

Quantum Computing and Simulations for Energy Applications: Review and Perspective

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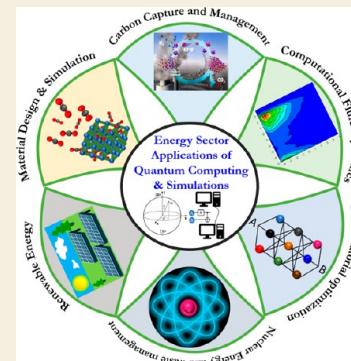
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ABSTRACT: Quantum computing and simulations are creating transformative opportunities by exploiting the principles of quantum mechanics in new ways to generate and process information. It is expected that a variety of areas ranging from day-to-day activities to making advanced scientific discoveries are going to benefit from such computations. Several early stage applications of quantum computing and simulation have already been demonstrated, and these preliminary results show that quantum computing and simulations could significantly accelerate the deployment of new technologies urgently needed to meet the growing demand for energy while safeguarding the environment. Exciting examples include developing new materials such as alloys, catalysts, oxygen carriers, CO₂ sorbents/solvents, and energy storage materials; optimizing traffic flows and energy supply chains; locating energy generation facilities such as wind and solar farms and fossil and nuclear power plants; designing pipeline networks for transporting hydrogen, natural gas, and CO₂; and speeding up tasks such as seismic imaging and inversion, reservoir simulation, and computational fluid dynamics. In this review, we introduce different aspects of quantum computing and simulations and discuss the status of theoretical and experimental approaches. We then specifically highlight a growing number of application areas in the energy sector. We conclude by providing an analysis of high-value application directions to address energy sector challenges.

KEYWORDS: Quantum information science, Quantum computing, Quantum simulation, Quantum sensor, Quantum networking and communications, Quantum entanglement and superposition



1. INTRODUCTION

The basic principles of quantum information science (QIS) are derived from quantum mechanics and make use of a number of physical and mathematical theories.^{1–4} In quantum mechanics, physical observables are described by probability to explore underlying chemical and physical phenomena. Such descriptions cannot be made in a classical regime.^{2,5,6} QIS theory is a basis for a system's entropic description. In the modern world, the QIS approach for entropy helps us to understand the performance of electronics and computing devices.^{7–9} Numerous scientific institutions and policy-makers around the world are showing a heightened level of interest in QIS because of the potential breakthroughs it may engender. Generally, QIS can be divided into four main pillars: quantum computing, quantum simulations, quantum sensing, and quantum networking. Table 1 summarizes their definitions, major attributes, and applications.

In previous work,¹⁵ we summarized the current status and future outlook of quantum sensing for energy applications. Here, we focus on summarizing the current status of quantum computing and simulations and their applications in the energy sector.

1.1. Basics of Quantum Computing and Quantum Simulations

The idea of quantum computing was first put forward by Russian mathematician Yuri Manin in 1980,¹⁸ whereas Richard Feynman independently proposed the concept of the quantum computer in 1981.¹⁹ Feynman realized that simulating quantum dynamics becomes impossible on classical computers beyond a certain simulated system size because of the exponential growth in the computational resources required.²⁰ Feynman, in advocating for quantum computer development, observed that “Nature isn’t classical and if you want to make a simulation of Nature, you’d better make it quantum mechanical, and by golly it’s a wonderful problem, because it doesn’t look so easy.”²⁰ In 1985, David Deutsch showed that quantum computers might have computational powers exceeding those of classical computers.²¹ Subsequently, Deutsch and

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Table 1. Four Pillars of Quantum Information Sciences

four pillars	definitions	main attributes	application
quantum computing	exploitation of collective properties of quantum states, such as superposition and entanglement, to perform the computation ¹⁰	qubit, quantum computer, quantum algorithm, analog and gate-based quantum computing ¹¹	computations surpassing classical capabilities ¹²
quantum simulations	using a “controllable quantum system to study another less controllable or accessible quantum system”; quantum simulation could be implemented with analog devices that would be easier to construct than quantum computers ¹³	programmable physical many-body quantum system such as spin-based system, quantum simulator	quantum chemistry problems, quantum many-body problems, superconducting qubits ¹⁴
quantum sensing	use of a quantum system, quantum properties, or quantum phenomena (coherence, entanglement) to perform a measurement of a physical quantity ^{15,16}	exploitation of quantum attributes of the coherent or entangled state	sensing beyond classical limits, atom interferometer, atom magnetometer, Rydberg atoms, atomic clocks, atom interferometer ¹¹
quantum networking	transmitting information with the help of “entangled” particles—whose quantum state cannot be described independently, even when they are separated by a large distance ¹⁷	exploitation of measurement induced collapse of the state such as by action of the eavesdropper	quantum cryptography, quantum key distribution (QKD) technology, quantum repeaters, telescopes connecting quantum sensors, quantum computers, quantum Internet ¹¹

