Review

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Bridging Computational Chemistry and Quantum Computing for Next-Generation Drug Discovery & Development

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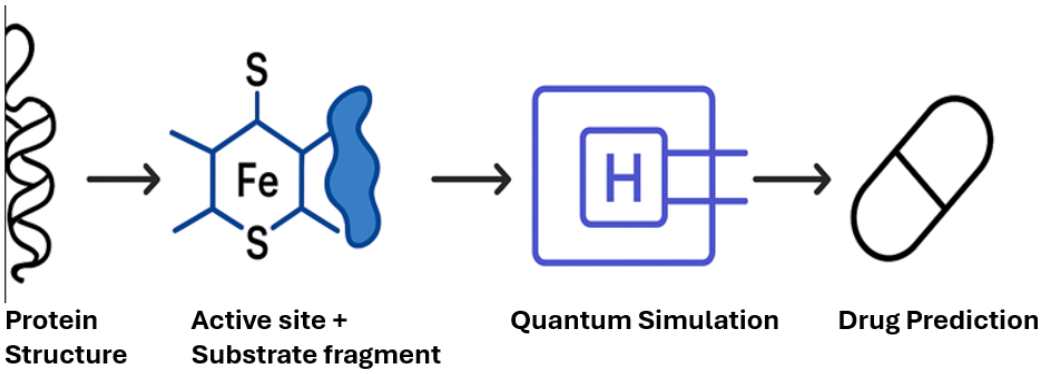

Abstract: Quantum chemistry plays a crucial role in advancing fundamental understanding of chemical processes and driving innovation in energy, medicine, and materials science. Recent progress in quantum computing has opened new possibilities for molecular simulations that are beyond the practical limits of classical approaches. Academic studies have demonstrated hybrid Density Functional Theory (DFT) and Variational Quantum Eigensolver (VQE) benchmarks on small transition-metal systems, such as iron porphyrin and heme analogues, using current noisy intermediate-scale quantum (NISQ) hardware. Although full-scale simulations of complex biological systems such as the complete Cytochrome P450 (CYP450) active site remain a long-term goal due to limitations

in qubit numbers, coherence times, and error correction, the underlying methodologies are now well established. At present, quantum chemistry applications in drug discovery remain largely experimental, and widespread practical medical impact is expected to require further technological advances over the next 5–10 years. Nevertheless, quantum software and algorithm development for chemical applications is progressing rapidly. This perspective summarizes recent advances in quantum computing algorithms, hardware, and software relevant to chemistry, and critically discusses the remaining challenges and opportunities for applying quantum computing to chemical problems, with particular emphasis on drug discovery and development.

Keywords: Quantum chemistry, Quantum physics, Quantum computing, Scientific exploration, technological innovation, Drug Discovery & Development

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Introduction

Quantum mechanics provides the fundamental framework for describing matter and energy at atomic and subatomic length scales, where classical physics is no longer adequate. At these scales, particles exhibit wave–particle duality, quantized energy levels, and probabilistic behavior, phenomena that are successfully captured by the mathematical formalism of quantum theory [1,2]. Rather than following deterministic trajectories, microscopic systems are described by wavefunctions whose measurable properties are obtained statistically through repeated observations.

Quantum chemistry applies the principles of quantum mechanics to chemical systems in order to describe electronic structure, chemical bonding, spectroscopy, and reaction dynamics. Established computational methods such as Hartree–Fock theory, density functional theory (DFT), and post–Hartree–Fock approaches have enabled accurate predictions for a wide range of molecular properties [3,4]. However, the computational cost of these methods increases rapidly with system size, particularly for strongly correlated systems such as transition-metal complexes, metalloenzymes, and excited-state processes. As a result, practical simulations often rely on approximations that can limit predictive accuracy [5,6].

Quantum computing offers a fundamentally different approach to molecular simulation by representing electronic wavefunctions directly on quantum hardware. Unlike classical bits, quantum bits (qubits) exploit superposition and entanglement, allowing quantum computers

to encode and manipulate many-body quantum states more naturally [11,12]. This has motivated the development of hybrid quantum–classical algorithms, such as the Variational Quantum Eigensolver (VQE), which are designed to operate on near-term noisy intermediate-scale quantum (NISQ) devices [15,18].

While quantum computers are still in an early stage of development, proof-of-concept studies have demonstrated their potential for quantum chemistry applications, including small-molecule simulations and transition-metal model systems [16-18]. These advances suggest that quantum computing may eventually complement classical electronic-structure methods, particularly in areas where strong electron correlation limits the accuracy of conventional approaches. In this context, quantum computing is increasingly viewed as a promising tool for molecular modeling and, in the longer term, for applications in drug discovery and development [19-21].

