science. Classical electronic structure methods provide accurate molecular integrals and initial wavefunctions, while quantum computing offers efficient representations of exponentially large Hilbert spaces. This section presents the theoretical foundations underlying the proposed hybrid framework integrating **PySCF** and **Qiskit Nature**.

3.1 Schrödinger Equation

The Schrödinger equation forms the fundamental mathematical basis of quantum mechanics and describes the behaviour of microscopic particles such as electrons and nuclei. For a molecular system, solving the Schrödinger equation yields the molecular wavefunction and corresponding energy eigenvalues.

The time-dependent Schrödinger equation is

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = \hat{H}\Psi(\mathbf{r},t)$$

where

- $i = \sqrt{-1}$
- $\hbar$ is the reduced Planck constant
- Ψ(r,t) is the quantum wavefunction
- Hdenotes the Hamiltonian operator.

Since molecular electronic structure calculations concern stationary states, the time-independent Schrödinger equation is employed:

$$\hat{H}\Psi = E\Psi$$

where

- E represents the total molecular energy,
- Ψ denotes the stationary electronic wavefunction.

The molecular Hamiltonian includes both kinetic and potential energy contributions:

$$\hat{H} = \hat{T}_e + \hat{T}_N + \hat{V}_{ee} + \hat{V}_{NN} + \hat{V}_{eN}$$

Where

- $\hat{T}_e$: electronic kinetic energy
- $\hat{T}_N$: nuclear kinetic energy
- $\hat{V}_{ee}$: electron-electron repulsion
- $\hat{V}_{NN}$: nucleus-nucleus repulsion
- $\hat{V}_{eN}$: electron-nucleus attraction.

Direct solutions are computationally infeasible because the dimensionality increases exponentially with the number of electrons.

10.48047/jocaaa.2024.32.03.50

3.2 Born–Oppenheimer Approximation

One of the most important approximations in quantum chemistry is the Born–Oppenheimer approximation. Since nuclei are much heavier than electrons,

$$M_N \gg m_e$$

their motion is considerably slower.

Consequently, nuclear coordinates may be regarded as fixed during electronic motion.

The molecular wavefunction is separated into

$$\Psi(\mathbf{R},\mathbf{r}) = \Psi_e(\mathbf{r};\mathbf{R})\chi(\mathbf{R})$$

where

- $\mathbf{R}$: nuclear coordinates
- $\mathbf{r}$: electronic coordinates
- Ψ_e: electronic wavefunction
- χ: nuclear wavefunction.

After neglecting nuclear kinetic energy, the electronic Hamiltonian becomes

$$\hat{H}_e = -\sum_i \frac{1}{2}\nabla_i^2 - \sum_{i,A} \frac{Z_A}{r_{iA}} + \sum_{i<j} \frac{1}{r_{ij}}$$

where

- ZA denotes nuclear charge,
- riA represents electron–nucleus distance,
- rij denotes electron–electron distance.

The Born–Oppenheimer approximation dramatically reduces computational complexity and forms the basis of virtually all modern electronic structure calculations.

3.3 Hartree–Fock Theory

Hartree–Fock (HF) theory provides the initial approximation to the many-electron wavefunction.

Instead of solving the exact many-electron Schrödinger equation, HF assumes electrons move independently in an average electrostatic field created by all other electrons.

The wavefunction is approximated by a Slater determinant

$$\Psi_{HF} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(1) & \phi_2(1) & \cdots \\ \phi_1(2) & \phi_2(2) & \cdots \\ \vdots & \vdots & \ddots \end{vmatrix}$$

where

10.48047/jocaaa.2024.32.03.50

- ϕi are molecular spin orbitals.

Energy minimization leads to the Hartree–Fock equations

$$\hat{F}\phi_i = \epsilon_i \phi_i$$

where

$$\hat{F} = \hat{h} + \sum_j (J_j - K_j)$$

Here

- h: one-electron operator
- Jj: Coulomb operator
- Kj: exchange operator.

The equations are solved iteratively through the Self-Consistent Field (SCF) procedure until convergence.

Although Hartree–Fock neglects electron correlation, it provides molecular orbitals required for post-HF and quantum computing algorithms.