Jozsa,²² Bernstein and Vazirani,²³ and Simon proposed quantum computing algorithms that provably outperformed classical algorithms. However, those algorithms solved problems with no practical applications. A major scientific achievement came in 1994 when Shor proposed a quantum computing algorithm for factoring large numbers,²⁴ which can break many popular encryption schemes. This provided great motivation for the development of quantum computers in the 1990s because the algorithm made possible provable exponential speed up²⁴ and allowed early stage quantum computers to outperform powerful classical supercomputers in solving specific problems for data encryption.²⁵ Interest in the quantum computer increased significantly in 1996 after Lov K. Grover proposed a search algorithm with provable polynomial speed up.²⁶ Moreover, the first technologically feasible design for a quantum computer was proposed in 1996.²⁷ These and other advances in quantum computing generated possibilities for its practical applications in information security, optimization, machine learning, and artificial intelligence. Currently, many quantum computing algorithms are available as, for example, can be seen at the quantum algorithm zoo.²⁸

In 1999, a Canadian company called D-Wave Systems built the first quantum computer based on superconductors.²⁹ The company demonstrated a 28 qubit quantum computer in 2007, followed by a few other quantum computers with higher numbers of qubits that were able to solve only optimization problems by exploiting a quantum annealing process. Subsequently, several companies developed universal quantum computers capable of solving a variety of problems. Recently, IBM has started cloud quantum computing called IBM-Q and has provided public access to a few universal quantum computers. In 2019, Google announced that it achieved quantum supremacy in computations using its 53 qubit Sycamore quantum computer. Today, a number of companies such as Microsoft, Intel, Rigetti, IonQ, Lockheed Martin, Honeywell, and others are building a universal quantum computer. In 2018, the European Commission announced the billion euro, 10-year Quantum Technologies Flagship. The metal oxide semiconductor (MOS)-based quantum information technology project was started after successful implementation of a complementary metal-oxide semiconductor (CMOS) compatible qubit in France.³⁰ Solid-state implementations have attracted attention in recent years due to their potential for scale up to a larger number of qubit systems. This class of qubits belong to the superconducting Josephson junctions and nitrogen-vacancy (NV) center in the nanodiamond. Spin qubits in silicon have become a great asset due to their compatibility with CMOS foundries.^{31,32} Each qubit in the system is individually interconnected to the outside world to perform the measurement. CMOS platforms provide greater flexibility while circumventing several technological problems. Table 2 provides examples of how various lab-built and commercial quantum computer platforms have evolved over the past 25 years, including the number and types of qubits used as well as some of the problems to which the computers were applied.

Quantum circuit operation in current quantum devices is limited to a small number of qubits due to noises and dissipations. Because thermal noise is the biggest threat to qubit stability, state-of-the-art qubits are maintained in a dilution refrigerator at sub-milliKelvin (~ 10 mK) temperatures. As part of the quantum error correction, several redundant physical qubits are required to encode a single

Table 2. Examples of Quantum Computing Platforms and Their Applications

year	qubit type	no. of qubits	problems investigated	ref
1998	H in deuterated cytosine	2	quantum search algorithm	33
2000	H in deuterated cytosine	2	fundamental studies on quantum computation	34
2004	¹³ C-labeled alanine	3	nonseparable 2 qubit operation	35
2010	trapped ⁹ Be and ²⁴ Mg ions	2	randomly chosen operations	36
2010	photonic	4	hydrogen molecule energy spectrum	37
2014	trapped ¹⁷¹ Yb ions	11	quantum correlations in long-range interactions	38
2014	trapped ⁴⁰ Ca ions	7	quantum dynamics	39
2015	Xmon transmon	9	simulation of fermionic models	40
2016	trapped ⁴⁰ Ca ions	4	simulation of lattice gauge theory	41
2017	trapped ¹⁷¹ Yb ions	53	non-equilibrium dynamics in the transverse-field Ising model	42
2017	transmon	6	small-molecule ground-state energy calculations	38
2018	trapped ¹⁷¹ Yb ions	5	Deutsch–Jozsa and Bernstein–Vazirani algorithms	43
2018	quantum dot electronic spins	2	Deutsch–Jozsa and Grover Search algorithms	44
2019	trapped ¹⁷¹ Yb ions	11	Bernstein–Vazirani and hidden shift algorithms	45
2019	transmon	53	quantum circuit simulations	12
2019	NV nanodiamond	2	Deutsch–Jozsa algorithm	46
2019	transmon	20	verifying multipartite entangled Greenberger–Horne–Zeilinger states	47
2021	hole spins in germanium quantum dots	4	generating Greenberger–Horne–Zeilinger states	48

logical qubit. The interconnect that addresses each qubit residing at 10 mK passes through a cryogenic dilution temperature of 4.2 mK followed by different levels all the way to ambient temperature. Thermal environments not only threaten the accuracy but also create a problem on running sophisticated quantum algorithms where an immediate action is required after the qubit is read.⁴⁹ Several proposals based on CMOS front-end electronics that can run at cryogenic temperatures have been developed to address the above challenges.^{50–53} One such example is Google's Bristlecone quantum computer where a CMOS prototype integrated circuit (IC) with a pulse generator was employed to communicate with qubits within 4 K temperature. This increased the possibility of realizing CMOS technology at the peripherals of qubits that are held at deep cryogenic temperatures.⁵⁴

