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Perspective

Quantum computing and chemistry

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SUMMARY

As the year-to-year gains in speeds of classical computers continue to taper off, computational chemists are increasingly examining quantum computing as a possible route to achieve greater computational performance. Quantum computers, built upon the properties of superposition, interference, and entanglement of quantum bits, offer, in principle, the possibility to outperform classical computers for solving many important classes of problems. In the field of chemistry, quantum algorithm development offers promising propositions for solving classically intractable problems in areas such as electronic structure, chemical quantum dynamics, spectroscopy, and cheminformatics. However, physical implementations of quantum computers are still in their infancy and have yet to outperform classical computers for useful computations. Still, quantum software development for chemistry is a highly active area of research. In this perspective, we summarize recent progress in the areas of quantum computing algorithms, hardware, and software, and we describe the challenges that remain for useful implementations of quantum computing for chemical applications.

THE TROUBLE WITH CLASSICAL COMPUTING AND COMPUTATIONAL CHEMISTRY

Computing, as we know it, has revolutionized science. From lab automation to data analysis to theoretical prediction, the level of understanding that can be achieved today far surpasses what could be accomplished even a decade ago due to advances in computational power. For almost a half-century, these advances in classical computing have closely followed Moore's law, a prediction based on the observations of Intel co-founder Gordon Moore in 1965.[1] Moore's law predicts that the number of transistors per square inch on a computer chip (or integrated circuit) doubles every 18–24 months, thereby increasing the speed of computers. However, in recent years, these advances have slowed down dramatically as integrated circuits approach their fundamental size limits. Components are becoming incredibly small, even approaching the atomic scale, where quantum effects become dominant.[2]

Though classical computers have had a monumental impact on science, there are still many types of computational tasks and problems that remain intractable in terms of scale even for the largest classical machines. In chemistry, for example, the many-body entangled states underlying the electronic structure of a molecule cannot be modeled fully even on today's most powerful computers. Instead, numerous approximations are required to make computations feasible for larger molecules. These approximations can miss important electronic or electron-nuclear effects, especially for complicated molecular systems such as complexes involving transition metals or heavy elements.[3]

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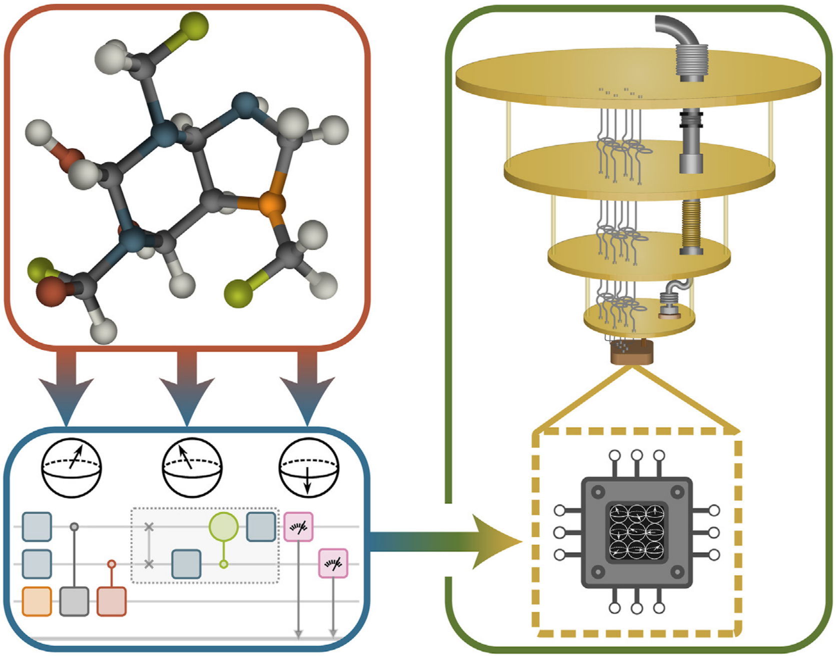

Figure 1. Illustration depicting a chemical simulation being performed on a quantum computer

For a molecular system of interest (image with red border), a computational method is chosen to compute a quantity of interest, such as an energy, property, or dynamical time evolution, for example. An algorithm is chosen to carry out the method, and, in the case of digital quantum computing, this algorithm is represented as a circuit diagram—a sequence of unitary operations performed on a set of qubits (image with blue border). Once the quantum circuit is constructed, it is sent to the quantum computer—or, more specifically, the quantum processor (dotted gold box)—where the operations from the algorithm are performed directly on the corresponding qubits within the processor. For superconducting qubits, these quantum processors reside on a chip inside a dilution refrigerator (image with green border) at a temperature of 10 mK.

Advances in classical computing have produced a number of powerful new computing strategies, including parallelization, graphics processing unit computing, and machine learning (ML). However, these developments still exhibit the same fundamental limitations of classical computing hardware for simulating complex quantum systems such as molecules. Given the slowing down of Moore's law and the clear need for more powerful computers, new computational paradigms are needed to further scientific achievements. Over the last few decades, quantum computing has emerged as a candidate to overcome the limits of classical computers. Some of the most exciting potential applications of quantum computers are in the field of chemistry, where more powerful computer simulations could directly lead to significant advancements in areas such as medicine, materials science, energy science, catalysis, and nanotechnology. As a result, chemistry has a prominent position at the forefront of quantum computing developments, and the idea of simulating chemical systems on quantum computers (Figure 1) is the subject of substantial ongoing efforts.

QUBITS AND THE QUANTUM REVOLUTION

It is rather remarkable that today's classically computerized world is built upon the foundation of the bit—the most basic unit of information in a computer, with the binary option of 0 or 1. From the perspective of modern silicon-based circuitry, this correlates to a transistor being in one of two states (i.e., being "on" or "off"). To illustrate, imagine this bit to be a light switch, where the only two options are for the light

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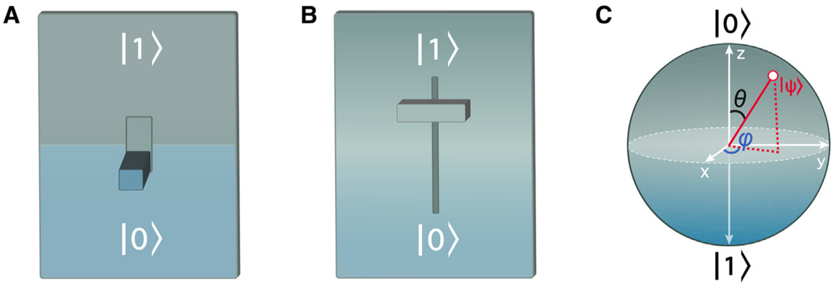

Figure 2. Representations of classical and quantum bits

An intuitive understanding of a classical bit to a quantum bit (qubit) can be made by comparing a binary on/off light switch and a dimmable light switch.