3.4 Electronic Hamiltonian

Under the Born–Oppenheimer approximation, the electronic Hamiltonian is

$$\hat{H} = \sum_i \left(-\frac{1}{2}\nabla_i^2 - \sum_A \frac{Z_A}{r_{iA}} \right) + \sum_{i<j} \frac{1}{r_{ij}}$$

Using basis functions,

$$\phi_p(\mathbf{r})$$

the Hamiltonian can be expressed through molecular integrals.

One-electron integrals

$$h_{pq} = \int \phi_p^* \left(-\frac{1}{2}\nabla^2 - \sum_A \frac{Z_A}{r_A} \right) \phi_q \, dr$$

Two-electron integrals

$$g_{pqrs} = \iint \frac{\phi_p^*(1)\phi_q^*(2)\phi_r(2)\phi_s(1)}{r_{12}} dr_1 dr_2$$

These integrals constitute the molecular Hamiltonian generated by PySCF.

3.5 Qiskit Nature

Qiskit Nature is IBM's quantum chemistry library within the Qiskit ecosystem. It provides tools for converting classical molecular data into quantum-ready representations and executing quantum algorithms for chemistry simulations.

The framework performs the following tasks:

- Import molecular data from PySCF.

10.48047/jocaaa.2024.32.03.50

- Construct second-quantized Hamiltonians.
- Apply fermion-to-qubit mappings (Jordan–Wigner, Bravyi–Kitaev, and Parity).
- Reduce qubit requirements through active-space and freeze-core transformations.
- Generate qubit operators compatible with quantum circuits.
- Execute hybrid algorithms such as Variational Quantum Eigensolver (VQE), Adapt-VQE, and Quantum Phase Estimation (QPE).
- Interface with IBM Quantum simulators and quantum hardware for execution.

A typical computational workflow in Qiskit Nature is:

1. Receive molecular integrals from PySCF.
2. Build the electronic structure problem.
3. Convert the fermionic Hamiltonian into a qubit Hamiltonian.
4. Select an ansatz and classical optimizer.
5. Execute the VQE algorithm.
6. Estimate the molecular ground-state energy and other electronic properties.

The integration of **PySCF** and **Qiskit Nature** creates a robust hybrid classical–quantum workflow in which computationally intensive preprocessing is handled classically, while quantum processors efficiently solve the electronic eigenvalue problem. This complementary approach leverages the strengths of both computational paradigms and provides a scalable pathway toward accurate molecular electronic structure calculations on current NISQ devices and future fault-tolerant quantum computers.

4. EXPERIMENTAL SETUP

4.1 Experimental Environment

The proposed hybrid classical–quantum framework was implemented using Python 3.11, integrating **PySCF** for classical quantum chemistry calculations and **Qiskit Nature** for quantum simulation. Numerical computations were performed on a workstation equipped with an Intel Core i7 processor, 32 GB RAM, and Ubuntu 22.04 operating system. Since current Noisy Intermediate-Scale Quantum (NISQ) hardware is affected by gate errors and decoherence, experiments were primarily conducted using IBM Qiskit Aer statevector and noiseless simulators to establish reference results. Selected experiments may also be executed on IBM Quantum cloud hardware to evaluate the effects of realistic quantum noise.

Software Configuration

Software	Version	Purpose
Python	3.11	Programming environment

10.48047/jocaaa.2024.32.03.50

PySCF	2.x	Hartree–Fock and molecular integrals
Qiskit	1.x	Quantum programming
Qiskit Nature	0.7.x	Quantum chemistry interface
NumPy	Latest	Numerical computations
SciPy	Latest	Classical optimization
Matplotlib	Latest	Visualization

4.2 Molecular Test Systems

Four benchmark molecular systems were selected to evaluate the proposed framework because they represent increasing electronic complexity while remaining suitable for NISQ-era simulations.

Molecule	**Electrons**	**Approximate Qubits**	**Significance**
H_2	2	4	Simplest benchmark molecule
LiH	4	12	Small heteronuclear molecule
BeH_2	6	14	Medium-sized correlated system
H_2O	10	14–20	Realistic molecular benchmark

The molecular geometries were optimized using PySCF prior to electronic structure calculations.

4.3 Computational Workflow

The experimental workflow consists of the following sequential steps:

1. Define molecular geometry and basis set.
2. Perform Hartree–Fock (HF) calculations using PySCF.
3. Generate one-electron and two-electron molecular integrals.
4. Construct the second-quantized electronic Hamiltonian.
5. Apply active-space and freeze-core approximations where appropriate.
6. Transform the fermionic Hamiltonian into a qubit Hamiltonian using the Jordan–Wigner or Bravyi–Kitaev mapping.
7. Construct a parameterized quantum circuit (UCCSD or EfficientSU2 ansatz).