1.1.1. Progress Overview on Quantum Computing and Simulations. Quantum simulation is a method to study a complex quantum system using a controllable and accessible model system. Several platforms such as neutral atoms, ions, polar molecules, electrons in semiconductors, superconducting circuits, nuclear spins and photons are possible quantum simulators. Experts currently believe that quantum simulations can provide near- or mid-term opportunities relative to quantum computers because fault-tolerant quantum computers that can perform such computations are currently not available.¹⁷

Quantum simulators consist of an array of qubits which could be represented using cold atoms in optical lattices, atoms in arrays of cavities, ions trapped by electric or magnetic fields in 2D crystals, electrons in arrays of quantum dots, Rydberg atoms, polar molecules, nuclear magnetic resonance (NMR), linear and nonlinear quantum optics, superconducting circuits, among others.⁵⁵ The defining feature of qubits is that they provide some means for encoding quantum information, such as internal energies and the vibrational modes of trapped ions, nuclear spins that can be manipulated and read-out by an NMR spectrometer, etc. For example, Geiger⁵⁶ described an experimental setup for creating ultracold ⁷Li atoms that can be used for quantum simulation of dynamical systems. Anderegg et al.⁵⁷ created an array of optical tweezers and trapped ultracold CaF molecules. They were able to control and image individual molecules and observe molecular collisions, enabling the simulation of chemical reactions.

Quantum computing is the process of computation with devices that process information using quantum mechanical laws such as quantum superposition states, photon squeezing, and entanglement. Quantum computation connotes the implementation of algorithms based upon the evolution of states under certain reversible operations using quantum logic gates, which are elementary circuits that operate on the qubit. Controlled NOT gate (CNOT), Hadamard (H), Pauli-X, -Y, and -Z, SWAP, and Toffoli gates are examples of elementary quantum logic gates.^{58–61} A sequence of quantum logic gates forms a block of the quantum circuit.

Quantum computers use quantum bits or qubits that represent the values of 0 or 1 or some combination of both at the same time (known as a "superposition"). Intrinsically interconnected ("entangled") qubits can access an exponentially large parameter space compared with classical bits. This enables quantum computers to solve problems that are impossible for classical computers to solve; for example, Shor's algorithm can factorize integers almost exponentially faster than the most efficient classical algorithm.⁶² When Shor's algorithm is implemented in a (as yet unavailable) quantum computer, it will be possible to break public key cryptosystems such as the Rivest–Shamir–Adleman (RSA) scheme,⁶³ which relies upon the fact that factorization of large integers is computationally intractable on classical computers. In recent years, several institutions have made significant contributions in the research and development of quantum computing. Google scientists demonstrated a long-sought milestone of quantum supremacy using a programmable superconducting processor.¹² This work is a demonstration of the exceptional power of quantum computation, and the benchmarks provide an idea of how future quantum systems will perform when solving similar but exponentially more complex simulations.

1.1.2. Past and Current Status: Web of Science Database Analysis. To explore the developmental trend of quantum computing and simulation, we conducted a Web of Science database analysis. Figure 1 shows the number of publications on quantum computers and simulations during the past 25 years. As one can clearly see, the number of publications on these topics have been increasing annually, demonstrating the rapid growth and development of quantum computers and algorithms. The research on quantum machine learning also increased during the last 5 years. Such trends indicate significant research efforts have been devoted to quantum computing and simulation.

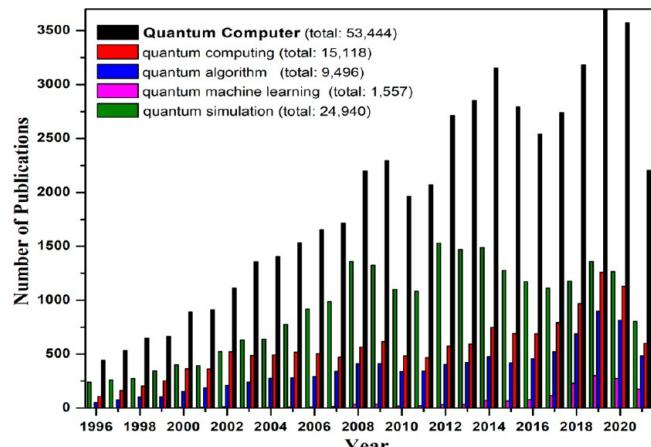


Figure 1. Number of publications on quantum computing. Searched from Web of Science database with keyword “quantum computer” first, then using other keywords to filter into four areas as shown. Only literature from the past 25 years is plotted in the figure. Data generated on October 14, 2021.