(A) An ordinary light switch can exist in two possible states, off and on. These two states are analogous to a classical bit being in the $|0\rangle$ or $|1\rangle$ state, respectively.

(B) A dimmable light switch can select between a continuous number of states, ranging from completely off to completely on. This characteristic is in part analogous to a qubit, whose state may be expressed as a linear combination of the $|0\rangle$ and $|1\rangle$ states.

(C) The state of a single qubit is best represented by a vector on the Bloch sphere.[4] In this representation, a state can be in a superposition of states $|0\rangle$ and $|1\rangle$ with complex phase in the two-level system's description, $|\psi\rangle = \cos\frac{\theta}{2}\,|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}\,|1\rangle$. When the qubit is entirely in its ground state, the state vector points north on the sphere and $|\psi\rangle = |0\rangle$, with $\theta = 0$. On the other hand, when the qubit is in the excited state, the state vector points south on the sphere and $|\psi\rangle = |1\rangle$, with $\theta = \pi$ and $\varphi = 0$.

to be on or off. Now, imagine a dimmable light switch, in which the brightness level can be controlled in a continuous manner. In this illustration, shown in Figure 2, the dimmable light switch is a naive representation of a single quantum bit, or qubit—many of which would be required to make a quantum computer. While the dimmable light switch provides a nice intuition for a qubit based on extrapolating from a classical bit, a single ideal qubit is better described mathematically as a vector on the surface of a Bloch sphere.

In contrast to classical bits, qubits inherently exhibit quantum mechanical effects such as superposition and entanglement. Superposition is a quantum mechanical phenomenon where quantum systems, such as qubits, can exist in a probabilistic linear combination of discrete states at a single time. In the dimmable light switch analogy, a superposition state of a single qubit is similar to the idea that the light can be in some state between entirely off and entirely on. Entanglement is another quantum mechanical phenomenon that describes how multiple qubits exhibit non-classical correlations with each other, such that the state of one qubit cannot be described independently from states of the others. Given the exponential scaling of the classical computational power required to solve these quantum mechanical problems, these unique properties of quantum mechanics have inspired the idea that using a computer that is itself quantum mechanical could be a better way to simulate quantum systems.[5,6]

The earliest ideas of quantum computation proposed to prepare a quantum system and evolve it in time in a manner that simulated the time evolution of a quantum Hamiltonian of interest. This method of computation, known as analog quantum computation, had the drawback that the qubits had to be specifically designed for the particular problem of interest—they could not be used in any other general quantum system simulation.

In contrast, a more general type of quantum computation was later proposed, which in some respects mimics the way classical computers are used to simulate arbitrary systems. In this approach, known as digital quantum computing,[7] algorithms are implemented using a consistent and familiar computing format. Starting with an initialized set of qubits, conditional operations using quantum logic gates are performed sequentially on one or more qubits. These gates are analogous to the classical bitwise logic gates used in classical computing. However, distinct from classical information processing, in quantum computing, the gates represent unitary transformations of qubit states and can be used to manipulate superposition (in single qubits) or entanglement (between multiple qubits) to encode a time-sequenced evolution of a multi-qubit state. At the end of a sequence of gates, a projective measurement of a qubit state is performed to obtain the final result. Unlike classical computing, each result of measuring the outcome of a quantum algorithm is probabilistic and represents only one of the possible outcomes of the gate-defined algorithm. This requires that the algorithm be repeatedly initialized and run multiple times to build the measurement statistics, which in aggregate ultimately encode the desired solution. Thus, in contrast to the analog quantum computing model, algorithms using the digital approach can, largely, be developed independently of hardware, making them more generally useful for a universal approach to quantum computation.

Other aspects of quantum computing also present novel challenges not found in the classical computing paradigm. To physically implement a particular algorithm, software known as quantum compilers will be needed to convert the sequence of quantum logic gates and measurements to specialized machine code needed for the physical manipulations and readout of different qubit systems. Additionally novel, and specialized, quantum memory solutions will likely need to be developed for storing information while computations are running. The quantum machines of the future will likely be heterogeneous systems made up of different physical components for qubits, memories, and communication channels. These future machines will also ultimately need highly non-classical error-correcting schemes, which will run continuously to tamp down both bit-flip and phase errors.[8]

Despite these differences from classical computing, digital quantum computation is ushering in significant advancements due to quantum algorithms no longer having to be tied to a specific qubit architecture. The digital model of quantum computing has become the dominant model at present for quantum computing implementations.

CHEMICAL APPLICATIONS OF QUANTUM COMPUTING

Successful implementations of quantum computing could bring about significant advancements for solving complex problems in science and engineering including cryptography, optimization, communications, quantum simulations, and large data analytics. However, perhaps the most promising application of quantum computing (the "killer app"), particularly in the near term, is in the field of quantum chemistry.[9–12] Recent algorithmic developments suggest that quantum computers are particularly useful for the simulation of the quantum many-body problem, a problem that manifests itself in many areas of quantum chemistry. For example, in electronic structure theory, efficient quantum algorithms exist for finding the ground state energies of molecules, such as the QPEA.[11] For chemical quantum dynamics, quantum computing offers natural ways for simulating the time evolution of molecular systems.[13] Exact solutions to these problems are infeasible on classical computers for molecules larger than a few atoms, at best, due to the exponential scaling in the computational resources required as the number of particles is increased.