Classical computers: Classical computers operate using bits, which can be either a 0 or 1. They process information step by step using algorithms, with each bit independent from the others. This makes them reliable and well-suited for most everyday tasks, but they can become slow when solving highly complex problems.In a classical computer, the bit is the most basic unit of information. Each bit can exist in only one of two states: 0 (off/low voltage) and 1 (on/high voltage) as shown in Figures 1 and 2. These bits are the building blocks of all digital operations [7-8]. Here's the role they play in classical computer operation:

1. Information Representation
    a. Numbers, text, images, and even videos are ultimately broken down into sequences of bits (binary code).
    b. For example, the letter A in ASCII is represented as 01000001.
2. Data Processing
    a. Bits flow through circuits made of transistors (tiny switches).
    b. Logic gates (AND, OR, NOT, etc.) use bits as inputs to produce outputs, enabling arithmetic operations, comparisons, and decision-making.
3. Memory and Storage
    a. Bits are stored in memory cells (RAM, hard drives, SSDs).
    b. Each cell records a 0 or 1, and groups of bits form larger units like bytes (8 bits).
4. Communication
    a. Bits are transmitted as electrical signals, light pulses (in fibre optics), or radio waves for data transfer between systems.
5. Deterministic Operation

a. At any point, a bit has a definite state (either 0 or 1).
b. This deterministic nature makes classical computers predictable and reliable but also limits their ability to handle extremely complex problems compared to quantum computers.

Bits are the foundation of classical computing, serving as the universal language that allows computers to represent, process, store, and transmit all kinds of information. In classical computing the bits of binary are represented by 1 and O. Let us consider there is a two-bit space to represent four combinations. Suppose it is a three-bit space we can represent 8 combinations. Hence there is n-bit space, we can represent 2^n combinations. But to change the states of the data from 00 to 10 as a sequence of operations (00, 01, 11, 10) the conventional process required four (04) clock pulses [9,10].

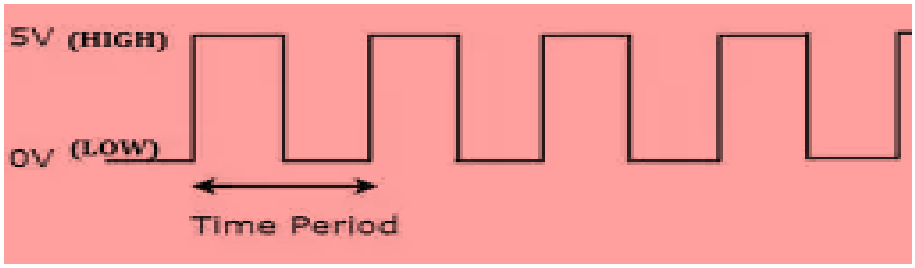

Figure 1. Conventional data representations

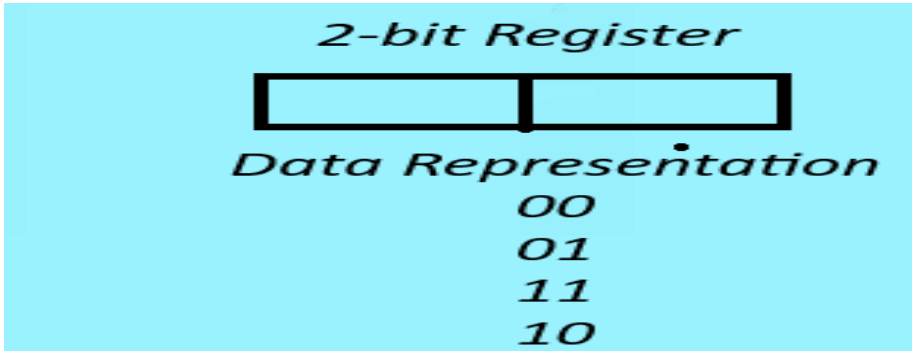

Figure 2. Low and High Conventional data representations

Quantum computers: Quantum computers on the other hand, use qubits. Unlike bits, qubits can exist in a superposition of 0 and 1 at the same time. Qubits also interact through a property called entanglement, which allows them to share information and influence one another In a quantum computer, the basic unit of information is the qubit (quantum bit). While it serves a similar purpose to a classical bit, its behaviour is very different because it is governed by the principles of quantum mechanics. In classical computing, representing all possible configurations requires sequential processing and large memory resources, leading to increased computational time and storage demands for complex problems. In Quantum

computing to represent the data in qubits we are using one fundamental technique, that is superimposition [11,12]. Here a quantum state is represented as a linear combination of conventional computing states. The following diagram shows the basic representation of Qubits 0 and 1 as shown in Figures 3 and 4.