1.2. Quantum Computing and Simulations for Energy Applications

Quantum computing is finding applications in numerous areas of basic sciences to further understanding of underlying physical phenomena. Studies have been performed in different research institutions worldwide to explore the utility of quantum computers in areas like high energy physics, nuclear science and energy,⁶⁴ quantum chemistry,^{65–67} economics,^{68,69} communications,⁷⁰ and optimization.^{71,72} The rapid progress of research in quantum computing has created opportunities for application in renewable energy, nuclear energy and nuclear waste management, fossil energy, geothermal energy, carbon management, and energy efficiency. Common themes can be identified that span many of these various areas of application, and these themes include:

1) Combinatorial optimization of energy infrastructure and materials science

Combinatorial optimization problems such as power systems design and operation as well as the search for new energy materials can be very challenging using classical computing approaches. As a long-term opportunity, the unique scaling properties (scalable with the system size) resulting from quantum entanglement and superposition could enable problems of combinatorial optimizations and material search to be solved using quantum computing machines with lower computational cost while maintaining high accuracy.⁷³

2) Accelerated and enhanced simulations of complex energy system processes

A fundamental challenge that exists in the synthesis and design optimization of energy systems is defining the design parameters and system configurations. Methods based on the superstructures (i.e., structures that embed all the possible configurations that fulfill a specified duty) have been developed for the design of chemical processing,^{74,75} mass and heat exchange networks,^{76,77} and distributed energy supply systems.⁷⁸ Such superstructure-based methods, for example, have been applied to find the best retrofit solution for CO₂ capture from exhaust gases in a pilot scale power plant in South Korea.⁷⁵ In a recent study, artificial intelligence

was applied in generating an open superstructure from a given set of rules.⁷⁹ The computational cost in simulating more complex energy systems would be too large to be feasible to perform such calculations on classical computers. Quantum computations could be useful as mid- to long-term opportunities for solutions to such problems.

3) Nuclear energy

Efforts are ongoing in formulating quantum mechanical descriptions of nuclei and field theoretic processes to enable realistic calculations. One such effort has continued to grow at Argonne National Laboratory (ANL), where quantum computing and quantum sensing are applied to solve complex problems of nuclear theory and experiments.^{80,81} For instance, Dumitrescu et al. used cloud quantum computing and reported a quantum simulation of the deuteron binding energy on nascent quantum devices.⁸² Highly sensitive QIS-enhanced devices not only detect early stages of radiation breaches but also provide avenues for remote monitoring of such specific safety-related issues in the power plant. In nuclear waste management, nuclear vitrification requires computational fluid dynamics modeling, which can benefit using quantum algorithms.⁸³

1.3. Scope of Review

The U.S. National Quantum Initiative Act (NQIA), which was signed into law in late 2018, instructs three U.S. agencies—the National Institute of Standards and Technology (NIST), the National Science Foundation (NSF), and the Department of Energy (DOE)—to work with academic institutions and private industry to catalyze the growth of QIS.⁸⁴ According to the NSF, in the next 10 years, several opportunities will be enabled in quantum processors, quantum sensors for biotechnology and defense, next-generation positioning and navigation, timing systems useful to military and commerce, new levels of understanding of complex problems in material science, chemistry and physics, machine learning and optimization, and robust cyber security systems that incorporate quantum cryptography and quantum key distributions. These applications have implications covering a wide range of areas such as energy and security that directly impact daily life.

In this article, we review the current development of quantum computing and simulations and discuss the potential opportunities offered by bringing this emerging technology into the different domains within the energy sectors. More specifically, we highlight potential opportunities where transitioning from classical computation to hybrid or quantum computation could help to enhance efficiency of energy production or consumption, as well as enhancing reliability and resiliency, and reducing environmental impacts from extraction, transportation, and utilization of energy resources. Although an emphasis is placed upon applications related to fossil energy and carbon management, an overview of relevance to other energy applications is also presented. Different areas within fossil energy and carbon management such as turbulent flows, catalysis, carbon capture and storage, oil and gas exploration, surface and subsurface characterization, and chemical sensing are all examples of applications where quantum technologies are potentially useful for enhancing safe, secure, and reliable extraction and utilization of energy

resources with net zero carbon emissions.^{85–88} Figure 2 highlights a general scope of this review. We discuss current

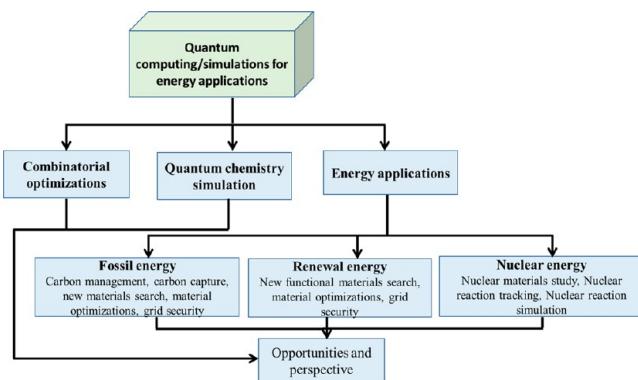


Figure 2. General scope of this review: Application areas of quantum computing and simulations in energy/fossil energy and carbon management with brief concepts for each and discussion on potential opportunities and perspectives.

developments of each QIS component, and present the recent status of energy sector applications. In addition, we also identify QIS opportunities for potential areas of energy (with emphasis on fossil energy) applications where currently available technologies will benefit from enhancement.