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The source of this exponential scaling lies in the very nature of the electronic structure and quantum dynamical problems. In conventional theoretical chemistry, the electronic structure problem primarily concerns the task of computing properties of ground and excited states of the electronic Hamiltonian. This can be done either through density matrix-based techniques[14,15] or wavefunction-based methods like active space-truncated configuration interactions[16] or several variants of coupled cluster,[17] which are both often considered gold standards. In the latter category, even though algorithms exists with superpolynomial runtime,[18,19] they are often faced with a persistent roadblock of insurmountable storage complexity given that the target wavefunction needs to be stored and manipulated classically. The size of this object increases dramatically with the size of the determinantal basis, and this basis, in turn, scales exponentially with the size of the system (or the size of the active space considered) and also the one-particle basis rank. For quantum dynamics, conventional wavefunction-based treatments like the multi-configurational time-dependent Hartree method have a similar problem, as the equation of motion for the coefficients of the target wavefunction in a determinantal basis is considered, which can be enormous depending on the basis rank and number of nuclear degrees of freedom.[20,21] Even though the quantum computing algorithms discussed herein may seem to obviate these problems by never explicitly retrieving the wavefunction from quantum memory, we shall see that direct claims about distinct quantum advantages need to be made with caution. Such algorithms belong to a different complexity class[22,23] and should be quantified by measuring sticks like circuit width (number of qubits), circuit depth (number of layers of non-commuting gate operations), and the number of measurements required to procure useful quantities—none of which have direct classical analogs.

The typical workflow for such quantum algorithms for chemical applications starts by encoding the fermionic states and operator space onto qubit states and operators. This can be done in several ways. The most popular method is known as the Jordan-Wigner transformation,[24] which directly translates a single determinant of r spatial orbitals to a single configuration of $2r$ qubits in the σ_z eigenbasis. This spin-orbital basis is usually chosen from a Hartree-Fock precursor done classically. The fermionic creation and annihilation operators map to strings of non-local Pauli words P_i where $P_i \in P = \{\otimes_{i=1}^{2r} \sigma_i | \sigma_i \in (\sigma_x, \sigma_y, \sigma_z, \mathbb{I})\}$ with correct anti-commutation algebra characteristic of fermions. Another way to map fermions onto qubits is parity mapping.[25] In this method, a binary vector consisting of the parity associated with the occupation number of the spin orbitals is treated as a state vector, which leads to occupation information being distributed non-locally. The fermionic creation and annihilation operators are converted to Pauli words affecting all sites non-trivially. A third mapping scheme, the Bravyi-Kitaev scheme,[25–27] is a combination of the first two, consisting of odd-indexed qubits storing parity and even-indexed qubits storing occupation. Fermionic operators are also grouped into two distinct categories, with the action of each affecting all sites. Other modes of mapping based on binary-addressing codes[28] or a compact encoding scheme, which reduces the non-locality of the operator space,[29] have also been developed recently. Once suitable mapping is performed by the user, the basic objective of all of the following algorithms discussed here is to prepare the quantum state (or electronic density) of interest and compute averages directly from the quantum circuit for retrieving various properties.

We shall now move on to discussing specific quantum algorithmic developments for applications in a wide variety of domains within the field of chemistry, including electronic structure, ML, quantum dynamics, spectroscopy, and cheminformatics, to name a few. We encourage the reader to refer to several helpful reviews for additional in-depth discussions of these topics.[10,30–34]

One of the earliest quantum algorithms applied to quantum chemistry is the quantum phase estimation algorithm (QPEA). A central component of many early quantum algorithms, the QPEA was first simulated for a chemistry problem in 2005 by Aspuru-Guzik et al.,[35] where a full configuration interaction Hamiltonian was simulated on a quantum computer based on a Hartree-Fock reference. A similar algorithm was developed in 2008, where the energy spectrum of molecular systems is obtained on a quantum computer from a multi-reference configuration interaction wavefunction based on a multi-configurational self-consistent field (MCSCF) reference.[36] These algorithms, however, assume the existence of a fault-tolerant quantum computer—one that is able to perform a quantum computation without the final result being affected by noise that will cause errors in the computational results. Despite ongoing efforts to advance in the areas of quantum error-correcting codes[37,38] and noise mitigation,[39] completely fault-tolerant quantum computers are still far from being realized. Thus, current implementations of quantum computing for chemistry are limited due to hardware challenges, especially the presence of noise (see the hardware section for more information on hardware implementations of quantum computers). This current era of quantum computing, in which noise plays a significant role and error-correcting schemes are still in their nascency, has been named the "noisy intermediate-scale quantum (NISQ)" era.[40]

One important new direction to advance the application of quantum computing algorithms for the simulation of chemical systems in the NISQ era is the development of hybrid classical-quantum algorithms. A hybrid approach to decompose the time-evolution operator of a molecular Hamiltonian into an optimal set of unitary basis gates was developed in 2011.[41] This work utilized the classical group leaders optimization algorithm[42] to decompose a given unitary matrix into a proper-minimum cost quantum gate sequence. The parameters, rotational angles in the quantum gates, are optimized to minimize the distance between the exact and approximate unitary matrix representation of a candidate approximation quantum circuit. Using this procedure, circuit designs were developed for the simulation of the unitary propagators of the Hamiltonians for the hydrogen and water molecules.[41]

Another important algorithm designed for NISQ devices is the variational quantum eigensolver (VQE).[43] The VQE algorithm is an example of another quantum-classical hybrid algorithm, in which the computation utilizes the strengths of both quantum and classical computing hardware. In the VQE approach to the electronic structure problem, a quantum processor evaluates the energy of a molecule based on a given wavefunction ansatz with inputted variational parameters. After each energy evaluation, the classical computer is used to optimize the variational parameters to minimize the energy. This variational process is repeated until convergence of the computed energy is reached, resulting in an estimation of the true ground state energy. This method was first developed for finding the ground state electronic energies of molecules,[44] and it has since been adapted to other areas such as linear system solvers,[45] matrix decomposition and numerical linear algebra,[46,47] and even non-linear analysis.[48] Early successes of the VQE algorithm have been in computing ground state energies of BeH_2,[49] the isomerization barriers of diazene,[50] and the energies of hydrogen chains up to 12 atoms.[50]