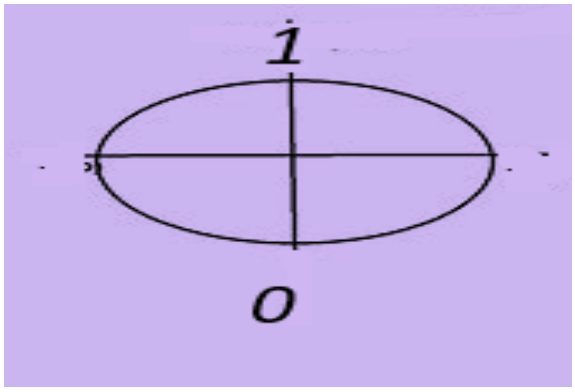

Figure 3. Quantum bit Representation

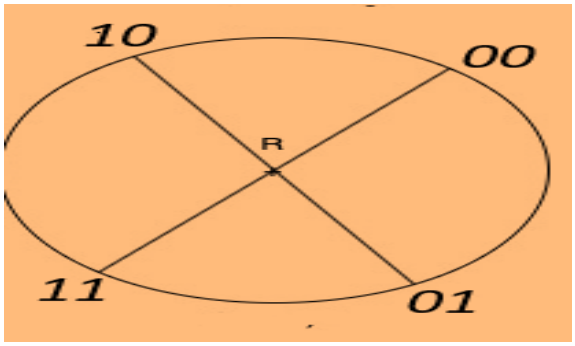

Figure 4. Quantum bit combination Through superimposition

To represent the combination of these two-bits that is (00, 01, 11 and 10) representation in the perspective of quantum computing is, suppose we represent the same thing in the layered structure [12,14]. That is at the same time or instinct all the combinations of 2-bits are possible as shown in Figures 5 and 6.

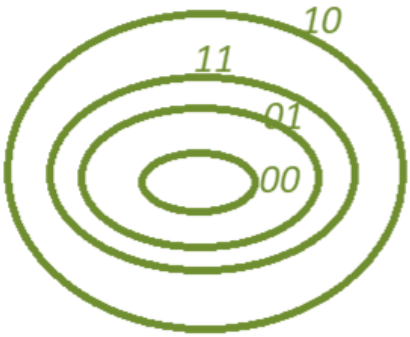

Figure 5. Two-dimensional view of layer structure

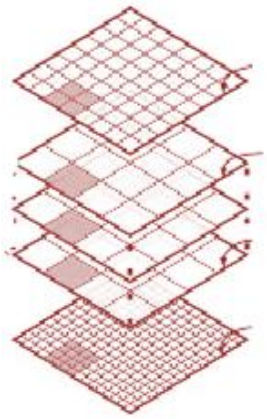

Figure 6. Multi-dimensional view of layer structure

Fundamental Concepts of Quantum Computing

1. Information Representation
   a) A classical bit can only be 0 or 1.
   b) A qubit can exist in a superposition of both states at once.
   c) Mathematically: $|\psi\rangle=\alpha|0\rangle+\beta|1\rangle$
      where α and β are probability amplitudes with $|\alpha|^2+|\beta|^2=1$
2. Parallelism in Computation
   a) A system of n qubits can represent 2^n states simultaneously.
   b) This parallelism allows quantum computers to process huge amounts of information, useful for tasks like optimization, cryptography, and molecular simulations.
3. Entanglement for Correlation
   a) Entanglement links qubits so that the state of one instantly affects the state of another, even across distance.
   b) This correlation is stronger than anything achievable with classical bits, enabling faster problem-solving and secure communication.
4. Quantum Interference
   a) Quantum algorithms rely on interference to amplify correct outcomes and cancel wrong ones.
   b) This "steering" of probabilities gives quantum algorithms their efficiency advantage.
5. Probabilistic Nature
   a) When measured, a qubit collapses to either 0 or 1 with probabilities $|\alpha|^2$ and $|\beta|^2$
   b) Before measurement, qubits hold multiple possibilities, which is the source of quantum computational power [13,14,15].