2. QUANTUM COMPUTING

While the classical computer has the power to solve many complex physics and chemistry problems to an acceptable level of accuracy, only the quantum computer has the power to simulate the so-called many-body problems from the quantum perspective. Classically intractable problems from material chemistry, which play a central role in fossil energy and carbon management technology development, provide an excellent test bed for early stage quantum computers. Challenges include the search for optimal carbon capture materials, small- to large-scale batteries, analyte sensing in harsh environments, and catalytic processes in complex reactions, where further understanding is necessary to advance technologies for maintaining the safe and secure utilization of energy. Classical computation of many of these problems is limited by either the size of the problem or the time to solution. With the advent of quantum computation, material chemistry problems of great interest and high technological importance for energy infrastructure are now within reach. In this section, we provide recent advancements in quantum computation from the hardware and algorithm development perspectives and present

its usefulness in material chemistry and physics relevant to carbon capture, sensing and other high-impact areas of fossil energy, and carbon management technologies. To provide an overview of the current status of the quantum computing industry, Table 3 lists the current state-of-the-art in commercially accessible quantum computers, as well as computers currently under development.

2.1. Problems Classification

Quantum computers are expected to speed up only certain type of problems, which are typically classified as “very hard” problems. The computational complexity of these very hard problems increases exponentially with the system size, making such problems intractable on today’s computers, even supercomputers. For some of those problems, quantum computing algorithms make the computational complexity scale polynomially with system size, making such problems tractable on quantum computers. Examples of such problems include optimization, simulating proteins, many-body quantum dynamics, highly energetic quantum particles, computational chemistry, machine learning, deep learning, artificial intelligence, and sampling of large data sets.

Even when a hard problem is theoretically solvable, it is important to know whether it can be solved within a given time using finite resources. Figure 3 depicts classes of problems that quantum computers would efficiently solve and their relation to other computational problems. A thorough explanation of computational complexity classes is beyond the scope of this review, but interested readers are referred to a book authored by S. Aaronson.⁹⁹ Quantum computation belongs to bounded-error quantum polynomial (BQP) time class problems, which do not include nondeterministic polynomial (NP) hard problems.⁹⁸ Examples of BQP class problems are the factorization of large numbers and the discrete logarithm. The BQP does not interface neatly with all other classes. The BQP class includes polynomial (P) and some of the NP time class, which are harder than P and are identified as time polynomials. Most of the NP and NP-complete problems are believed to be outside the BQP class and intractable on quantum computers because solving them with a quantum computer would require more than a polynomial number of steps. Figure 3 also shows that all the above classes fall within PSPACE, the class of problems that require a polynomial amount of memory (but unlimited time). Most complexity classes usually consist of decision-making problems categorized according to the time or memory requirements. Note that even more complex problems are not contained within PSPACE.

Classes of problems are defined by computational complexity, hardness, quantum speed up and quantum supremacy:

Table 3. Commercially Accessible Quantum Computers

company	year	model	no. of qubits	type of qubits	ref
IBM	2019	Quantum System One	27	Transmon	89
Google	2019	Sycamore	53	Transmon	12
D-Wave	2020	Advantage	5640	SQUIDs	90
IonQ	2020		32	Trapped Ions	91
Honeywell	2020	System H1	10	Trapped Ions	92
Alpine Quantum Technologies	2020	Quantum Simulator (with noise)	10	Trapped Ions	93
SpinQ	2020	Gemini	2	NMR	94
PSI Quantum	under development		1000000	Photonic	95
ColdQuanta	under development	Hilbert	100	Cold Atom	96
Universal Quantum	under development			Trapped Ions	97

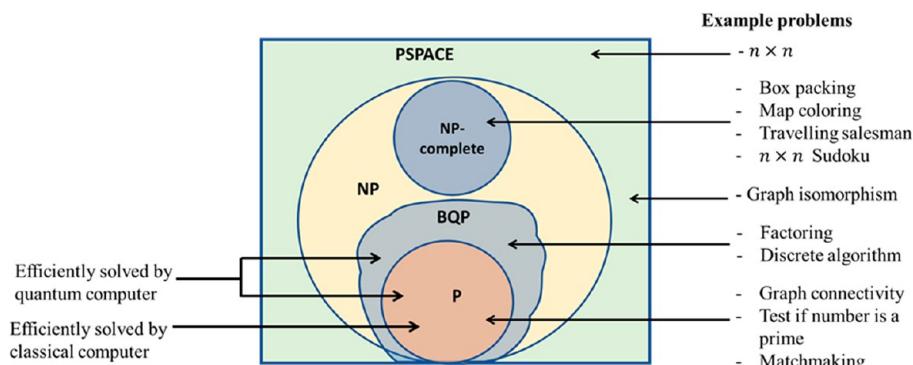


Figure 3. Illustration of the class of problems that can/cannot be solved using classical and quantum computers. BQP problems are classified as harder than P problems and can be solved efficiently by quantum computers. Example problems are also shown on the side.⁹⁸