VQE is a highly active area of research, and new developments of this method are being formulated that hold enormous promise for further improvements. Such developments can be broadly classified into two categories. The first category is implementing new ansatzes, including circuit unitaries representing the target state like unitary coupled cluster,[51,52] hardware-efficient ansatzes,[49] tensor-network inspired designs,[53,54] and methods based on reduced density matrix theory.[55] The second category is prescribing modifications in the overall algorithmic flow like the Adaptive Derivative-Assembled Pseudo-Trotter ansatz Variational Quantum Eigensolver (ADAPT-VQE) method,[56] partitioning the system mimicking embedding protocols,[57] adapting the Hamiltonian through orbital rotations,[58] and optimizing the orbitals within the VQE routine,[59] in analogy with the MCSCF procedure in conventional quantum chemistry. Powered by such developments, in recent years, variants of the algorithm with reduced measurement count, more expressive state-preparation strategies, and clever initialization have enabled extending the list to interesting systems such as the benzene molecule under deformations,[60] *trans*-butadiene and the bimetallic chromium complex $[Cr_2(OH)_3(NH_3)_6]^{+3}$,[61] a large active space simulation of NH_3,[62] keto-enol tautomers,[63] ground and excited state energies of indoaniline dyes such as phenol blue,[64] molecules in solution,[65] and transition metal complexes like PtCO.[66] The development of variants of VQE has even enabled extending the paradigm to compute vibrational levels of both ground and excited electronic states in CO_2, HCHO, and HCOOH.[67]

Along similar lines, parallel efforts are being made to improve quantum-enabled ML algorithms for a variety of applications in physics and chemistry.[68–71] An example of such efforts is neural network encoding of a quantum state in, for example, restricted Boltzmann machines,[72–74] where the network is used to represent the amplitude and phase field of the components of the wavefunction of the target state. Algorithms to train such a network on a quantum device with quadratic resources have been developed and successfully applied in constructing properties of two-dimensional (2D) materials,[72,75] molecular systems, and spin assemblies in Rydberg-excitation-based sensing on cuprous oxide hosts[76] and spin liquids.[77]

Apart from the wavefunction-based methods indicated above, digital quantum algorithms for retrieving the electronic density, which forms the cornerstone of density functional theory, have also been recently developed.[78] One of the early efforts in this area[79] proposed constructing the wavefunction on the quantum circuit using adiabatic real-time evolution[80] for a given instance of the external ion-electronic interaction potential as input. Appropriate measurements on the wavefunction are subsequently performed that can retrieve the electronic energy and electronic density, which are then fed into a classically trained ML algorithm to generate a new instance of the external potential to be used in the next cycle. However, refined protocols exist now[81] wherein oracular access to Hamiltonian matrix elements in first quantization on a grid is assumed. The algorithm outputs an updated electronic density with a user-defined error threshold ϵ when the oracle is interrogated $O\left(\frac{sN_l}{\epsilon}\right)$ times, wherein s is the sparsity of the Hamiltonian matrix and N_l denotes the number of grid points defining the resolution. The crux of the algorithm involves block encoding of the Hamiltonian matrix,[82] which embeds it within a unitary, followed by generating polynomials through quantum singular value transformations[83] to approximate a Fermi-Dirac distribution, which essentially defines the electronic density. This protocol has been successfully exemplified by performing simulations on H_2O and $BaTiO_3$ for various grid sizes.

Besides the digital simulation algorithms mentioned above, analog protocols have also been designed recently for simulating and understanding electronic structures. In analog simulations, the primary focus is on mapping the terms of the Hamiltonian of the system of interest (in this case, the many-body fermionic systems arising in physicochemical applications) to terms of the Hamiltonian of a secondary system, which is directly implementable and can be manipulated experimentally efficiently. In this regard, one of the early proposals was to define a map for converting a Jordan-Wigner-transformed fermionic Hamiltonian to a *k*-local, but a diagonal Ising Hamiltonian, in an expanded dimension (i.e., with an enhanced number of qubits[84,85]) with the hope of simulating such Hamiltonians directly on an analog device. Local variants of such Ising Hamiltonians are routinely employed in quantum annealers such as those used by D-Wave[86,87] for solving a variety of binary optimization problems. A more direct and recent analog proposal[88] relies on using fermionic atoms hopping in an artificially engineered optical lattice to mimic electrons. The potential generated from the optical lattice plays the role of one-body interactions (nuclear-electronic), and a second set of trapped atomic species mediates repulsive interactions between the aforementioned fermionic atoms in the Mott-insulating phase. This interaction serves as a proxy for Coulombic repulsion among electrons in atoms and molecules.

Apart from electronic structure information about the ground state potential energy surface (PES), which is important in understanding available reaction pathways, the knowledge of excited state PESs is also very important in chemistry. This is due to the fact that it enables the study of optical excitations in spectroscopy, branching due to conical intersections in quantum wavepacket dynamics, and even understanding optically induced reaction pathways such as isomerization, light-harvesting properties of photosynthetic complexes, and excitonic properties of materials. Excited state PESs can be computed on a quantum computer by variational means, either through sampling the orthogonal complement of the ground state[72] or by computing averages between commutators of excitation operators and the Hamiltonian with such commutators acting on the prepared ground state.[89]

In either case, once the PES is obtained, the next step is studying dynamical evolution. To this end, one can use a grid-based approach in the first quantization, as illustrated in a recent report with two coupled diabatic surfaces and a wavepacket initialized on either surface.[90] However, such techniques require large numbers of qubits owing to the discretized encoding of the spatial grid, a problem that can be readily solved using a basis set and second quantization. To this end, proposals for using a prototypical spin-boson model[91] exist that involve coupling a two-level atom (energy levels are the energies of the coupled PES in the system of interest) to a collection of harmonic modes (degrees of freedom for nuclear motion), each truncated at a given maximum occupation. The ansatz involves a parameterized sequence of gates (with time-dependent parameters) much like the Trotterized evolution of the Hamiltonian under consideration. The MacLachlan scheme[92] is used for norm minimization to optimize parameters of the ansatz such that the evolved wavepacket follows the Schrödinger equation temporally.[93]

Such proposals are only beginning to gain attention and have been far less investigated or explored compared to usual eigenstate preparations. These are especially gaining attention in the context of dynamical evolution for open quantum systems[94,95] wherein the usual non-unitary evolution of the system is unitarized for implementation on a quantum device.[13] Treatments like these are important in illustrating the mechanistic details of exciton transport in photosynthesis,[96] which can be mimicked to develop efficient artificial light-harvesting devices. Another particularly interesting area would be to compute the branching ratio of the wavepacket across conically intersecting PESs—a phenomenon seen in many different areas of chemistry/chemical biology including photophysics of vision[97,98] and bioluminescence in fireflies.[99] In addition to these quantum molecular dynamics (MD) studies, even classical MD can be studied on a quantum computer, whereby nuclear coordinates are propagated by solving Hamilton's equations on a precomputed PES from the electronic structure. This workflow is typical of *ab initio* MD simulations. Indeed, computing nuclear gradients (which act as forces in Hamilton's equations) for such simulations using quantum computers is being investigated as a possibility.[100]