Qubits allow quantum computers to store and process information in ways far beyond classical bits. Through superposition, entanglement, and interference, qubits make it possible to solve problems that would take classical computers millions of years. Because of these features, quantum computers can explore many possible solutions simultaneously instead of sequentially as shown in Figure 7 and comparison of bits vs qubits as shown in Table 1. This parallelism is what gives them the potential to solve certain types of problems such as drug discovery, cryptography, and optimization much faster than classical computers [13,14].

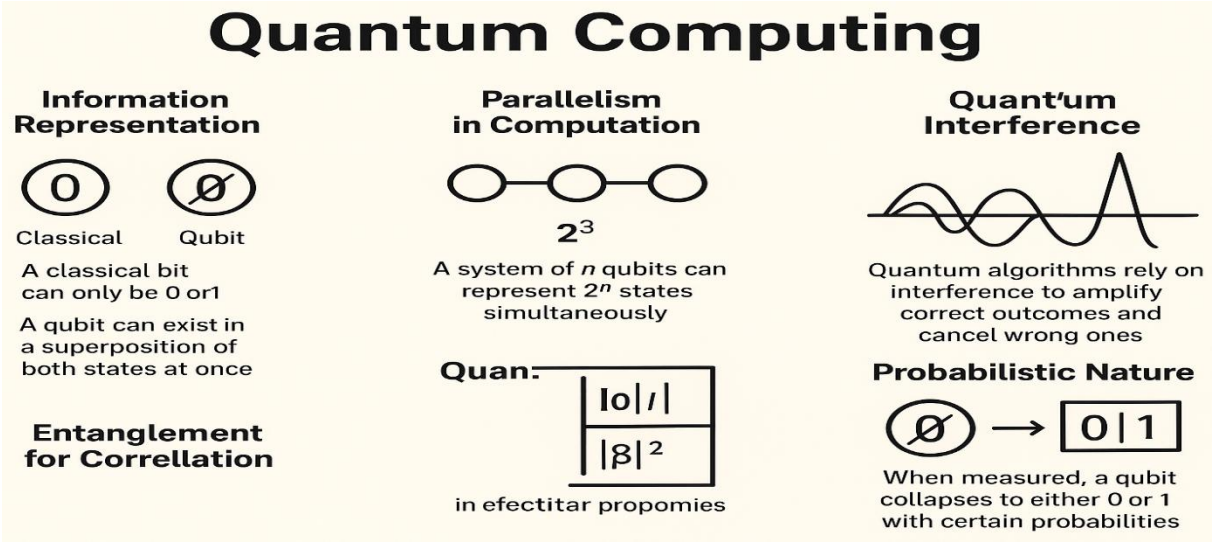

Figure 7. Transformation of conventional to quantum computing

Table 1. Classical Bit vs. Quantum Bit (Qubit): Feature-by-Feature Overview

Feature	Classical Bit	Quantum Bit (Qubit)
Basic state	Either 0 or 1	Can be 0, 1, or a superposition of both
Representation	Binary values (0 = off, 1 = on)	Quantum state
Parallelism	Represents one state at a time	Represents many states simultaneously
Correlation	Independent unless	Can be entangled (strongly correlated)
Computation	programmed	Probabilistic, uses interference to find solutions
Storage	Deterministic, step-by-step	1 qubit stores a combination of 0 and 1
Scalability	1-bit stores either 0 or 1	(more information capacity)
Measurement	n bits = n pieces of information	n qubits = 2n2^n states simultaneously
Technology	Directly reveals stored value	Collapses to 0 or 1 with certain probabilities
Examples of	Transistors, silicon circuits	Superconductors, trapped ions, photons, etc.
use	Word processing, web browsing, standard computation	Quantum simulation, cryptography, optimization, drug design

Computational Framework

The quantum-enhanced drug discovery workflow integrates classical electronic-structure methods with near-term quantum algorithms [15,16]. Initially, biologically relevant targets such as enzyme active sites or ligand–receptor complexes are identified and pre-processed using classical techniques, including molecular docking, molecular dynamics, and density functional theory (DFT), to generate optimized geometries and representative conformations. From these calculations, a chemically meaningful active space is constructed by selecting orbitals with significant deviation from full or empty occupation, typically guided by automated approaches such as atomic valence active space (AVAS) selection or orbital entanglement measures [35,36]. The resulting second-quantized electronic Hamiltonian is mapped onto qubits using standard fermion-to-qubit transformations (e.g., Jordan–Wigner or Bravyi–Kitaev mappings), with symmetry exploitation employed to reduce qubit counts. Ground- and low-lying excited-state energies are then evaluated using hybrid quantum–classical algorithms, primarily the Variational Quantum Eigensolver (VQE) with chemically motivated or adaptive ansätze. Quantum circuits are executed on simulators and available noisy intermediate-scale quantum (NISQ) hardware with appropriate error-mitigation strategies. Finally, quantum-derived energies and wavefunctions are validated against classical high-level methods and reintegrated into the drug discovery pipeline for ligand ranking, reaction-barrier estimation, and metabolism prediction [31,34].