- (1) *Computational complexity:* A problem's computational complexity is defined in terms of different Turing machines that can simulate all types of problems in PSPACE. The BQP class of problems pose computational complexity for classical computers due to the time polynomial nature of the problems.
- (2) *Hardness:* Can the hardest problems in nature be solved using a Turing machine? An existing notion is that unconventional adaptive analogue computers can give solutions to NP-hard problems, which require exponential resources in time and memory for classical machines to solve.^{100–104} A more detailed description on the hardness of the problem can be found in refs 98 and 105.
- (3) *Quantum speed up:* Quantum speed up can be achieved, by definition, if quantum computation is successful. Dewes et al. described this process using a Grover algorithm with a transmon 2 qubit system.¹⁰⁶ Polynomial speed up has not been achieved because current state-of-the-art quantum computing is limited to only a few high-fidelity qubits. Achieving quantum speed up is currently a strong area of interest.
- (4) *Quantum supremacy:* Quantum supremacy is the demonstration of computations that can be conducted on a quantum computer, but cannot be conducted on existing classical computers with available memory in any reasonable time frame.^{107,108} As previously discussed, Google first demonstrated quantum supremacy in 2019 with a 53 qubit machine that far surpassed Summit, which was the world's fastest supercomputer at that time.

2.2. The DiVincenzo Criteria

In practice, a multitude of physical implementations of quantum computation that utilize different type of qubits, including solid-qubit, spin qubits, trapped ions, time-bin, and photon, can be realized. In 2000, D. DiVincenzo formulated a set of requirements for the physical realization of a quantum computer, which has guided researchers trying to build quantum computers over the past two decades:¹⁰⁹

- a) A scalable and well-characterized qubit system: To realize quantum computation practically, the first step is to identify how the qubit is defined in the chosen system and whether that is scalable so that a larger system is achieved by maintaining the same level of fidelity and efficiency.
- b) Possibility of qubit initialization: Initializing the qubit precisely to one of the well-defined states (register)

should be possible. A precise initialization of the qubit in the register is required also for detection and correction errors caused by decoherence.

- c) Long qubit decoherence time: "Long" decoherence time is defined as time long enough to do gate operations required for performing a quantum computation. This is rather a "strict" requirement on the physical systems implementing quantum computation. A lack of coherence in the qubits introduces quantum errors. In the 1990s, quantum error correction was proposed^{110,111} as a mitigation strategy and applied successfully in quantum computation.¹¹²
- d) Well-defined universal quantum gates: Gates are the core of both classical and quantum computation. Quantum gates are unitary transformations applied on the qubits. For example, based on the Hamiltonian H_i of the system, a unitary operator $U_i = e^{\frac{i}{\hbar} H_i t}$ is used to simulate the dynamics from the time t_1 to t_2 .
- e) Capability to read out stored information: After performing the computation, the specific qubits should be read out with the highest accuracy possible. The measurements are done by probing the system directly or indirectly and are obtained in terms of outcome 0 with probability p and 1 with probability $1 - p$.
- f) Possibility of qubit interconversion: The qubit should be able to interconvert between a stationary qubit, such as for memory purposes, and a flying qubit, such as for on-chip communication between quantum registers.
- g) Quantum interfaces for quantum entanglement and information processing: There should be quantum interfaces that allow for quantum entanglement and long-distance communication of quantum information.

2.3. Qubit Representation in a Quantum Computer

- 2.3.1. **Basic Concept of the Qubit.** The quantum bit, or "qubit", is the heart of quantum computation. A qubit can be represented by a quantum two-level system. Although analogous to a classical bit taking a value of 0 or 1, a qubit could exist in more complex states as explained here. The initial state thus prepared is manipulated using quantum logic gates, and the final state is read out. The state of a classical bit is either deterministic (0 or 1) or stochastic, where non-negative real numbers α and β represent the probabilities of 0 and 1 and $\alpha + \beta = 1$. Unlike a classical bit, a qubit could exist in a *superposition* of 0 and 1. This means that the qubit will take the value of 0 or 1 only at the time of measurement. The