Another interesting and extremely understudied area is using quantum algorithms for computing spectroscopic parameters. In this regime, quantities such as vibronic coupling parameters, Franck-Condon factors for vibronic spectroscopy,[101] transition moment integrals,[102] molecular response properties,[103] 2D electronic spectroscopy,[104] condensed-phase spectroscopy,[105] and spectral response functions for electronic spectroscopy could be obtained. Beyond academic research, such projects are of immense importance to pharmaceuticals, paint-based industries, cosmetic industries, and chemical industries (or their raw-material-supplying partners), where spectral information is required for characterization of chemical compounds. Recently, some work has been done in this regard, such as the preparation of zero-temperature as well as finite-temperature vibronic spectra.[106] The key idea is computing the overlap between vibrational states of the ground and excited PESs using a phase estimation scheme. A complication that arises in such computations is the fact that creation and annihilation operators of the two PESs are not identical due to the change in shape and frequency of the associated normal mode, but they are related through a Duschinsky transform.[101] In another report, the temporal autocorrelation function for a time-ordered perturbation string is computed directly through the appropriate Pauli decomposition and use of phase estimation.[107,108] The Fourier transform of such functions gives the frequency domain response from which properties like spectral lineshapes can be calculated.

However, given that the use of phase estimation is impractical in the NISQ era, a recent work[109] presents an approach to directly compute the frequency domain response function. The primary workhorse is to construct a solution vector $|\psi(\omega)\rangle$ for each frequency ω from the previously prepared ground state of the system using a variational framework, i.e., through an appropriate cost function. The frequency-domain response function is then computed through a simple observable average in this newly prepared state directly. The method was applied to compute the real and imaginary parts of dynamic polarizabilities of H_2 at different bond distances as well as the absorption spectrum of acenes.

Recently, Asthana et al.[110] formulated another recipe for computing electronic excitation energies wherein the ground state is obtained using unitary-coupled cluster ansatz. A sequence of excitation operators is considered for arbitrary excited states, and their nested commutators with the Hamiltonian are used to obtain the excitation energy, similarly to how the quantum equation of motion approach is used in traditional excited state variants of coupled-cluster theory. The method is exemplified using H_2, LiH, H_2O, and the symmetric stretching of H_4 into two H_2 clusters. The method was extended by the group[111] to obtain transition dipole matrix elements/oscillator strength for singlet and triplet states of small molecular systems under the linear response limit.

Typical computations of finite-temperature response functions (the effect of line broadening in the spectrum would not be captured otherwise) would need system-environment coupling, which eventually leads to a framework of dynamical evolution

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of open systems. The dynamics of open quantum systems under the Born-Markov scheme has been amply studied on a quantum computer either variationally[96,112,113] or otherwise. Recently, such a scheme for computing current-voltage (*I-V*) transport characteristics for electronic transport has been presented.[114] The work describes the dissipative dynamics of an externally driven system coupled to a fermionic bath. The Kraus operators of the system are implemented on a quantum circuit using ancillary qubits for purification. The output of the circuit directly gives the non-equilibrium steady state, from which steady-state current versus voltage characteristics can be obtained. While the work is presented on a model system, an extension to realistic systems can be made using the previously illustrated dynamical frequency-dependent response study[109] to compute AC Kubo conductivity. The motivation for extending such studies comes from the fact that transport characteristics (thermal as well as electronic) are extremely important for studying transistor-logic operations,[115–117] valleytronics, and spin-valley polarization in certain classes of 2D materials like MoS_2,[118–121] switching action in heatronics,[122] and spintronics devices.[123,124] Each of these domains can benefit the materials science industry, nanotechnology, and energy sectors immensely. Besides, electronic transport and ion transport are important for understanding the functioning of lithium-ion batteries such as $LiMnO_2$[125,126] and anode materials as in Liu et al.[127] and Meng et al.[128] Techniques for performing quantum simulations of environment-assisted quantum transport in complex chemical systems have also been developed.[129,130]

Apart from technological advances, such investigations may even lead to new platforms for quantum computing itself. A recent report[131] explores this intriguing possibility wherein quantum gates (both single and two-qubit unitaries) are constructed using system-electrode configurations and their mutual coupling in a molecular electronics setup. Single-qubit gates can be constructed using two-electrode output configurations, into which the scattering of an electron happens from a separate input electrode inter-separated by a molecular bridge (system) in between. The output electrodes correspond to two states of a qubit, and a general superposition state between the two can be created by engineering the system-electrode coupling. The inclusion of interacting matrix elements between electrons of a particular electrode can lead to two-qubit gates. Such possibilities allow the use of molecular electronics as a platform for quantum computing and should be a subject of further investigation.

Exploring chemical space and classifying molecules using a supervised learning protocol trained from a given dataset have also gained enormous momentum in recent years. Kernel-based classification/regression techniques are very useful in this regard. Kernel estimates can be obtained from a quantum computer from the inner products of two states (each encoding a classical data vector). One way that this has been implemented is by using the SWAP test.[132] A qubit-efficient version of such SWAP protocols with at most 2 registers being used at a time is explored in Yirka and Subaşı[133] through judicious qubit resets. After such estimation, the typical pipeline involves feeding the quantum-enabled kernel matrix estimate to a classical ML task.[134–138] Reports claim that, depending on the data-encoding unitary, certain correlations can be introduced in the state that are not attainable from classical resources.[139–141] Accordingly, kernel estimates from such states on a quantum device are believed to be more expressive in performing the task.[138,142]

A second type of typical workflow is framing a quantum ML (QML) problem with a parameterized unitary following a data encoder. The data encoder maps a given classical data vector onto a quantum state (amplitude encoding, phase encoding, or any other relevant schemes can be used). The parameterized unitary is responsible for

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transforming this mapped quantum state encoding classical data into an ansatz state. A suitable user-defined observable is then measured in this ansatz state to obtain an average value. This average is directly used to construct an appropriate task-specific cost function, which is subsequently variationally optimized with respect to the parameters of the unitary. Again, quantum computers are useful, as certain reports claim such functions can be universal depending on the nature of the encoding.[143] In general, both workflows can benefit from the fact that certain recent reports provably demonstrate (analytically as well as through numerical experiments)[144–146] that QML models require less training data than their classical counterparts.

