A Perspective on Quantum Computing Applications in Quantum Chemistry using 25–100 Logical Qubits

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The intersection of quantum computing and quantum chemistry represents a promising frontier for achieving quantum utility in domains of both scientific and societal relevance. Owing to the exponential growth of classical resource requirements for simulating quantum systems, quantum chemistry has long been recognized as a natural candidate for quantum computation. This perspective focuses on identifying scientifically meaningful use cases where early fault-tolerant quantum computers, which are considered to be equipped with approximately 25–100 logical qubits, could deliver tangible impact. We highlight near- to mid-term opportunities in algorithm and software design, discuss representative chemical problems suited for quantum acceleration, and propose strategic roadmaps and collaborative pathways for advancing practical quantum utility in quantum chemistry.

I. INTRODUCTION AND MOTIVATION

This year marks a significant milestone—roughly a century since the formulation of quantum mechanics fundamentally reshaped our understanding of matter at the atomic and molecular level [1–3]. The Schrödinger equation, introduced during this transformative period, provided the theoretical bedrock for quantum chemistry, enabling, in principle, the prediction of chemical properties and reactivity from first principles, famously demonstrated for the hydrogen molecule [4]. Over the subsequent 100 years, the field has witnessed impressive advances, with the development and application of sophisticated classical computational methods, such as Density Functional Theory (DFT) [5–7] and wave function-based approaches like Coupled Cluster (CC) theory [8–10], achieving remarkable success in explaining and predicting chemical phenomena [11, 12].

Despite a century of progress and the power of established classical algorithms, substantial challenges remain. The inherent complexity of the quantum many-body problem, the very challenge laid barely by quantum mechanics itself, continues to limit the accuracy and applicability of classical methods, particularly in the treatment of (i) strongly correlated electronic systems (e.g., modeling complex catalytic sites like FeMoco [13]), (ii) the description of complex excited states crucial for photochemistry and materials science [14], (iii) the simulation of open quantum dynamics governing system-environment interactions [15], and (iv) the accurate prediction of weak interaction and thus transition state, which is critical to describe reaction kinetics [16]. These enduring limitations, stemming di-

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rectly from the exponential growth of the Hilbert space with system size, motivate the exploration of fundamentally different computational paradigms. Quantum computational approaches, which leverage quantum phenomena directly, offer a potential pathway to supplement or even surpass classical techniques by tackling these intrinsically quantum problems more naturally, as envisioned early on by Feynman [17] and Lloyd [18], and extensively reviewed ever since [19–21].

This perspective focuses on identifying strategies, opportunities, and roadblocks relevant to performing quantum chemistry simulations using quantum hardware anticipated in the near-to-intermediate future—specifically, devices possessing approximately 25–100 logical qubits. This regime represents a crucial transitional phase, bridging the current era of noisy intermediate-scale quantum (NISQ) devices [22] and the long-term vision of large-scale, fully fault-tolerant quantum computing [23], known as Fault-Tolerant Application-Scale Quantum (FASQ) [24]. This intermediate scale presents a unique window of opportunity to potentially demonstrate impactful quantum computations, possibly achieving quantum utility for specific, well-chosen chemical problems. Success in this era will likely hinge on leveraging resource-aware algorithm design [25], developing robust hybrid quantum-classical workflows [26], and fostering interdisciplinary co-design between quantum algorithms, chemistry domain expertise, and hardware capabilities [27].

Realizing this opportunity necessitates a clear-eyed understanding of both the burgeoning capabilities, demonstrated by recent hardware milestones [28–31], and the significant constraints of near-term fault-tolerant quantum hardware platforms. Before delving into specific quantum chemistry applications and the algorithms tailored for this 25–100 logical qubit regime, we first briefly overview the rapidly evolving landscape of quantum hardware development and further articulate the motivation for concentrating efforts within this specific computational resource range.

II. THE 25–100 LOGICAL QUBIT REGIME: A TRANSITIONAL LANDSCAPE

Recent advances in quantum hardware have significantly improved the prospects for achieving early fault-tolerant quantum computations. While current NISQ devices have achieved important milestones, including small-scale quantum simulations [32, 33] and sophisticated error mitigation [34], scalable quantum utility requires logical qubits protected by quantum error correction (QEC) [22, 35].

Implementing a single logical qubit today demands thousands of physical qubits, depending on error rates and the chosen code, such as the surface code [23, 36, 37]. Nevertheless, improvements in coherence times, gate fidelities, and system integration across leading platforms—including superconducting qubits [29, 38], atom array [30], trapped ions [39, 40], and photonic architectures [41, 42]—suggest that processors comprising 25–100 logical qubits could become available within the next several years [28, 43–45].

In comparison with long-term strategic directions, the 25–100 logical qubit regime marks a pivotal near-term threshold in the evolution of quantum computing applications in quantum chemistry (see Figure 1). Devices in this range may be the first to enable meaningful quantum chemistry simulations that are intractable on classical computers, such as accurately modeling complex molecules [13, 25]. However, the opportunity comes with substantial caveats: these early fault-tolerant systems will still face non-negligible logical error rates, limited coherence times relative to computation depth, and practical constraints on connectivity, measurement, and classical I/O [46].

Progress in this regime demands a re-evaluation of what constitutes "quantum utility" in chemistry [47]. It is not solely about outperforming classical solvers in compute time or accuracy for all problems, but rather about delivering new scientific insights into problems that are intrinsically quantum and difficult to treat or beyond classical methods—including strongly correlated electrons [10], quantum coherence in dynamics [48], and environmental interactions [15].

Development efforts are therefore increasingly centered around hybrid algorithms [26], embedding techniques [49–60], and variational methods [61] that operate with shallow circuits or make optimal use of limited logical qubit counts. These strategies aim to optimize the use of limited quantum resources while interfacing seamlessly with classical simulation frameworks.