Drug Discovery Target and Computational Objective

The biological target is defined as a chemically relevant subsystem, such as an enzyme active site or ligand–receptor binding pocket, extracted from experimental crystal structures (resolution ≤ 2.5 Å) or high-quality homology models. The primary computational objectives include prediction of relative binding energies (ΔE or ΔG), spin-state energetics, and reaction barriers (ΔE‡) with a target accuracy of ∼1 kcal·mol^{-1}, which is typically required for chemically meaningful ranking of drug candidates.

Classical Pre-Screening and Model Preparation

Initial structure preparation and conformational sampling are performed using classical molecular docking and molecular dynamics (MD) simulations. MD trajectories of 50–100 ns are generated to identify representative conformations of the binding site. Geometry optimizations of the chemically active region are carried out using DFT (e.g., B3LYP or PBE0 functionals with a double-ζ or triple-ζ basis set), providing reference orbitals and electron densities for subsequent quantum calculations. QM/MM partitioning is applied where the quantum region

typically contains 50–150 atoms, while the remaining protein environment is treated classically [32].

Active-Space Construction for Quantum Simulation

Selection of the active space is guided by quantitative criteria derived from classical electronic-structure calculations. Orbitals with natural orbital occupation numbers deviating significantly from 2.0 or 0.0 (typically >1.98 or <0.02 excluded) are prioritized. In practice, orbitals with occupations in the range of ~0.02–1.98 are considered active. Automated approaches such as the Atomic Valence Active Space (AVAS) method or orbital entanglement analysis (based on single-orbital entropy values >0.1) are used to identify chemically relevant orbitals. For near-term quantum hardware, active spaces are typically limited to 8–20 spatial orbitals (corresponding to 16–40 spin orbitals), requiring approximately the same number of qubits after mapping [35].

Hamiltonian Mapping and Qubit Encoding

The second-quantized electronic Hamiltonian constructed from the selected active space is mapped onto qubits using standard fermion-to-qubit transformations, such as Jordan–Wigner or Bravyi–Kitaev mappings. Symmetry exploitation, including particle-number conservation and spin-parity symmetries, enables qubit tapering, reducing the total qubit requirement by 2–6 qubits depending on the system. For example, an active space with 20 spin orbitals can often be reduced from 20 to ~14–16 qubits after symmetry reduction [33].

Quantum Algorithm Selection

Hybrid quantum–classical algorithms are chosen based on accuracy and hardware constraints. The Variational Quantum Eigensolver (VQE) is employed for ground-state energy calculations, targeting convergence thresholds of 10^{-3}–10^{-4} Hartree. For excited states, extensions such as state-averaged VQE or equation-of-motion VQE (EOM-VQE) are applied. Quantum Phase Estimation (QPE) is discussed as a future approach for high-precision energies, requiring fault-tolerant hardware and circuit depths exceeding 10^6 logical gates [18,22-24].

Ansatz and Circuit Optimization

Parameterized ansätze are selected to balance chemical expressiveness and circuit depth. Chemically motivated ansätze such as UCCSD or its truncated variants (e.g., UpCCGSD) are used, with parameter counts typically ranging from 50 to 300. Adaptive methods (ADAPT-VQE) are employed to construct problem-specific circuits, often reducing circuit depth by 30–50% compared to fixed ansätze. Initial parameter values are seeded using classical Hartree–Fock or CASSCF amplitudes to accelerate convergence.

Quantum Hardware Execution and Error Mitigation

Quantum circuits are executed on both noiseless simulators and real NISQ devices with gate fidelities in the range of 99.5–99.9%. Measurement shot counts of 10^3–10^5 per expectation value are used to control statistical error below ~1 mHartree. Error mitigation strategies include readout calibration, symmetry verification, zero-noise extrapolation, and measurement grouping, which together can reduce total energy errors by a factor of 2–5 relative to unmitigated results [37,38].

Classical Post-Processing and Validation

Quantum-computed energies and wavefunctions are validated against classical high-level methods such as CASSCF or CCSD(T) for reduced models, with acceptable deviations typically within 1–2 kcal·mol^{-1}. For binding or reaction studies, quantum results are combined with classical free-energy methods (MM/PBSA or thermodynamic integration) to obtain chemically relevant observables.