The kind of benefits chemistry, in particular, can enjoy through such models are also highlighted in section 4 of our recent review.[68] In fact, a direct benefit has already been seen in reduced training time for the classification of active versus inactive ligands in *M. tuberculosis* using just two features[147] using a quantum support vector machine (QSVM) algorithm on IBMQ-Rochester. In a drug-discovery pipeline, apart from the activity of a ligand against a target protein, one is also interested in screening ligands based on drug-induced toxicity and predicting ligand-target protein binding affinity. Inspired by the tremendous success of classical ML techniques like regression and kernelized classification, straightforward quantum extensions of these classical ML methods can be directly adapted for these applications too. In addition, developing such classification techniques for other applications like sieving molecular and material properties, e.g., optical activity or electrical and thermal conductivity, given information about the band structure in materials, can be investigated as a straightforward extension of such protocols.

Given this vast array of quantum algorithm development for the field of chemistry, the question of how much advantage could quantum computers be expected to provide over classical computers for chemical applications remains. Even though this question is being increasingly examined, the answer is not yet clear. A good place to start addressing this question is by analyzing the runtime complexity of some of these algorithms. A typical starting point of a VQE method, aimed at solving molecular/atomic electronic structure problems, consists of r_o occupied and r_{uo} unoccupied spin orbitals in a classically computed Hartree-Fock reference ($N_{elec} = r_o$). For such a setup, the more commonly used unitary coupled-cluster singles and doubles (UCCSD) ansatz[148] requires $O(r_o)$ qubits, $O(r_o^2 r_{uo}^2)$ cluster amplitudes as parameters of the ansatz, and $O(\chi r_o^4)$ gates where $\chi = O(r_o)$ or $O(log(r_o))$, depending on the mode of mapping. For a problem-agnostic structurally layered ansatz[149,150] repeated over D layers with $O(poly(r_o + r_{uo}))$ gates in a single layer, the number of parameters used is $O(Dpoly(r_o + r_{uo}))$. If the encoded fermionic Hamiltonian $H = \sum_k^M d_k P_k$, where P_k are Pauli words defined before and $d_k \in \mathbb{R}$, then $O(M \approx (r_o + r_{uo})^4)$ measurements are necessary to determine $\langle H \rangle$ (this number can be further optimized[151,152]) with an overall precision of $O\left(\sqrt{\sum_k^M |d_k|^2 \frac{Var(P_k)}{N_s}}\right)$ when N_s shots are used for each Pauli measurement.[153] For variational dynamical simulations on closed or open quantum systems, additional measurements are necessary to retrieve elements of the propagator for constructing an equation of the motion of the parameters.[94,95,154] None of these methods retrieve the full quantum state from quantum memory, and hence all of them meet a polynomial storage requirement.

However, this apparent illusion of advantage needs to be examined carefully, as an analysis of the VQE method has found that the method in its current form should not

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be expected to ever outperform classical computations for useful problems in chemistry.[155] Besides, such variational methods are also sometimes plagued by the menace of barren plateaus,[156–160] which render them untrainable for large system sizes. Several strategies to mitigate barren plateaus are being actively pursued,[160–163] but this issue is far from being completely solved. In addition, there is always the known problem of the expressibility of the chosen ansatz, which is tough to gauge *a priori* and difficult to characterize.[164,165] The alternative is the more traditional QPEA, which requires exceptionally deep quantum circuits, making it unfriendly to the NISQ era. Moreover, a recent work by Lee et al.[166] provided numerical evidence showing that the QPEA—even in the fault-tolerant setting—may not be favorable for generic chemistry problems due to high state preparation costs and circuit repetition protocols, thereby questioning the usually accepted hypothesis that the QPEA can furnish exponential speedup over classical ones for solving ground state quantum chemistry problems. However, it should be noted that even just a polynomial speedup could be a major benefit for many chemical applications. More broadly, quantum advantage is a multi-faceted issue comprising a wide variety of factors beyond algorithmic complexity, involving state initialization, information storage and retrieval, the overhead of repeated measurements, and even energy consumption. All of these elements—and their scaling with increasing system size—must be considered on balance to determine if a given algorithm achieves an advantage.[167–169] The continued steady improvements in algorithms, coupled with advances in error mitigation, error correction, and hardware, will continue to narrow the performance gap between quantum and classical computational chemistry. Exactly when the two approaches reach parity is an open question, but the intrinsic nature of the quantum chemistry problem is an ideal paradigm for investigating the promise of quantum speedups for chemical simulation.

HARDWARE

In classical computers, at the most basic hardware level, binary information is stored in the state of transistors built into silicon. These transistors function effectively as two-state switches, which can be controlled with the application of appropriate voltages, and are arranged to form logic gates. At a higher level, logic modules are bundled together into task-specific integrated circuits, which are the backbone of modern classical processors ranging from the laptops and smart phones we use every day to the largest supercomputers.

While no physical system can be completely isolated from external noise, in classical computing, environmental noise has no significant contribution to the ability to carry out a computation, nor to the accuracy of the computational results. This is due in large part to the robustness of modern transistors to noise in the control voltages and to the mature, and relatively straightforward, techniques of classical error correction. On the other hand, while initial implementations of quantum computing for chemical applications suggest promise for future quantum advantage, the advancement of quantum computing in the relatively near future remains limited by challenges associated with the noisy quantum hardware characteristic of the NISQ era. In this section, we review the essential properties needed to make quantum computing hardware, provide a brief overview of hardware implementations currently in use for computational chemistry, and discuss the ongoing challenges in the experimental realizations of quantum computations for chemical applications.

The main requirements needed to build a robust and functional quantum computer are captured in DiVincenzo's criteria,[170] which state the following.