This regime is particularly well-suited for active space quantum simulations, where a judiciously chosen set of orbitals—often those associated with strong correlation or reactive behavior—is treated on a quantum computer, while classical components handle the weakly correlated environment. Techniques such as downfolding [62–72] and quantum embedding [49–60] provide viable pathways to construct effective Hamiltonians for such active spaces.

In addition to ground-state energy estimation, quantum dynamics is emerging as an area where early utilities may arise [21, 48]. Simulating time-dependent processes, especially in open systems or photoinduced transformations, poses considerable challenges for classical methods due to memory bottlenecks and entanglement growth [73, 74]. Quantum processors may offer more efficient routes for handling such inherently quantum phenomena using algorithms like Trotterization or Qubitization [75–77].

Collectively, these considerations underscore the need for focused, resource-aware, and problem-specific approaches in the early fault-tolerant era of quantum computing. The following sections explore these directions in detail, with an emphasis on bridging algorithmic innovation, hardware development, and domain relevance.

III. OPPORTUNITIES IN QUANTUM CHEMICAL SIMULATIONS

Quantum chemistry presents a set of grand challenges where quantum computers—even at the scale of 25–100 logical qubits—are expected to make meaningful contributions. Rather than aiming for a wholesale replacement of classical electronic structure methods, progress is anticipated through hybrid approaches that integrate quantum computing with classical techniques, high-performance computing

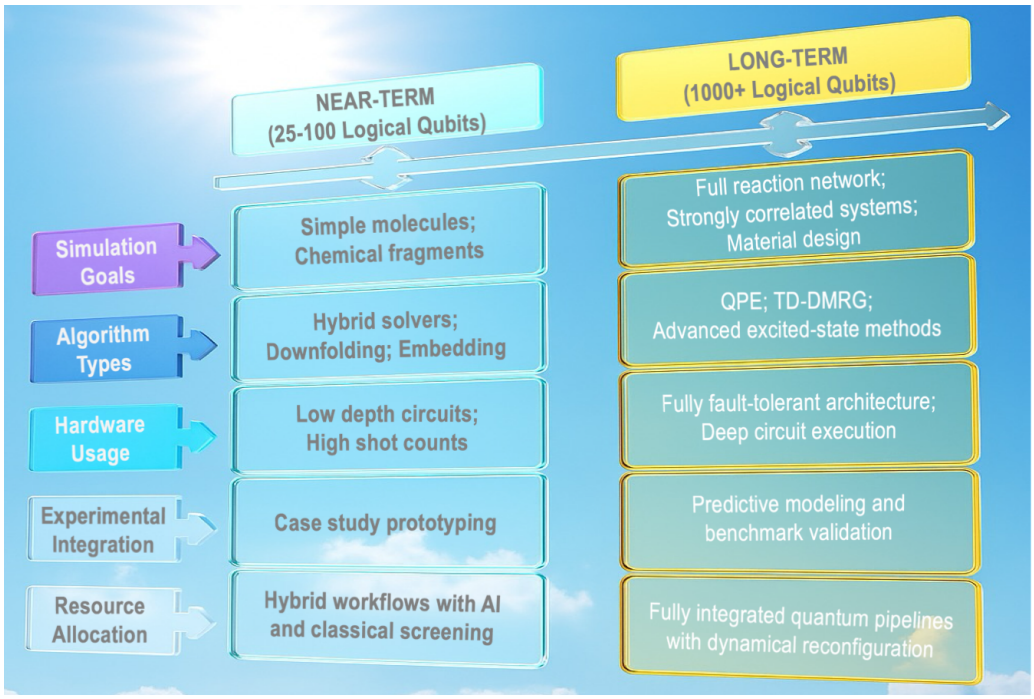

Figure 1. Strategic directions for quantum chemical simulation at different scales.

(HPC), and artificial intelligence (AI). This synergy enables both targeted enhancement of computational workflows and the exploration of scientific regimes where classical models break down. In the following, we highlight several directions that offer promising opportunities for near- to mid-term demonstrations of quantum utility in quantum chemical simulations.

A. Strong Correlation and Active Space Decomposition

Many chemically and industrially important systems—such as open-shell transition metal complexes [78–80] and f-electron materials [81–83]—exhibit strong electronic correlation. This characteristic poses significant challenges for standard classical simulation methods. Density functional theory, for instance, while widely used in catalysis [84], faces limitations in quantitatively describing strong correlations, electron spin states in magnetic catalysts, and weak intermolecular forces, which can impact the accuracy of predicted reaction barriers. Single-reference wavefunction approaches also struggle with strong correlation [85, 86]. These limitations become particularly pronounced when high precision is essential, such as in modeling intricate catalytic mechanisms where quantitative accuracy is critical for mechanism identification and catalyst design, electronic excitations spanning valence and core levels [14, 87], and relativistic effects in heavy elements [88–90]. Capturing these properties often requires computationally demanding multi-reference methods, whose cost scales prohibitively [91, 92]. Consequently, these strongly correlated systems are prime candidates for quantum-accelerated solvers [20, 21, 93] and advanced embedding strategies [49–60], potentially overcoming classical barriers and handling complexities (like multiple active sites or interfaces in catalysis) currently beyond reach. Quantum algorithms applied within carefully chosen active spaces, derived via embedding or selection protocols, are already being explored for catalytic problems such as molecule-surface interactions [94, 95].

A key insight facilitating these approaches is that electron correlation is often spatially localized within molecular fragments. This motivates fragment-based methods like the Localized Active Space (LAS) approach, which has emerged as a particularly promising framework [96–99]. LAS constructs the total wavefunction as an antisymmetrized product of local active space wavefunctions defined on weakly entangled fragments. Each fragment is treated with high-level methods, while inter-fragment interactions are captured at a mean-field level. The LAS State Interaction (LASSI) refinement recovers spin symmetries by diagonalizing the full Hamiltonian within a basis of LAS-configured states. Notably, the inclusion of charge transfer (CT) configurations between fragments within the LASSI Hamiltonian can be crucial for achieving quantitative accuracy, for example, when calculating magnetic coupling constants in multinuclear complexes. The applicability and scalability of LAS/LASSI have been demonstrated through calculations on systems like Cr(III) dimers [98, 100, 101] and spin ladder in Fe_3 compound [97], and large-scale LASSCF calculations are being applied to systems with over 1000 orbitals (e.g., Fe_4S_4, Cr_2, $NiFe_2$, and Ni_2). LAS is part of a broader family of embedding techniques; related methods like Density Matrix Embedding Theory (DMET) [102] are also being combined with high-level solvers for large systems and specific applications such as core-level spectroscopy [103]. Together, these strategies provide a scalable foundation for integrating classical and quantum work-

flows, potentially targeting specific active sites identified by classical methods with high-accuracy quantum calculations [99, 104, 105].