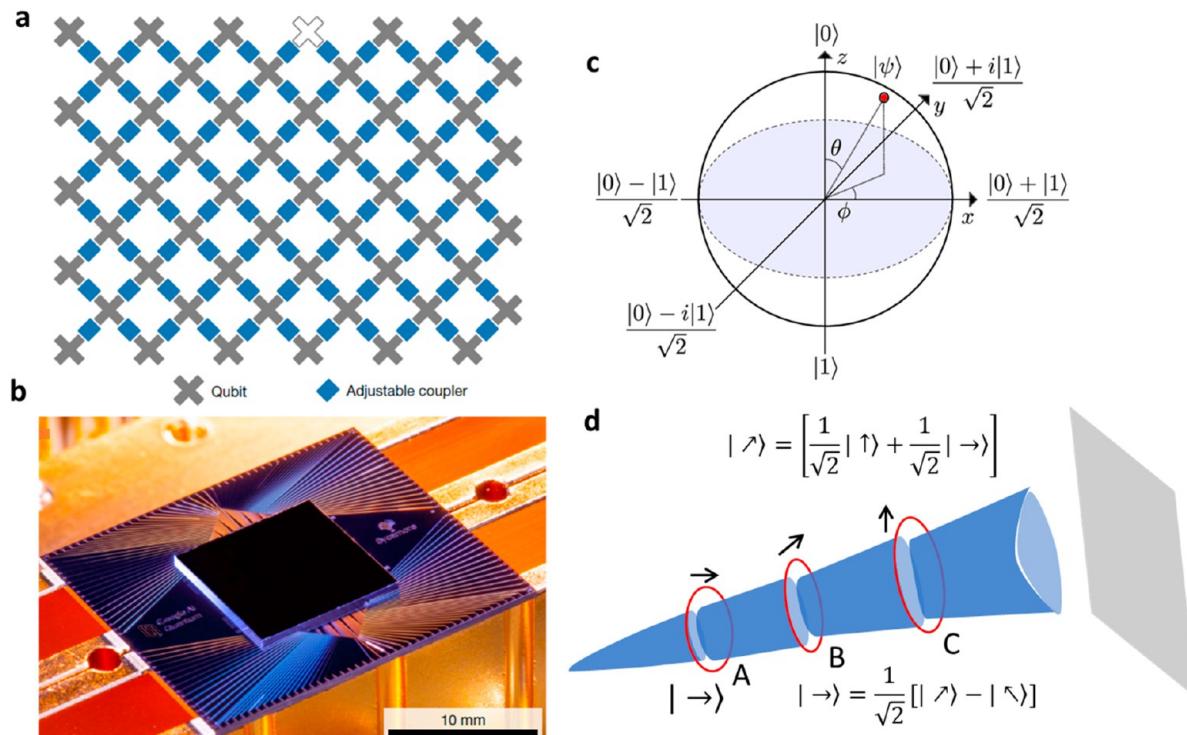


Figure 4. Layout of Google’s 53 qubits (gray) operational Sycamore processor (a). Each qubit is connected to the four nearest neighbor couplers (blue rectangles). A nonfunctional qubit is also shown. The actual Sycamore chip (b).¹² The definition of qubits as represented in a Bloch sphere where $|0\rangle$ and $|1\rangle$ represent the reference axes (c). A schematic of a simple experiment showing pure quantum mechanical effects, where polaroid B with 45° polarization is inserted between two polaroids A and C, respectively, with 0° (horizontal) and 90° (vertical) polarization of the resulting photon intensity on the screen (d). Reprinted with permission from ref 12. Copyright 2019 Springer Nature.

superposition is represented as $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, where the amplitudes α and β are complex numbers, and their mod square gives the respective probability that a measurement yields either 0 or 1. Therefore, $|\alpha|^2 + |\beta|^2 = 1$ because only two states are possible upon measurement. A significant difference compared to classical probabilities is that the amplitudes represented by complex numbers could cancel out, a phenomenon known as *quantum interference*. The notation $|\psi\rangle$, called a ket vector, represents the 2D vector $\begin{bmatrix} \alpha \\ \beta \end{bmatrix}$.

The state of a multiqubit quantum system can, in some cases, be described in terms of its component qubits, specifically, as the tensor product of the component qubits. However, in other cases, that is not possible because the qubits are said to be *entangled*, which is a purely quantum mechanical phenomena. To elucidate, consider an entangled 2 qubit state $|\phi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$. This state cannot be decomposed because it is impossible to find a_1 , a_2 , b_1 , and b_2 such that $(a_1|0\rangle + b_1|1\rangle) \otimes (a_2|0\rangle + b_2|1\rangle) = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ where \otimes indicates a tensor product. Therefore, the 2 qubit state is considered to be entangled. To achieve computational advantages using quantum computation, the concept of entanglement must be exploited, which results in a dramatic reduction in the mathematical complexity that exists in the classical representation of a quantum system. Entanglement is a basic quantum mechanical phenomenon observed when the quantum state of a particle in a pair or group of interacting particles at spatial proximity cannot be described independently from the quantum state of other particles, even when they are separated by a large distance. Feynman first realized

that it would be impossible to simulate the behavior of entangled states of even modest sizes in a classical computer, leading to his proposal for the development of the field of quantum computing.¹⁹ The quantum systems like electrons and photons can exist in the superposition of their possible observable states before a measurement is performed. In tracking the probability of particles in different superposition states, a classical computer would quickly run out of memory as the number of quantum particles exceed, say, 60.