Integration into the Drug Discovery Workflow

Validated quantum-enhanced results are reintegrated into the drug discovery pipeline for ligand ranking, lead optimization, and metabolism prediction. Performance is benchmarked against purely classical workflows in terms of accuracy, computational cost, and scalability. Reporting includes explicit disclosure of active-space size, qubit count, circuit depth, number of parameters, and achieved energy errors to ensure reproducibility and meaningful comparison across studies.

Quantitative Criteria for Active-Space Selection

Active-space selection is guided by explicit numerical thresholds derived from preliminary classical electronic-structure calculations. Natural orbitals obtained from Hartree–Fock, DFT, or CASSCF calculations are analyzed, and orbitals with occupation numbers significantly deviating from closed-shell values are selected. In practice, orbitals with natural occupation numbers in the range 0.02–1.98 are included in the active space, while orbitals with occupations >1.98 (doubly occupied) or <0.02 (virtual) are excluded. For automated selection, the Atomic Valence Active Space (AVAS) method is employed to include orbitals with significant overlap (typically >10–15%) with predefined atomic valence orbitals relevant to the chemical problem. Alternatively, orbital entanglement analysis is used, where orbitals with single-orbital entropy values exceeding ~0.1 are identified as strongly correlated and retained. To ensure feasibility on near-term quantum hardware, the final active space is typicall restricted to 8–20 spatial orbitals (corresponding to 16–40 spin orbitals), resulting in a comparable number of qubits after fermion-to-qubit mapping and symmetry reduction [35-36].

Computational Results and Implications

Hybrid quantum–classical simulations reported in the literature demonstrate that near-term quantum algorithms can reproduce chemically meaningful trends for small molecular systems and reduced models of transition-metal complexes relevant to drug discovery. Benchmark studies using the Variational Quantum Eigensolver (VQE) on noisy intermediate-scale quantum (NISQ) hardware show that ground-state energies for small molecules and active-site fragments can be obtained with errors on the order of a few millihartree to a few kilocalories per mole when compared with high-level classical references, depending on active-space size, circuit depth, and error-mitigation strategy. For strongly correlated systems, such as iron–porphyrin and FeMoco fragments, quantum approaches are able to capture qualitative features of electronic structure, including spin-state ordering, that are challenging for standard density functional approximations. Although present hardware limits simulations to reduced active spaces, these results indicate that quantum methods scale more favorably with increasing electronic complexity than exact classical treatments. When integrated into drug discovery workflows, quantum-derived energies and wavefunctions can enhance the description of metal-center reactivity, enzyme catalysis, and ligand–binding interactions, complementing classical DFT and QM/MM approaches. Overall, current results confirm that quantum computing does not yet replace established computational chemistry methods, but it already provides a viable and systematically improvable framework for treating strongly correlated electronic problems that are central to future applications in drug discovery and development.

Quantum Computers in Drug Discovery & Development

Quantum computers operate directly on quantum states, enabling a natural representation of electronic wave functions. This allows algorithms such as VQE to estimate molecular ground-state energies with accuracy that is less dependent on empirical approximations than conventional DFT methods. ”Algorithms like the Variational Quantum Eigensolver (VQE) and Quantum Phase Estimation (QPE) can compute the ground-state energy of molecules, a critical step in predicting stability and reactivity [15,16,17-18].

Molecular Simulation & Quantum Chemistry

a. Traditional computers struggle to simulate complex molecules due to exponential scaling.
b. Quantum computers can directly model electronic structures and molecular interactions, enabling accurate prediction of chemical properties.
c. This accelerates identification of promising drug candidates.
d. At the heart of drug discovery is understanding how a drug molecule interacts with a biological target (like a protein or enzyme).
e. This requires simulating electronic structures, bonding, and chemical reactions at the atomic level.
f. Classical computers use approximations (like Density Functional Theory, DFT), but for large molecules these calculations become impossibly complex because the number of interactions grows exponentially.

Simulation of the FeMoco Enzyme (Nitrogenase)

The FeMoco (iron–molybdenum cofactor) enzyme is responsible for nitrogen fixation in nature (turning atmospheric nitrogen into ammonia). Simulating FeMoco is extremely difficult for classical computers due to its complex electron interactions [19-21]. A quantum computer, using VQE, has been demonstrated (IBM & Google research) to better approximate its electronic structure. This kind of simulation can be extended to drug molecules binding to protein active sites, helping design drugs with better binding affinity [22-25].