To further reduce complexity, downfolding methods can be employed to derive effective Hamiltonians that retain essential many-body physics within minimal active spaces [62–72]. Chemically motivated diagnostics—such as orbital occupation analysis and entanglement entropy—guide the selection of these reduced spaces [106], enabling the targeting of chemically significant regions using limited quantum resources.

B. Quantum Dynamics and Noise-Informed Simulation

Real-time quantum dynamics, particularly for open quantum systems (OQS), has been highlighted as a promising domain for near-term quantum utility [107]. Simulating processes such as photoinduced charge transfer, vibrational energy redistribution, and nonadiabatic transitions provides critical insights into reaction mechanisms and non-equilibrium phenomena beyond static approximations [108]. However, these simulations are computationally intensive for classical methods. Techniques like Multiconfigurational Time-Dependent Hartree (MCTDH) [109] and Hierarchical Equations of Motion (HEOM) [110] face the "curse of dimensionality," scaling poorly with system size, while tensor network approaches can be limited by the area law in capturing highly entangled dynamics compared to quantum circuits [111, 112].

Quantum devices may be well-suited to this regime due to their natural ability to implement unitary time evolution and sample from high-dimensional entangled states. Methods such as Trotterized real-time evolution, variational dynamics [113], and Krylov-subspace propagation (related to quantum signal processing, or Qubitization) have been proposed as viable quantum algorithms (see e.g. Ref. 107 for a recent overview). However, challenges remain, including the accurate preparation of initial states (which can be non-trivial and propagate errors), significant measurement overhead due to wavefunction collapse, and the difficulty of accurate Trotterization, especially for coupled, time-dependent systems.

Simulating OQS presents the additional challenge that quantum computers naturally perform unitary evolution, while open systems exhibit non-unitary dynamics due to environmental interaction. Standard quantum approaches to OQS include embedding the system within a larger environment simulated unitarily (ancilla-based methods), using stochastic quantum trajectories, or implementing Kraus operators [114–120]. Intriguingly, noise, traditionally viewed as an impediment, has been proposed as a resource [121]. Hardware-induced decoherence, if properly characterized or engineered, may serve as a proxy for environmental interactions, thereby facilitating OQS simulation. This "noise-assisted" approach has been explored in analog and digital quantum computing [122–125], potentially reducing overhead compared to full error mitigation by using techniques like partial error correction [126, 127] or pulse control.

The encoding of bosonic modes—representing vibrational, solvent, or bath degrees of freedom—also requires careful consideration. Strategies include truncated Fock spaces, coherent-state encodings, and squeezed-state representations [128]. Opportunities arise from the potentially simpler Hamiltonian structures in exciton-boson systems ($\mathcal{O}(N^2)$ or $\mathcal{O}(N)$ terms) compared to standard electronic structure ($\mathcal{O}(N^4)$ terms). Furthermore, embedding approaches and the development of advanced Gaussian ansatzes are being explored to reduce the resource requirements for representing these bosonic degrees of freedom [129]. Non-Hermitian Hamiltonians are also relevant for modeling dissipation, although simulating their dynamics on quantum hardware often involves mapping back to larger unitary systems or specific simulation techniques [119].

C. Hybrid Pipelines and AI Integration

The integration of quantum computing (QC) with artificial intelligence (AI) and high-performance computing (HPC) is rapidly advancing, with major initiatives developing platform-level solutions for accelerating chemistry and materials discovery [47, 130–134]. At the forefront of innovation is NVIDIA's DGX Quantum system, which enables low-latency, tightly coupled execution between quantum processing units (QPUs) and GPUs to support real-time AI-assisted quantum error correction (QEC), calibration, control, and readout [130]. To program such heterogeneous quantum–classical systems, NVIDIA introduced the CUDA-Q platform [135], a single-source, hardware-agnostic programming framework that unifies quantum and classical workflows, leveraging NVIDIA's existing CUDA and AI ecosystems. Another approach is provided by Microsoft's Discovery platform (formerly, Azure Quantum Elements), which offers a cloud-based solution that integrates access to multiple quantum hardware backends with Azure's HPC infrastructure and specialized AI tools, enabling users to build scalable hybrid quantum applications within a managed cloud environment [131].

In such hybrid ecosystems, AI models—often trained on large synthetic datasets generated via HPC simulations or augmented with quantum data—are used to accelerate discovery by enabling rapid screening, property prediction, and system-level optimization. For example, AI models deployed within Azure Quantum Elements have been used to evaluate millions of potential battery materials [136], while NVIDIA has developed generative AI approaches such as GQE [137] and QAOA-GPT [138] to automate the synthesis of optimal quantum circuits with desirable characteristics, such as low depth and high expressivity. In addition to algorithm development, NVIDIA has also demonstrated the use of AI for QEC in collaboration with QuEra [139].

This tiered, adaptive computational approach allocates quantum resources to the most challenging subproblems where classical methods struggle—such as transition states poorly captured by DFT or systems with strong multireference character [140, 141]. AI is integral across this hybrid workflow: from hardware design and calibration to device control, algorithm optimization, QEC decoding, and post-processing [142, 143]. Diagnostic tools—including uncer-

tainty quantification in AI models, convergence analysis of classical solvers (e.g., DMRG), and AI-driven screening and circuit optimization—support dynamic resource allocation across the classical-quantum-AI stack [144–146].