(1) The hardware implementation must be scalable, such that the addition of the necessary number of qubits does not affect the overall robustness and accuracy of the quantum computation.
(2) The set of well-characterized qubits must be straightforwardly initializable to some known state, or "fiducial state," before computation begins.
(3) The qubits comprising the computer must have coherence times long enough that all the gates necessary to complete a computation can be carried out before the qubits decohere.
(4) The quantum system must be able to host a "universal set of quantum gates," where the system's interaction mechanisms are well defined and robust enough to be able to control with gates, i.e., unitary transformations, within a quantum algorithm.
(5) Lastly, the quantum system must have readout capabilities to determine the results of the computation. Ideally, a readout will have a high level of measurement accuracy, or fidelity, and the readout measurement will be within a reasonable time frame with respect to the qubit coherence time.

These criteria are widely accepted as the foundation for gate-based quantum computing and must be met by any actual physical realization of a quantum computer.

In order to build a quantum processor, one needs a robust quantum system that can be used as a qubit. The main ingredient for a qubit is a discrete energy-level spectrum to provide the computational basis states. While there are many quantum systems that have discrete energy levels, an additional criterion is imposed by the need to control the occupation of these states. In particular, the energy levels need to be distinguishable from one another, and the state of the qubit must be deterministically controllable. Typically, the computational subspace used for quantum computing is confined to two dimensions, i.e., two addressable energy levels or (in an ideal case) a simple two-level system. However, there are also physical platforms that consider d-dimensional computation subspaces using qudits.[171–175]

While a wide variety of qubit platforms are being investigated and implemented, several quantum hardware platforms have already been used extensively to simulate molecules; these are superconducting qubits,[49,50,176–178] trapped ions,[179,180] spins in semiconductor devices,[181,182] neutral atom arrays,[183] and photons.[184–186]

To understand the basics of how simple logic gates are implemented in quantum hardware, and how these can be combined into more complex quantum processing units, it is useful to describe how one of these platforms works in order to build an intuition for what controlling and manipulating qubits looks like. As a concrete example, we will focus this discussion around superconducting qubits since a variety of multi-qubit systems using this hardware platform have already been demonstrated for NISQ-era quantum chemical applications.[49,50,176–178] Additionally, superconducting qubit processors have also been used to demonstrate purported advantage in other computational arenas, such as in sampling random quantum circuits[187] and IBM's array of quantum processors, which include the "Eagle" 127-qubit processor that has claimed quantum utility in the NISQ era[188] and the 27-qubit "Falcon" processor, demonstrating the creation of magic states as a key step toward fault tolerance with error mitigation.[189]

The foundation of the superconducting qubit relies on the control and readout techniques of circuit quantum electrodynamics (cQED)[190,191]—the circuit analog of

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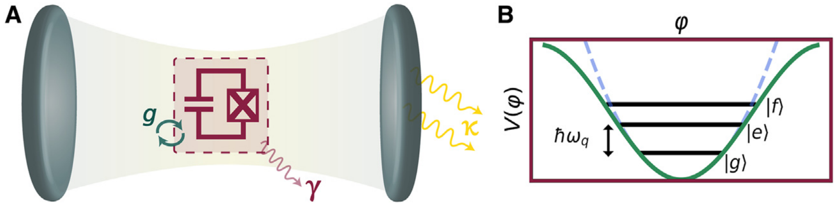

Figure 3. Representation of a superconducting transmon qubit coupled to a microwave cavity with a corresponding anharmonic potential energy-level diagram

(A) Superconducting qubit (represented by a Josephson junctions shunted by a capacitor) inside a resonator cavity for cQED-based control and readout. The qubit is coupled to the cavity field (yellow shaded region) with a strength g. The cavity and qubit both have individual loss rates κ and γ, respectively, where the loss rate of the cavity can be thought of as an imperfectly reflective mirror.
(B) The qubit-level spacing is anharmonic to allow for individual state distinguishability. This anharmonicity arises from the non-linear current-to-voltage relationship of the Josephson junction (red x in circuit in A).

cavity QED[192,193]— which describes the interaction of a two-level atom with a bosonic cavity control field (see Figure 3). In contrast to cavity QED, in which a real two-level atom is confined in an optical cavity, in cQED, a circuit containing a capacitive element in parallel with a non-linear inductor acts as an artificial atom and is coupled to a microwave resonator cavity. Like any classical inductor-capacitor (LC) resonant circuit with fundamental frequency $\omega = \frac{1}{\sqrt{LC}}$, this quantum LC circuit has a resonant frequency, ω_q, defined by its capacitive and inductive components. These circuits can be designed to have discrete anharmonic energy levels (left, Figure 3), where the anharmonicity is provided by the non-linear inductor, called a Josephson junction,[194–196] in which Cooper pairs—two electrons bound together acting as the "supercurrent particle" intrinsic to superconductivity—can tunnel across the junction with some probability. The ability to control this type of qubit relies on engineering the coupling between the capacitively shunted Josephson junction circuit and the electromagnetic control signals of the cavity field.[197] With these basic circuit elements, a wide variety of superconducting qubits can be created having various levels of coherence and functionality.[198]

Typically, these superconducting qubits are designed to operate at microwave ($\simeq 3 - 8$ GHz) frequencies. In essence, a single qubit can be manipulated on the Bloch sphere via sequences of microwave pulses having appropriately defined amplitude, phase, and duration. These microwave signals are typically synthesized at room temperature and supplied to the qubits via on-chip microwave transmission lines and resonator structure. The superconducting qubit chips are housed in the cryogenic environment ($T \simeq 10$ mK) provided by a dilution refrigerator (see Figure 1). This level of cooling is needed in order to passively initialize the qubits into their quantum mechanical ground state. To generate two-qubit logic, one needs additionally to control the interaction between two individual qubits, generate deterministic entanglement, and detect that an entangled state has been created.[199] There are multiple ways for coupling two qubits—via ancillary qubits,[200–203] coupling resonators,[204–206] or tunable couplers,[207–209] for example. Finally, as with their classical counterparts, larger-scale quantum integrated circuits and processors are then composed of many such qubits coupled together with varying levels of connectivity depending on a particular chip architecture.