FeMoco is hard for classical computers

a. Many electrons, many orbitals: The FeMoco active site has multiple metal centers (Fe, Mo, S clusters) with strong electron correlation.
b. Exponential scaling: Classical methods like Full Configuration Interaction (FCI) scale exponentially with the number of orbitals; approximations (DFT, coupled cluster) break down for such strongly correlated systems.

Quantum approach: Variational Quantum Eigensolver (VQE)

Regarding Quantum parta parameterized quantum circuit prepares a trial wavefunction for the molecule's electronic structure [26-28]. Latera classical optimizer updates the circuit parameters to minimize the expected energy $\langle\psi(\theta)|H|\psi(\theta)\rangle$. Then it works like Quantum hardware can naturally encode the full electronic state (which is huge for classical computers) with a polynomial number of qubits [29]. The results so far areIBM, Google, and academic groups have demonstrated proof-of-concept simulations of fragments of FeMoco, achieving better approximations than comparable classical resources [30].

Extending to drug discovery

Drug–target binding involves with Accurate binding energies and Conformational flexibility of the drug and protein active site. Solvent effects point of view Quantum algorithms like VQE (and more advanced ones such as Quantum Phase Estimation, q-DRIFT, or quantum machine learning models) can:

a. Compute highly accurate interaction energies of drug molecules with protein active sites.
b. Model transition states and reaction pathways (important for enzyme inhibitors).
c. Provide better potential energy surfaces than current DFT or MM/GBSA approximations.

Because quantum computers can natively represent the molecular wavefunction, they could, at scale, give drug developers a much more faithful picture of how a small molecule binds to a protein or enzyme site leading to:

a. Better ranking of candidate molecules (affinity prediction).
b. Rational design of modifications to improve potency or selectivity.
c. Reduced reliance on trial-and-error wet-lab screening [31].

Present & near-term picture

Current quantum hardware is "noisy intermediate scale" (NISQ): tens to hundreds of qubits, limited coherence. Hybrid quantum–classical workflows (like VQE) are the most promising now. Early industry pilots (e.g., pharmaceutical companies partnering with IBM, Google, Quantum) are testing quantum algorithms on small drug-like fragments and active-site models as shown in Table 2.

Table 2. Comparison of Classical and Quantum (VQE) Approaches for Molecular Simulation

Aspect	Classical Simulation	Quantum (VQE) Simulation
Scaling	Exponential with system size	Polynomial with qubits
Accuracy for FeMoco	Approximations break down	Can represent full correlated state
Drug Binding Simulation	Force fields / DFT approximations	Direct quantum-mechanical binding energies
Stage	Mature	Early but rapidly advancing

3.8 Role of Quantum Computers in medicine

Quantum computing in medicine is a rapidly growing research area, and while still in early stages, it holds huge potential to transform healthcare. The other two key areas of quantum technology are quantum communication, which focuses on ultra-secure information transfer using the principles of quantum entanglement and quantum key distribution, and quantum sensing, which leverages quantum states to achieve measurements of unprecedented precision in fields like navigation, medical imaging, and environmental monitoring. Together, these three areas computing, communication, and sensing are forming the backbone of the

so-called second quantum revolution. Unlike the first, which gave us transistors, lasers, and MRI machines, this new wave is expected to transform industries by harnessing the unique properties of superposition, entanglement, and quantum coherence at a practical scale. Quantum computers will be able to simulate a key structure of Cytochrome P450, an enzyme found in humans, with higher accuracy in less time than classical computers [32,33].

Cytochrome P450 (CYP450) enzymes are heme-containing monooxygenases involved in drug metabolism and biosynthesis.

a. The active site is a heme iron coordinated by a porphyrin ring and axial ligands (often cysteine).
b. It binds and activates O_2 and transfers it to substrates a reaction very sensitive to electronic structure.
c. Understanding the spin states, intermediate species (Fe(III)/Fe(IV)=0), and ligand binding is critical for drug design and toxicity prediction [32,33].

Classical quantum chemistry (DFT, multireference methods) gives insights, but for the highly correlated iron–oxo centre (like in FeMoco) approximations can miss key states.

Quantum approach for CYP450 active site

The key cluster of the CYP450 active site (e.g., the heme + Fe + cysteine + substrate fragment) and map it to a quantum algorithm [34,35].

a) Hamiltonian building:
    a. Choose an appropriate active space (e.g., Fe - d orbitals + porphyrin π orbitals + substrate orbitals).
    b. Derive the electronic Hamiltonian in second quantization.
b) Quantum algorithm:
    a. Use VQE on a quantum processor to find ground and excited states.
    b. Calculate potential energy surfaces for different spin and oxidation states.
    c. Predict reaction barriers for O_2 activation or substrate hydroxylation.
c) Classical optimizer:
    a. Classical computer tunes the quantum circuit parameters.
    b. Combine with QM/MM to include the protein environment as shown in Table 3.