AI's role spans the entire quantum computing stack [130]. In hardware development, it accelerates qubit characterization, architecture exploration, and control pulse optimization. During operation, AI automates calibration and tuning, enabling closed-loop control strategies adaptive to evolving noise environments. In software, AI aids circuit synthesis and compression, variational optimization, and hybrid workload scheduling. It enhances QEC by improving decoder performance [29] and enabling scalable, low-latency strategies. In post-processing, AI reduces measurement overhead and mitigates errors in tasks like tomography [147], observable estimation, and readout classification. This end-to-end integration of AI is essential for scalable, fault-tolerant quantum computing and efficient use of hybrid resources.

D. Benchmarking and Experimental Validation

Robust benchmarking remains essential for validating quantum methods and ensuring reproducibility. A three-way validation framework—incorporating quantum simulations, high-level classical reference data, and experimental observations—has been endorsed [21, 43, 44]. This framework allows for iterative refinement of algorithms and facilitates the identification of performance gaps.

Benchmark systems that are well-defined chemically relevant, experimentally tractable, and computationally challenging have been proposed as community-wide testbeds. These systems allow simulations at different levels and experiments to interact closely, enabling to guide method development, hardware requirements, and software stacks across multiple disciplines. Table I summarizes several classes of model systems identified as focal points for algorithm validation and workflow integration. These span catalysis, photochemistry, and energy materials.

IV. ALGORITHMIC INNOVATIONS

The development of quantum algorithms capable of addressing chemically relevant problems using 25–100 logical qubits must be guided by co-design principles that account for fault-tolerant constraints. These include limited circuit depth, restricted qubit connectivity, noise resilience, and modular architecture [167, 168]. The goal is to create a unified framework for evaluating algorithms across diverse problems, establishing robust metrics and methodologies to uniformly measure performance [169]. Rather than converging on a single dominant paradigm, the current landscape favors the parallel exploration of diverse algorithmic strategies tailored to specific problem structures and hardware capabilities [20, 21, 142]. Many algorithms exist, balancing accuracy and efficiency, as exact solutions scale exponentially and are often impractical for large systems. Below, we highlight several promising algorithmic directions in this context.

A. Structured Ansatzes and Adaptable Methods

Traditional variational quantum eigensolver (VQE) approaches [61] employing unitary coupled-cluster (UCC) ansatzes face challenges such as barren plateaus, spin contamination, and instability across geometries [26]. Developments in areas like neural network ansätze for solids [170], most innovation has been focused on more chemically inspired and hardware-efficient ansatzes [32, 171]:

- **Real, imaginary, and complex parameterizations of the unitary Cluster Jastrow (uCJ) ansatz** [172, 173]. For instance, the real antisymmetric uCJ form is widely used and offers a more physically meaningful treatment of strong correlation than the generalized unitary coupled-cluster with singles and doubles (GUCCSD) [174], while significantly reducing quantum resource requirements [173]. Alternative parameterizations—such as the imaginary symmetric (Im-uCJ) and general complex (g-uCJ) forms—are also promising, particularly in challenging scenarios like bond dissociation. These findings suggest that tuning the parameterization strategy can improve accuracy and robustness, though care must be taken to evaluate potential drawbacks, such as spin contamination.

- **Optimization-free and adjustable subspace construction methods.** Representative examples include quantum subspace expansion [175], non-orthogonal configuration interaction approaches [167], hybrid and quantum Krylov/Lanczos methods [176–179], quantum computed moment techniques [180], the quantum equation-of-motion approach [181, 182], and generator coordinate-inspired strategies [183]. The subspace basis can range from individually optimized determinants (e.g., Hartree–Fock states) to coherent states, enabling access to multiple eigenstates while reducing circuit depth and enhancing sampling efficiency. Notably, error mitigation techniques such as shadow tomography may also help reduce measurement overhead.

- **Adaptive, parallel, and heuristic enhancements to VQE.** Adaptive strategies like ADAPT-VQE and operator pooling dynamically construct compact ansatzes tailored to the correlation structure of the system, minimizing circuit depth without sacrificing accuracy. In parallel, recent work has introduced techniques for parallel parameter optimization to accelerate convergence in VQE [184, 185]. Heuristic methods inspired by quantum annealing have also been explored to guide variational optimization and improve initial state preparation [186]. Complementing these efforts, quantum-information-informed approaches such as PermVQE [187] and ClusterVQE [188] exploit mutual information to reduce circuit depth via entanglement-aware qubit per-

Table I. Representative chemical systems in quantum chemical simulations, including scientific context and simulation goals.

Model/System	Category	Scientific Significance and Features	Simulation Target
CO/CO_2 on a catalyst [94, 148, 149]	Surface catalysis	Surface-supported reaction network; Activation barriers	Reaction barrier; Intermediate species and energetics
Transition metal oxides [78, 80, 100, 150]	Metal complexes	Strong correlation; Oxygen atom transfer	Spin states; Oxidation potentials
Chromophores in solvents [151–153]	Photochemistry	Intramolecular proton transfer; Fluorescence; Vibronic and nonadiabatic effects	Excited-state spectra; Charge/exciton recombination
PCET in enzymes [115, 121, 154]	Open quantum systems	Coupled nuclear-electronic dynamics; Tunneling and dissipation	Vibronic coupling; Solvent decoherence
$Li[Fe/Mn/Ni/Co]_yO_x$ [155–157]	Battery materials	Redox-driven polymorphism; Multiconfigurational complexity	Phase transitions and Jahn-Teller effect; Polaron hopping
Benzene, OLED molecules [158–160]	Correlated organics	π-electron delocalization; Singlet-Triplet Inversion and gaps	Benchmarking correlated methods; Gap prediction
Iron-sulfur clusters [161, 162]	Strong correlation testbeds	Magnetic coupling and spin frustration in bioinorganic settings	Multi-reference solver performance
Alkali metal hydrides (NaH, KH, RbH) [27]	Quantum computing benchmarks	Evaluation of quantum computing performance for electronic structure calculations	Ground-state energy calculations on quantum hardware
QM9 molecules with QH9, MultiXC-QM9 datasets [163, 164]	Machine learning in quantum chemistry	Prediction of Hamiltonian matrices using supervised learning	Accelerated electronic structure predictions
VQM24 dataset molecules [165]	Large-scale quantum chemical datasets	Comprehensive coverage of small molecules for benchmarking	Evaluation of quantum chemical methods across diverse molecules
Non-equilibrium non-covalent complexes [166]	Non-covalent interactions	Benchmarking interaction energies in non-equilibrium geometries	Assessment of computational methods for weak interactions

mutation and to enable scalable parallel VQE through graph-based decomposition, respectively.