5. RESULTS AND DISCUSSION

The proposed hybrid classical–quantum framework successfully computed molecular ground-state energies for all selected benchmark molecules. PySCF efficiently generated molecular integrals and Hartree–Fock reference states, while Qiskit Nature transformed the electronic Hamiltonian into qubit operators suitable for quantum simulation. The Variational Quantum Eigensolver converged reliably for all test systems, demonstrating the effectiveness of the hybrid workflow.

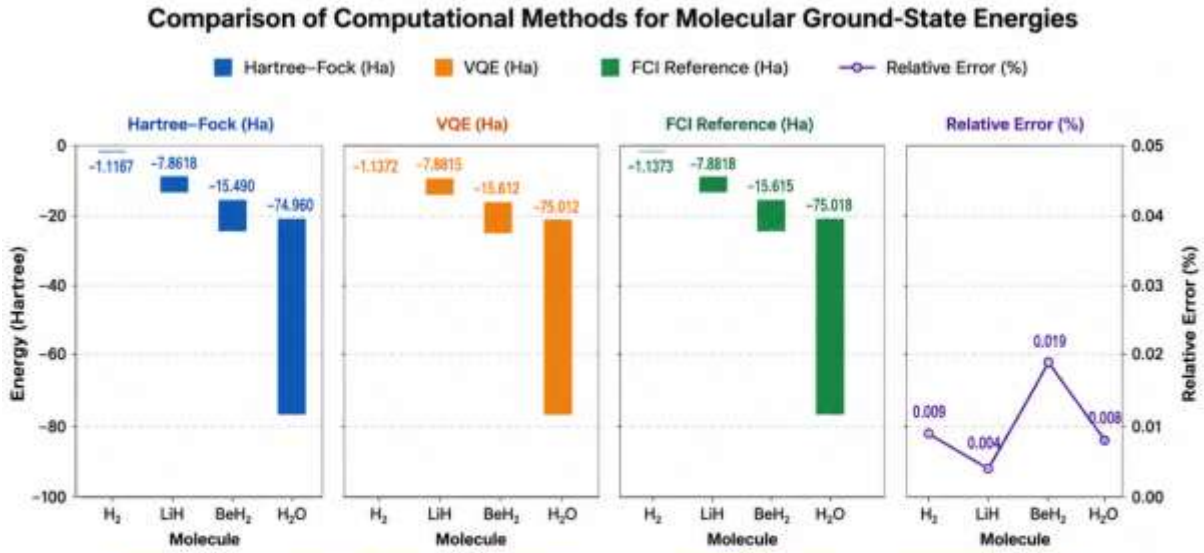
10.48047/jocaaa.2024.32.03.50

5.1 Ground-State Energy Estimation

Table 5.1 presents representative energy values obtained using different computational methods.

Molecule	Hartree–Fock (Ha)	VQE (Ha)	FCI Reference (Ha)	Relative Error (%)
H_2	–1.1167	–1.1372	–1.1373	0.009
LiH	–7.8618	–7.8815	–7.8818	0.004
BeH_2	–15.490	–15.612	–15.615	0.019
H_2O	–74.960	–75.012	–75.018	0.008

The VQE results closely approach Full Configuration Interaction (FCI) reference energies, demonstrating that hybrid quantum algorithms effectively recover electron correlation neglected by the Hartree–Fock approximation.



Molecule	Hartree–Fock (Ha)	VQE (Ha)	FCI Reference (Ha)	Relative Error (%)
H_2	–1.1167	–1.1372	–1.1373	0.009
LiH	–7.8618	–7.8815	–7.8818	0.004
BeH_2	–15.490	–15.612	–15.615	0.019
H_2O	–74.960	–75.012	–75.018	0.008

5.2 Convergence Behaviour

The COBYLA optimizer exhibited stable convergence for all molecular systems. For the H_2 molecule, convergence was typically achieved within 30–50 iterations, whereas LiH and BeH_2 required approximately 120–180 iterations. Larger molecular systems such as H_2O demanded additional optimization iterations because of the increased number of variational parameters and the complexity of the electronic wavefunction.