Table 3. Classical vs Quantum (VQE) Approaches to Transition-Metal Chemistry

Problem	Classical Approach	Quantum Approach (VQE)
Electronic correlation (iron–oxo states)	Multireference CI but limited to small active spaces	Larger active spaces, direct correlated wave function
Spin-state energetics	Often DFT-dependent, may miss predict	Can directly compute singlet/triplet/quintet states
Drug metabolism Predictions	Empirical or approximate QM/MM	More accurate transition states for substrate oxidation

Pipeline (visual idea)

Protein structure (CYP450)

→ Extract active site + substrate fragment

→ Build molecular Hamiltonian

→ Encode into qubits (Jordan–Wigner / Bravyi–Kitaev mapping) [26,27]

→ Quantum circuit (VQE)

→ Energies, spin states, reaction barriers

→ Feed back into drug design (predict metabolism, design inhibitors)

This is exactly analogous to the FeMoco case, but now for an enzyme relevant to drug metabolism. Pipeline Representation of Protein structure (CYP450) as shown in Figure 8.

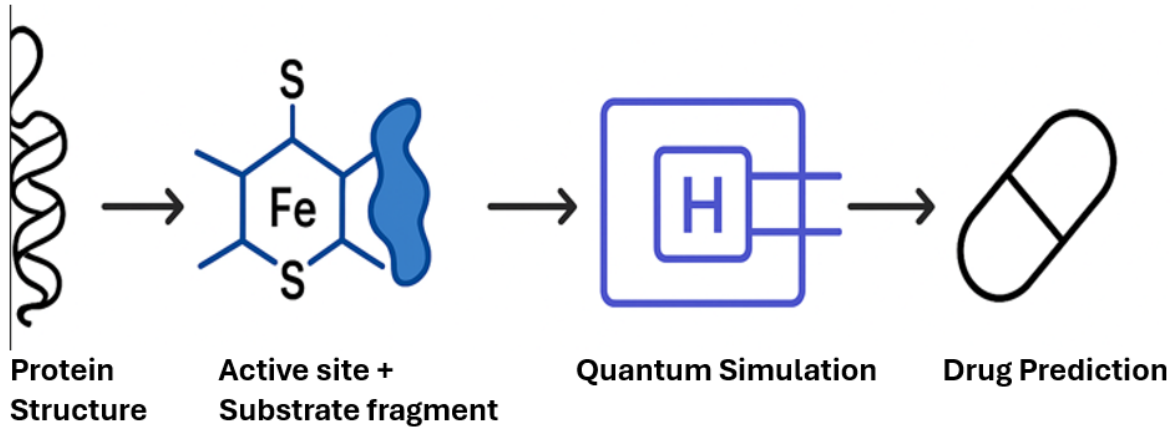

Figure 8. Pipeline Representation of Protein structure (CYP450)

Current status

- Academic groups have done DFT + VQE style benchmarks on small heme analogues (like iron porphyrin complexes) on today's hardware.
- Full CYP450 active site simulations are still future work because of qubit and error-correction limitations, but the methodology is established [36,37,38-39].

Conclusions

1. Bits are the foundation of today's classical computers: simple, reliable, deterministic. Qubits are the building blocks of quantum computers: complex, probabilistic, and vastly more powerful for certain specialized tasks.Quantum molecular simulation allows researchers to study drug–target interactions with unprecedented accuracy, at present it is a cutting down trial-and-error lab work.

2. Quantum computing is emerging as a transformative tool in pharmaceutical research. By enabling highly accurate simulation of molecular structures, protein–ligand interactions, and reaction pathways, quantum computers can significantly reduce the time and cost required for early-stage drug discovery. Their ability to handle complex combinatorial problems allows faster screening of drug candidates, optimization of molecular properties, and prediction of adverse effects, which are often challenging for classical computers.

3. Although practical, large-scale quantum computers are still under development, early demonstrations using hybrid quantum–classical approaches (such as VQE and QAOA) already show promising improvements in molecular modelling and lead optimization. As hardware scales and error rates drop, quantum computing is expected to complement traditional computational chemistry and AI methods, accelerating the journey from concept to clinic. Ultimately, this technology could shorten development timelines, lower R&D costs, and enable the discovery of safer and more effective therapies.

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