- **Automation and user-accessible deployment of quantum solvers.** Recent efforts have focused on automating the ansatz and subspace construction process to facilitate the broader adoption of non-orthogonal quantum solvers [189]. These efforts aim to make quantum algorithm deployment more accessible to non-experts by reducing the manual complexity of circuit design, subspace definition, and error mitigation integration.

B. Downfolding and Renormalization Techniques

Effective Hamiltonian construction via downfolding offers a powerful way to reduce resource requirements while maintaining chemical accuracy [71]. By integrating out external degrees of freedom and targeting compact active spaces, these approaches bridge high-level accuracy with qubit efficiency:

- **Coupled Cluster Downfolding:** Techniques like subsystem embedding subalgebras (SES) [62, 69] and Double Unitary Coupled Cluster (DUCC) downfolding [65, 72] construct effective Hamiltonians in reduced active spaces. The accuracy depends on the treatment of commutator terms [70]. These can be applied to ground [69] and excited states [67] and dynamics [68].

- **Quantum Flow (Q-Flow)** and related **renormalization flow methods** transform Hamiltonians into energy-dependent effective models [63].

- **Tensor Factorization:** Recent approaches use tensor factorizations within recursive downfolding to optimize the scaling complexity on classical and quantum computers [190].

- **Hybrid Green's function and wave function methods** In recent development, wave function and Green's function methods are combined [191, 192]. The latter is used for the quantum bath (environment),

while wave-function solvers are used for the active space. The embedding is somewhat different as the bath is derived from a Green's function.

These techniques enable scalable embedding schemes [49, 53, 60] and are compatible with classical solvers and quantum subspace diagonalization methods. Combined with Green's function embedding and self-energy projection, they provide access to spectral and dynamic properties beyond ground states [193].

C. Quantum Phase Estimation (QPE) and Variants

QPE remains the gold standard for precision energy estimation [19] but typically exceeds available fault-tolerant resources. It is a key subroutine in many quantum algorithms [20, 21, 35]. Several modified QPE protocols have emerged to address resource constraints:

- **Iterative QPE** and **Bayesian QPE** minimize ancilla qubits and circuit depth, trading circuit depth for more measurements [194–196]. Here, Bayesian approaches can optimize parameter selection, and improve efficiency and robustness against errors.
- **Statistical Phase Estimation:** Alternatives to standard QPE that use lower-depth circuits and fewer auxiliary qubits, making them more suitable for early fault-tolerant devices and error mitigation techniques [197]. Recent methods improve accuracy for a given circuit depth compared to earlier analyses.
- **Filtered QPE**, involves enhancing QPE algorithms by incorporating filtering techniques, like Gaussian and subspace filters, to improve precision and robustness [198–200]. These filters help to refine the estimation of eigenphases, especially in the presence of noise or when dealing with complex systems.
- **Hybrid QPE-VQE workflow** that employs VQE for initial state preparation and then incorporating QPE techniques to accelerate the optimization process [201].

These variants improve scalability, particularly when paired with classical compression techniques such as classical shadows or active error mitigation [34, 197]. Recent experimental demonstrations include Bayesian QPE on trapped-ion systems [196] and statistical phase estimation on superconducting processors [197]. Simulations are also advancing, for instance, using tools like QPESIM for ground and core-level states [202]. Fault-tolerant algorithms based on QPE are also being developed for other properties, such as interaction energies via symmetry-adapted perturbation theory [203].

D. Benchmarking, Resource Modeling, and Modular Execution

Realistic resource estimation and performance assessment are critical for determining algorithm viability in early fault-tolerant conditions and understanding progress towards utility-scale problems [27, 204]. Benchmarks mapped across problem complexity and solver classes help identify promising targets, compare solver capabilities, and understand what makes specific problems challenging for different algorithms. The QB GSEE Benchmark [169], for example, aims to provide a cohesive and unified framework for evaluating algorithms across diverse problems using robust, standardized metrics. This involves incorporating problem instances of various sizes, from small examples to utility-scale challenges, sourced from established datasets like Varbench [205], the Gaussian-2 (G2) set [206], transition metal studies [207], and other high-utility systems.

- **Difficulty-feature space maps:** To understand problem similarity and complexity, instances are characterized by Hamiltonian features chosen for their relevance to algorithm complexity [27, 130, 169]. These features include electron/orbital counts, norms, graph properties (vertex degree, weight, edge order distributions), number of terms, estimated Full Configuration Interaction (FCI) dimension, and double-factorized properties (rank, eigenvalue gap). Techniques like Principal Component Analysis or Nonnegative Matrix Factorization can visualize this high-dimensional feature space.
- **Solver performance assessment:** Evaluating algorithm performance under realistic conditions, incorporating noise models and hardware constraints where feasible, is crucial [208, 209]. Machine learning tools offer complementary approaches for assessing performance, potentially by building surrogate models or evaluating performance on high-utility problems that lack exact classical reference solutions [130]. Establishing robust and uniform performance metrics across diverse algorithmic approaches is a key goal to enable fair comparisons.
- **Active learning protocols:** Active learning strategies can potentially optimize the curation and evolution of benchmark suites by efficiently identifying the most informative or challenging problem instances [130]. This allows for systematic targeting of known hard areas in computational chemistry, such as strongly correlated transition metal complexes [100, 101], complex excited state phenomena [14, 87], and open-shell systems [78–80], thereby focusing benchmarking efforts where they are most needed. Specific protocols tailored for quantum benchmark curation represent an ongoing area of research.
- **Benchmarking Toolkits and Programs:** Community efforts aim to standardize resource estimation and performance evaluation. Examples include the DARPA Quantum Benchmarking (QB) program [210] and open-source toolkits like BenchQC [208]. Benchmarking specific components, such as classical optimizers used within VQE under noise, is also crucial [209].