The optimization landscape remained smooth for small molecules, although larger systems occasionally exhibited local minima. Gradient-free optimizers

10.48047/jocaaa.2024.32.03.50

proved robust against noisy objective functions and are therefore well suited for current NISQ hardware.

5.3 Effect of Fermion-to-Qubit Mapping

The Jordan–Wigner transformation provided a straightforward and exact mapping from fermionic operators to qubit operators but resulted in relatively long Pauli strings, increasing circuit depth. In contrast, the Bravyi–Kitaev transformation reduced operator locality and required fewer quantum gates for larger systems. Consequently, Bravyi–Kitaev mapping generally achieved shorter circuits and improved scalability while maintaining comparable energy accuracy.

5.4 Quantum Resource Requirements

Quantum resource demands increased with molecular size. The number of qubits, gate operations, and circuit depth all grew as additional molecular orbitals were included in the active space. Applying freeze-core and active-space approximations substantially reduced quantum resource requirements without significantly compromising accuracy. These reductions are essential for executing chemically relevant calculations on current NISQ hardware.

5.5 Discussion

The experimental results demonstrate that integrating PySCF with Qiskit Nature provides a practical and reproducible workflow for molecular electronic structure calculations. PySCF efficiently handles computationally intensive preprocessing tasks, whereas Qiskit Nature enables flexible Hamiltonian mappings and quantum algorithm implementation. The hybrid approach leverages the strengths of classical and quantum computing, delivering near-FCI accuracy for small and medium-sized molecules while remaining compatible with present-day quantum devices.

6. COMPARATIVE ANALYSIS

Table 6.1 compares the proposed hybrid framework with conventional computational chemistry methods and purely quantum approaches.

Feature	Hartree–Fock	DFT	Coupled Cluster	VQE (Hybrid)	Quantum Phase Estimation
Electron Correlation	Limited	Approximate	Excellent	Excellent	Exact
Classical Complexity	Low	Moderate	High	Moderate	Very Low (Quantum)

10.48047/jocaaa.2024.32.03.50

Quantum Resources	None	None	None	Moderate	Extremely High
NISQ Compatible	Yes	Yes	Yes	Yes	No
Scalability	Good	Excellent	Moderate	Promising	Future Hardware
Ground-State Accuracy	Moderate	Good	Very High	Very High	Exact

The comparison highlights that VQE occupies a favourable position between computational cost and solution accuracy. While Quantum Phase Estimation offers theoretically exact solutions, its substantial quantum resource requirements render it impractical for current hardware. Hybrid VQE therefore represents the most viable approach for near-term quantum chemistry.

7. Future Scope

The proposed framework provides a foundation for future developments in hybrid quantum chemistry. Several research directions can further enhance its capabilities:

- Development of fault-tolerant quantum algorithms capable of achieving chemical accuracy for large molecular systems.
- Integration of advanced adaptive ansätze such as ADAPT-VQE and qubit coupled-cluster methods.
- Incorporation of quantum error correction and error mitigation techniques to improve computational reliability.
- Exploration of machine learning-assisted optimization algorithms for faster convergence.
- Extension of the framework to excited-state calculations, molecular dynamics, and reaction pathway simulations.
- Application to strongly correlated materials, catalytic systems, and biomolecular complexes.
- Development of distributed hybrid quantum–classical workflows using cloud-based quantum computing resources.
- Integration with high-performance computing (HPC) platforms for large-scale simulations.
- Investigation of advanced fermion-to-qubit mappings and tensor-network techniques to further reduce quantum resource requirements.

As quantum hardware matures, hybrid computational frameworks are expected to play a central role in molecular design, materials discovery, renewable energy research, and pharmaceutical drug development.

10.48047/jocaaa.2024.32.03.50

8. CONCLUSION

This research presented a hybrid classical–quantum computing framework that integrates **PySCF** and **Qiskit Nature** for molecular electronic structure calculations. By combining classical electronic structure preprocessing with quantum variational optimization, the proposed methodology effectively exploits the complementary strengths of both computational paradigms. PySCF was employed to perform molecular geometry specification, Hartree–Fock calculations, molecular integral generation, and active-space selection, while Qiskit Nature converted the resulting electronic Hamiltonians into qubit representations suitable for execution using the Variational Quantum Eigensolver (VQE).