While superconducting qubits represent just one type of quantum computing platform, qubits can be made from a variety of physical systems. For trapped ions and neutral atoms, qubits are formed from the states and configurations of the electrons

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orbiting the ions/atoms, and excitation and manipulation are provided by laser fields instead of microwave pulses.[210–216] On the other hand, spin qubits in semiconductor devices are like the quantum mechanical cousins of the classical bits in our current classical computers. In these devices, the qubit states are the spin projections of an electron subjected to an external magnetic field and confined within a nanoscale gate-defined region, called a quantum dot.[217,218] In these quantum dots, voltages applied to surrounding electrodes can be used to control and manipulate the electron spin.[219,220] Beyond these platforms, even more novel types of qubits are carving a path in the race for building a robust large-scale quantum computer, such as optical devices that encode information in photons[221,222]; color-center defects in diamond[223,224]; single electrons trapped above the surface of superfluid helium[225–231] or neon[232,233] or in radio-frequency traps[234,235]; and anyon-based topological qubits.[236–239] For more complete descriptions of these hardware platforms, we refer the reader to helpful reviews for further information on this highly active area of research.[240,241]

Although these various qubit platforms have their own unique characteristics that make them good candidates for quantum processors for different reasons, one thing all these qubit platforms have in common is their sensitivity to environmental noise. As mentioned earlier, several hardware platforms have already demonstrated practical use toward chemical applications, particularly with variational quantum algorithms due to their usability on current NISQ-era devices. Through cloud capabilities provided by IBM, one can run quantum algorithms on any of their available superconducting devices. Moreover, cloud-based quantum computing services are also available through Microsoft Azure and Amazon BraKet, where one can choose quantum computers from various companies and run algorithms on superconducting, trapped ion, or neutral atom devices. With the widening availability of these platforms, many algorithms for chemistry applications are being developed and tested.[242–245]

While current implementations of quantum computing devices have yet to outperform classical computers in these chemical applications, advances in quantum processor performance continue,[187,246,247] which generally bodes well for future applications to quantum chemistry. Estimates for the necessary number of logical qubits for quantum computers to outperform their classical counter parts are placed at around $50 - 100$[40]; however, the number of physical qubits required to do necessary error correction will likely require millions at least, depending on the algorithm and the specific error correction protocol.[7,248–251] In the end, the device platforms that will provide the most benefits for not only chemistry but all purposes will be the ones that can mitigate and/or correct errors efficiently, process information quickly with respect to qubit lifetimes, and overcome the detrimental effects of noise. While a single platform has yet to prove supremacy over the others, a large area of research in quantum software aims to make do with the current state-of-the-art devices and attempt to extract value from today's NISQ devices.

SOFTWARE

As quantum computing hardware continues to develop, another component that is required in order to make quantum computers useful for chemistry is software. The goal of software is to convert human-inputted instructions into a format that can be carried out on a computer chip. For classical computers, the physical realization of this process corresponds to manipulations of voltages of classical bits on electronic circuits. For quantum computers, software is needed to transform human input into

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physical manipulations of qubits. Effective software is crucial to any scientific field, as it makes it possible for those who are not experts in computer engineering or programming to still perform useful computations and gain the resulting insight. For example, classical quantum chemistry software packages have been developed over decades, and they allow chemists—both experimentalists and theorists alike—to perform useful computations of molecular systems without having to know all the details of classical computing processors, bits, or logic gates. The goal of quantum computing software for chemistry is to produce a similar type of software that allows any chemist—both experts and novices—to make use of quantum computers for their own work. The software for performing computations of chemical systems on quantum computers is still in the early stages. In this section, we summarize the vast amount of progress that has occurred in this area over the last few years.

While quantum computers are believed to be useful for solving certain classes of problems, they are not expected to be better than classical computers for all types of computations. As a result, the practical implementations of quantum computing do not use quantum computers for all aspects of the computation. Instead, much of the work that goes into the computation, including writing the code, setting up the qubit parameters, and loading the input data, occurs on classical computers, and only the most demanding part of the computation is performed on the quantum processor. Thus, quantum computations are inherently hybrid processes that take advantage of both classical and quantum hardware. Therefore, the software that is needed for quantum computing involves many different layers, which together are known as the quantum software stack, consisting of both classical and quantum components.

The quantum software stack consists of tools such as programming languages, libraries, compilers, error correction software, and debuggers. Several quantum simulation packages exist that include many or all of these software categories in one package. These ‘‘full-stack’’ software packages handle all aspects of running a quantum computation, starting from the initial algorithm specification and continuing all the way to the instructions that directly manipulate the qubits. Full-stack software packages with explicit support for quantum chemistry computations include Google's OpenFermion,[252] IBM's QISKit,[253] Quantinuum's InQuanto,[254] Microsoft's Quantum Development Kit (QDK),[255] and Tequila.[256] Fortunately, these software packages are either completely open source or contain open-source components, which is an important feature for expediting the improvement of these codes and extending the overall quantum computing user base. For a more complete list of open-source software components for quantum computing, see Fingerhuth et al.,[257] Bharti et al.,[258] and Quantum Open Source Foundation.[259]

Many interfaces exist between quantum computing software and classical quantum chemistry software packages. These interfaces allow for classical programs to easily provide input data for the quantum algorithm, including molecular geometries, integrals, orbitals, or starting wavefunctions. For example, OpenFermion has plugins for Psi4, PySCF, Dirac, and QChem; QISKit interfaces with Psi4, PySCF, Gaussian, and PyQuante; QDK interfaces with NWChem; and Tequila interfaces with Psi4, PySCF, and Madness. The existence of these quantum chemistry interfaces in commercial quantum computing software from, e.g., Google, IBM, and Microsoft serves as an indication of the high amount of attention that chemistry is receiving in near-term quantum computing efforts.

CONCLUSIONS AND OUTLOOK

Quantum computing in chemistry holds immense promise, offering the potential to revolutionize our understanding of the structure and dynamics of complex molecular systems, thus accelerating scientific discovery across various fields. This encompasses simulating molecular structures and chemical reactions and advancing drug discovery and design, catalyst design, materials science, QML, and data analytics, among other applications. Realizing this potential necessitates ongoing development of quantum computing algorithms for both electronic structure and dynamics. These efforts must be coupled with the advancement of scalable hardware devices and the resolution of technical challenges. These challenges encompass developing efficient error correction methods to mitigate the effects of noise and errors in quantum hardware, enhancing the reliability and scalability of quantum computing algorithms, and integrating quantum computers with classical computational methods. As the field of quantum computing continues to evolve, applications in chemistry are poised to be at the forefront of innovation.

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