Modular workflows, like the one implemented in the GSEE benchmark (Problem Database $\rightarrow$ Solution Genera-

tion → Feature Computation → Performance Analysis → Reporting/ML Tools), decompose quantum algorithms into reusable and trackable stages (e.g., using unique identifiers for provenance). Emphasizing qubit-efficient state preparation, error-mitigated measurements, and standardized post-processing pipelines promotes modularity. Furthermore, the development of open-source toolkits and standardized datasets is vital for supporting community-wide contributions and ensuring reproducibility.

V. COMPUTATIONAL DESIGN AND HYBRID INTEGRATION

Realizing practical quantum simulations in the 25–100 logical qubit regime necessitates deep integration across quantum algorithms, classical computing resources, and emerging hardware architectures [131]. Quantum utility in this intermediate scale is unlikely to be achieved by quantum processors in isolation but is increasingly viewed as contingent on well-orchestrated hybrid systems that enable co-designed, end-to-end workflows [47, 132]. Understanding the interplay between algorithms, software stacks, and hardware is paramount.

A. Hardware-Aware Algorithm Design and Execution Frameworks

Quantum chemistry simulations impose specific architectural demands, including high two-qubit gate fidelities, error correction throughput, and fast classical control [95]. Emerging platforms—such as NVIDIA's accelerated quantum supercomputing framework [211]—are designed to address these demands by coupling GPUs with QPUs via low-latency interconnects. Understanding hardware limitations (gate speeds, fidelities, error rates, connectivity, coherence times across different platforms like superconducting, ion traps, or neutral atoms) is crucial for near-term algorithm design. AI-powered error correction decoders [130] and real-time control loops are incorporated into such platforms to support scalable execution and circuit calibration. Frameworks like the Transpiler-Architecture Codesign Optimization explore hardware-informed circuit optimization (e.g., using native gates like $RX(\pi/4)$ alongside T gates) and cost-aware transpilation, recognizing the different resource costs of gates like RZ vs CX in the fault-tolerant regime [212]. Heterogeneous error correction architectures, potentially combining surface codes with quantum low density parity check codes like the Gross code, are also being investigated to optimize resource usage [213].

Key enablers for hardware-aware quantum computing include:

- **Compact fermionic encodings**, such as Bravyi-Kitaev and parity mappings, requiring minimal ancilla overhead.
- **Mid-circuit measurement support** and layout-aware transpilation.
- **Noise-informed scheduling and AI-based decoder models**, enabling rapid inference for fault-tolerant circuits. Collaboration with hardware providers can yield high-fidelity noise models for simulation and tailored error management strategies [34].

Runtime orchestration must coordinate tasks across QPUs, GPUs, and CPUs, potentially requiring latencies on the order of hundreds of nanoseconds [211]. Compiler stacks must bridge the quantum-classical interface and ideally incorporate chemistry-aware abstractions and recognize important pre-compiled primitives (like Trotter steps or block encodings [75–77]).

B. Hybrid Workflows and Adaptive Execution Models

The modular hybrid model—where classical computation handles pre- and post-processing while quantum routines solve reduced subproblems—remains the most feasible strategy in the near term. Quantum acceleration is typically applied to chemically active subsystems, such as multiconfigurational fragments or correlated sites [54, 55, 60], identified through classical methods or machine learning heuristics. Techniques like quantum embedding [49, 51–53, 56, 57, 59, 60] and downfolding [63, 66, 69, 71, 190] are crucial for partitioning the problem. Green's function methods can provide high-fidelity descriptions of the environment (bath) for embedding or downfolding approaches [50, 193]. Accordingly, workflows increasingly leverage:

- **Active space identification** using methods like DMRG-based entropy diagnostics [145], orbital entanglement entropy [214], or automated schemes such as AutoCAS [215–217].
- **Post-processing** using high-level classical solvers (e.g., Semistochastic Heat-bath Configuration Interaction [218–220], CCSD(T) [10]) for result validation or refinement. Molecuiar energetics can be improved beyond VQE via post-processing by invoking perturbation theory in a manner analogous to CCSD(T) [221, 222].
- **Runtime task delegation** across heterogeneous resources with shared memory and synchronization [132].

Furthermore, classical pre-processing can extend beyond problem decomposition to optimizing the quantum routine itself; for instance, the stabilizer bootstrap technique leverages classical simulation of stabilizer circuits to pre-optimize parameters and analyze the potential for improvement in quantum machine learning models before quantum execution [223, 224]. These methods may offer a framework for integrating fault-tolerant quantum computing techniques with NISQ-era devices [225].

C. Hybrid qubit–qumode devices and gates

Qumodes or quantum harmonic oscillators are known for their infinite-dimensional Hilbert space and offer a compelling resource beyond the two-level systems of conventional qubits [226]. In practice, the Fock basis of a qumode within an energy cutoff represents a discrete multi-dimensional generalization of a qubit, also known as a qudit [227]. There has been significant progress on quantum devices consisting of qumodes coupled to a qubit, based on the circuit quantum electrodynamics (cQED) approach [228], where the qumodes are realized as microwave cavities dispersively coupled to a superconducting transmon acting as the qubit [229]. In addition to more resources than qubit-only architecture, cQED devices provide a diverse range of universal gate sets [230–233] such as echoed conditional displacement (ECD) with qubit rotations [231], selective number-dependent arbitrary phase (SNAP) gates with displacements and beamsplitters [230], and conditional-not displacement gates [232], to name a few. These gates have been recently explored for chemistry [234–236], optimization [237], and quantum machine learning [238] applications. These hybrid qubit-qumode gates are also hard to mimic using shallow qubit-only circuits [239, 240], so have a potential advantages for specific problems suitable to bosonic problems [239] or optimization landscapes favourable to these circuits [241]. The high-quality and long-lived cavity qumodes have already demonstrated quantum error correction beyond break-even for both logical qubits [242] and qudits [243]. However, these benefits can be undermined by the noise originating from the ancillary qubit coupled to the qumodes [244]. This is where a logical qubit dispersively coupled to multiple qumodes will be highly impactful.