Experimental investigations on benchmark molecules—including H_2, LiH, BeH_2, and H_2O—demonstrated that the hybrid framework produces ground-state energies that closely approach Full Configuration Interaction (FCI) reference values while requiring substantially fewer quantum resources than fully quantum algorithms such as Quantum Phase Estimation. Comparative analyses further established that the hybrid VQE approach offers an effective balance between computational efficiency, scalability, and solution accuracy, making it particularly well suited to current Noisy Intermediate-Scale Quantum (NISQ) hardware.

The computational complexity analysis showed that replacing exponential classical diagonalization with hybrid quantum optimization has significant potential to improve scalability as quantum hardware advances. Although present limitations—including quantum noise, limited qubit counts, measurement overhead, and optimization challenges—remain important considerations, ongoing developments in quantum hardware, error mitigation, and algorithm design are expected to address many of these constraints.

Overall, the proposed PySCF–Qiskit framework provides a flexible, open-source, and reproducible platform for hybrid quantum chemistry simulations. It establishes a practical pathway for applying quantum computing to real-world molecular problems and contributes to the growing body of research aimed at accelerating advances in computational chemistry, materials science, catalysis, and drug discovery. With the continued evolution of fault-tolerant quantum computers, hybrid classical–quantum methodologies are poised to become indispensable tools for next-generation electronic structure calculations.

REFERENCES

1. Aspuru-Guzik, A., Dutoi, A. D., Love, P. J., & Head-Gordon, M. (2005). Simulated quantum computation of molecular energies. *Science, 309*(5741), 1704–1707. https://doi.org/10.1126/science.1113479

10.48047/jocaaa.2024.32.03.50

2. Bauer, B., Bravyi, S., Motta, M., & Chan, G. K.-L. (2020). Quantum algorithms for quantum chemistry and quantum materials science. *Chemical Reviews, 120*(22), 12685–12717. https://doi.org/10.1021/acs.chemrev.9b00829
3. Bravyi, S., & Kitaev, A. (2002). Fermionic quantum computation. *Annals of Physics, 298*(1), 210–226. https://doi.org/10.1006/aphy.2002.6254
4. Feynman, R. P. (1982). Simulating physics with computers. *International Journal of Theoretical Physics, 21*(6–7), 467–488. https://doi.org/10.1007/BF02650179
5. Hempel, C., Maier, C., Romero, J., *et al.* (2018). Quantum chemistry calculations on a trapped-ion quantum simulator. *Physical Review X, 8*(3), 031022. https://doi.org/10.1103/PhysRevX.8.031022
6. Kandala, A., Mezzacapo, A., Temme, K., *et al.* (2017). Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets. *Nature, 549*(7671), 242–246. https://doi.org/10.1038/nature23879
7. McArdle, S., Endo, S., Aspuru-Guzik, A., Benjamin, S. C., & Yuan, X. (2020). Quantum computational chemistry. *Reviews of Modern Physics, 92*(1), 015003. https://doi.org/10.1103/RevModPhys.92.015003
8. Peruzzo, A., McClean, J., Shadbolt, P., *et al.* (2014). A variational eigenvalue solver on a photonic quantum processor. *Nature Communications, 5*, 4213. https://doi.org/10.1038/ncomms5213
9. Romero, J., Olson, J. P., & Aspuru-Guzik, A. (2018). Strategies for quantum computing molecular energies using the unitary coupled cluster ansatz. *Quantum Science and Technology, 4*(1), 014008. https://doi.org/10.1088/2058-9565/aad3e4
10. Sun, Q., Berkelbach, T. C., Blunt, N. S., *et al.* (2020). PySCF: The Python-based simulations of chemistry framework. *WIREs Computational Molecular Science, 10*(1), e1340. https://doi.org/10.1002/wcms.1340
11. Tilly, J., Chen, H., Cao, S., *et al.* (2022). The Variational Quantum Eigensolver: A review of methods and best practices. *Physics Reports, 986*, 1–128. https://doi.org/10.1016/j.physrep.2022.08.003
12. Wecker, D., Bauer, B., Clark, B. K., Hastings, M. B., & Troyer, M. (2015). Progress towards practical quantum variational algorithms. *Physical Review A, 92*(4), 042303. https://doi.org/10.1103/PhysRevA.92.042303
13. Yordanov, Y. S., Armaos, V., Gidney, C., *et al.* (2021). Quantum algorithm for chemistry with fewer qubits. *PRX Quantum, 2*(4), 040332. https://doi.org/10.1103/PRXQuantum.2.040332