D. AI-Augmented Simulation Pipelines

AI plays a multifaceted role in enabling efficient hybrid quantum chemistry workflows [130, 133]:

- **Preprocessing**: circuit compilation, active space scoring, and orbital selection using trained models [92, 141], and techniques like the stabilizer bootstrap for optimizing variational circuits [223].
- **Quantum Circuit Generation**: approaches such as the Generative Quantum EigenSolver use transformer models to synthesize low-depth circuits without optimization loops. Quantum autoencoders can compress quantum states, optimizing qubit usage [137].
- **Error correction and control**: AI decoders for surface codes can exceed classical maximum likelihood performance, essential for QEC scalability [37, 130].
- **Post-processing and compression**: learning-based estimators, like projected quantum kernels or classical shadows, can reduce quantum measurement overhead and enable real-time observable estimation [245].

AI–quantum integration, sometimes termed Quantum Machine Learning (QML) [246, 247], is seen as critical not only for enhancing performance but also for overcoming training bottlenecks (like barren plateaus [26]) and generalizing algorithms across molecule types or basis sets [248].

E. Co-Design Strategies and Modular Architecture

Realizing quantum utility requires a shift from isolated algorithm development to full-stack engineering and co-design [131]. Co-design efforts span:

- **Cross-platform modular workflows**—supporting portable components for state preparation, encoding, and measurement compression [132, 169].
- **Tensor network abstraction and recursive optimization**—to manage circuit scaling and problem decomposition [111].
- **AI-in-the-loop runtime control**—for latency-aware scheduling and dynamic resource allocation [130].
- **Bridging Algorithmic Paradigms**—Leveraging insights and efficient classical simulation techniques from fault-tolerant approaches (e.g., stabilizer formalism) to optimize and analyze near-term variational algorithms like QML [223].

Leveraging chemical insights, such as partitioning based on weakly interacting fragments, can inspire developments lower down the software/hardware stack. Ultimately, the trajectory toward fault-tolerant quantum chemistry hinges on tight coupling of chemical knowledge, hardware constraints, and scalable computing infrastructure [44].

VI. ROADMAP AND COLLABORATIVE PATHWAYS

Achieving quantum utility in quantum chemical simulation is not solely a technical endeavor but also a challenge in strategic alignment and realistic assessment [44, 47]. Realizing utility in the 25–100 logical qubit regime requires coordinated efforts across algorithm development, hardware architecture, software integration, and cross-sector collaboration. The roadmap outlined below reflects both immediate opportunities and long-term visions grounded in chemistry-driven use cases [120].

A. Benchmark Design and Problem Class Prioritization

The need for chemically grounded benchmark problems will go beyond idealized or academic systems [27, 169]. Prioritized use cases include challenging electronic structure problems relevant to the model systems relevant to energy and materials science as described in Table I.

Benchmarks can further be organized into classes [249] based on the evaluation metrics distinguishing moderately correlated systems tractable in the near-term from strongly correlated systems requiring large-scale fault tolerance:

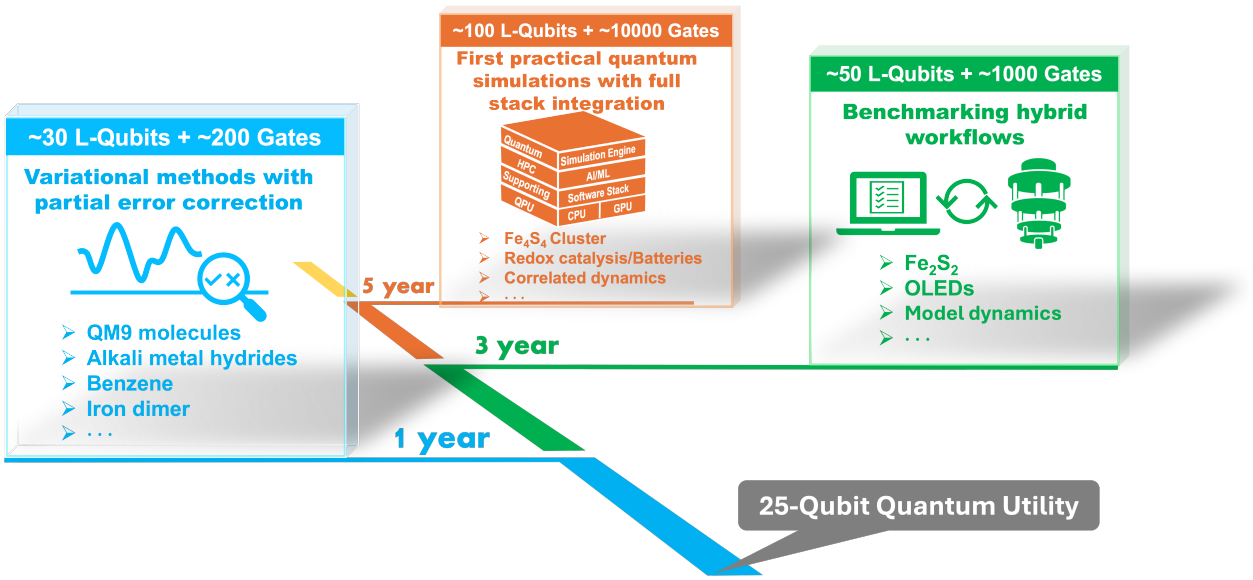

Figure 2. Strategic roadmap for quantum chemistry simulation with increasing logical qubit budgets.

- **Class 1:** Moderately multireference systems with localized correlations—potentially tractable within 25–100 logical qubits (e.g., cyclobutadiene [250], Fe_2S_2 clusters [161, 162]).

- **Class 2:** Strongly multiconfigurational systems with global entanglement—requiring >1000 logical qubits and full fault tolerance (e.g., FeMoco [13]).

Class 0 systems (weakly correlated ones) also remain important targets for verifying methods [249].

Notably, the evaluation metrics were encouraged to include quantitative agreement with experiment, convergence behavior, scaling trajectories, and chemical observables such as excitation energies, spin state gaps, and phase boundaries.

B. Community Infrastructure and Interoperability

Community-driven infrastructure is considered essential for enabling reproducibility and scaling collaboration. Critical components include:

- Modular, open-source codebases for hybrid quantum-classical workflows (e.g., frameworks integrating classical chemistry packages with quantum libraries [251]).

- Interoperable APIs and intermediate data formats for quantum and classical backends.

- Public benchmark repositories with problem instances, convergence criteria, and reference outputs [163, 165, 169].

- Cloud-accessible simulation environments and emulators, potentially integrated with HPC ecosystems [132].

We encourage efforts to bridge the language gaps between chemists, software engineers, and hardware developers, as well as build up compiler tool chains with chemistry-aware abstractions (domain-specific languages) and automated translation between Hamiltonians and quantum circuits [251].

C. Strategic Roadmap and Time-Phased Goals

Staged roadmaps have typically been discussed to guide the evolution of capabilities across the next five years, though specific timelines remain speculative [47]. Public roadmaps from hardware vendors also inform expectations [28]. Here, we emphasize realistic targets tied to hardware constraints (e.g., progress in error correction [37, 38]), software stack maturity, and community readiness, as summarized in Figure 2.

Reverse engineering of hardware requirements from target applications, such as defining chemical accuracy thresholds to determine necessary qubit counts and gate fidelities [149, 204, 252, 253], can be employed as a guiding principle. Also, defining realistic capabilities requires understanding the practical performance limits and optimization potential of near-term algorithms. For variational approaches like QML, techniques such as the stabilizer bootstrap are being developed to assess when and how these circuits might offer utilities or be efficiently optimized, informing feasibility assessments along the roadmap [223].

D. Collaborative and Cross-Disciplinary Models

Progress toward these goals was linked to structured collaboration across institutions and disciplines [44]. Suggested models include:

- Shared fellowships and postdoctoral exchanges across chemistry, computer science, and physics.

- Multi-institutional consortia aligned around benchmark testbeds (e.g., DOE National Quantum Information Science Research Centers [254], DARPA Quantum Benchmarking Program [210], and NSF National Quantum Virtual Laboratory [255] and Quantum Leap Challenge Institutes [256]).
- Hackathons and challenge problems with well-defined resource and accuracy targets.
- Standardized terminology (e.g., logical vs. physical qubits, QEC-protected operations) to improve communication.

Notably, we realize that it is also important to disseminate negative results, clarify failed optimization strategies, and share classical-quantum crossover boundaries for guiding future design.

VII. CONCLUSION AND OUTLOOK

A. A Pragmatic Shift Towards Quantum Utility in Chemistry

The field of quantum computing for quantum chemistry is undergoing a significant strategic shift. Rather than awaiting the arrival of large-scale, fault-tolerant machines, the community is coalescing around a more pragmatic approach focused on the emerging regime of 25–100 logical qubits [44]. This scale is viewed not as a temporary constraint but as a crucial proving ground for demonstrating tangible quantum utility in the coming years. The emphasis has moved towards hybrid, modular, and application-aware strategies that maximize the utility of currently available, limited quantum resources. These strategies often involve techniques like embedding, downfolding, adaptive algorithm design, and importantly, principled integration with classical HPC and AI tools [130, 132, 257].

The central goal has been refined towards achieving "Quantum Utility"—demonstrating that a quantum device can outperform the best classical methods for specific, well-chosen tasks, considering metrics like speed, accuracy, efficiency, and resource costs [258]. This means prioritizing niche but meaningful problems where quantum computers are most likely to provide an impact, such as strongly correlated systems, quantum dynamics, and catalysis. Recent demonstrations, like simulating H_2 using logical qubits with error detection [259], signal tangible progress towards fault tolerance. Quantum chemistry continues to be a cornerstone application driving these advancements [20, 21, 142].

B. Co-Design, Collaboration, and Building the Foundation

Looking ahead, progress hinges critically on the principle of **co-design**. This involves deep collaboration: between algorithm development and hardware capabilities, across different stages of simulation workflows, and among diverse disciplinary communities [44, 120, 131]. Continued innovation in theory, hardware, and software is essential, particularly focusing on techniques like downfolding, low-depth subspace methods, renormalized embeddings, and novel fault-tolerant frameworks (e.g., combining fermion and qubit codes) [260]. Integrating quantum workflows with efficient classical pre-processing and optimization strategies, potentially leveraging structural properties or fault-tolerant concepts even for near-term methods [223], will also be key.

The near-term roadmap prioritizes several concrete actions:

- Design of chemically relevant, resource-annotated benchmarks to guide development and measure progress [27, 169].
- Development of efficient classical pre-processing and optimization strategies tailored for quantum algorithms [223].
- Creating modular, testable hybrid workflows that are explicitly co-designed with hardware constraints and capabilities [131, 251].
- Integration of AI and classical HPC as scalable partners within quantum simulation workflows [130, 132].
- Building a robust ecosystem, including open infrastructure and community benchmarks, to ensure reproducible and reliable scientific outcomes.

Ultimately, the work ahead is inherently collaborative. Achieving production-quality quantum chemical simulations requires a shared vision, coordinated investment, and a commitment to open science [44, 120]. The current momentum indicates that the era of practical quantum chemistry enabled by quantum computers is rapidly approaching, and its foundations—built on pragmatic goals, collaborative co-design, and targeted applications—are being firmly established today.

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