Figure 4a,b shows Google’s Sycamore two-dimensional layout with 53 qubits and an actual Sycamore chip. The concept of qubits and the functioning of such chips is clearer if we visualize them in a three-dimensional Bloch sphere, as shown in Figure 4c.¹ A vector (qubit) pointing in any arbitrary direction in the Bloch sphere can be simply written as a linear combination of 0 and 1, each with a complex coefficient: $|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle$. As an example, a vector with an angle of $\theta = \frac{\pi}{2}$, $\phi = \frac{\pi}{2}$ represents a qubit $|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle)$. Qubits can be represented using different physical properties such as polarization, magnetic domain, trapped ions, atomic ensembles and optical modes. Figure 4d represents a simple experiment that shows a qubit representation by a photon’s polarization. The polaroids A and C are horizontally ($|\rightarrow\rangle$) and vertically ($|\uparrow\rangle$) polarized, which means that the polarization states of photons that pass through A and C are $|\rightarrow\rangle$ and $|\uparrow\rangle$, respectively. If only polaroid filters A and C are present, no light reaches the screen. Polaroid A puts the photons in the $|\rightarrow\rangle$ state, and when they reach polaroid C, they are blocked because they do not have a component in the (orthogonal) $|\uparrow\rangle$ direction of C.

Surprisingly, when we insert a polaroid B with a polarization angle of 45° ($|/\!\rangle$) between A and C, light reaches the screen. The explanation is as follows. The state of a photon passing through A, $| \rightarrow \rangle = \frac{1}{\sqrt{2}}[|/\!\rangle - | \nwarrow \rangle]$, is a superposition of $|/\!\rangle$ and $| \nwarrow \rangle$ states. When passing through polaroid B ($|/\!\rangle$ measurement), 50% of the photons pass through and they will be in the $|/\!\rangle$ state, which in turn is a superposition of horizontal and vertical polarization states: $|/\!\rangle = \frac{1}{\sqrt{2}}[|/\!\rangle + | \rightarrow \rangle]$. Therefore, 50% of the photons pass through polaroid C ($|/\!\rangle$ measurement) and reach the screen. The space of possible polarization states of a photon in the above example represents a *qubit*. A classical bit, even if stochastic, cannot mimic this behavior.

2.3.2. Qubit Decoherence. One of the fundamental challenges in building quantum computers is maintaining the coherence of qubits. Coherence is a qubit's ability to maintain its state of superposition. If a quantum system were perfectly isolated from the environment, it would maintain coherence indefinitely. But perfect isolation is impossible; radiation, light, sound, vibrations, heat, and magnetic fields interact with qubits, and they lose information or decohere over a period, called coherence time. The noise introduced in the computations through decoherence must be mitigated with quantum error correction or with the help of algorithms that are error-tolerant, such as variational quantum eigensolver, first introduced in ref 113. Here, we briefly discuss the concept of qubit decoherence in superconductivity.

High-fidelity computation requires a balance in quantum coherence, connectivity, and proper control of the qubits. Superconductivity is a promising technology for developing a quantum computer with a relatively high fidelity.¹⁰⁵ Superconductivity also allows for scalability: electrons can remain in a microscopic quantum state, allowing a large number of integrated circuits to be built with individual control lines.¹¹⁵ Superconducting qubits are easily disturbed by material defects, phonon excitations, and radiative coupling to external wiring.^{116–118} These factors limit the quantum coherence time, as denoted by T , which is the amount of time qubits remain in the superposition state. The coherence of qubits can be lost either by energy relaxation or by dephasing. The time of energy relaxation is denoted by T_1 , whereas the time of dephasing is denoted by T_2 , as shown in Figure 5.¹¹⁴ In general, the coherence time of a qubit is calculated as $\frac{1}{T} = \frac{1}{T_1} + \frac{1}{T_2}$. The longer the coherence time the greater the ability of the qubits to do computations. T for superconducting qubits has been determined to be on the order of tens of microseconds.^{115,119,120} Figure 6a,b shows qubit energy decay and spin-echo relaxation measured by phase tomography.¹¹⁵ Figure 6c–f presents qubit relaxations due to quasiparticle excitation in superconductors.¹²⁰ Qubit populations are seen to decay non-exponentially in several tens of microseconds.

2.4. Physical Implementations of Qubits in Quantum Computation

In the last three decades, researchers have devised many physical implementations for qubits that satisfy the DiVincenzo criteria.¹⁰⁹ NMR and ion traps are two of the earliest implementations of qubits.^{33–36} In addition to its use in quantum simulation as discussed before, NMR can be used in universal quantum computers, as well, using the spin of atomic nuclei to implement the state of a qubit. The quantum

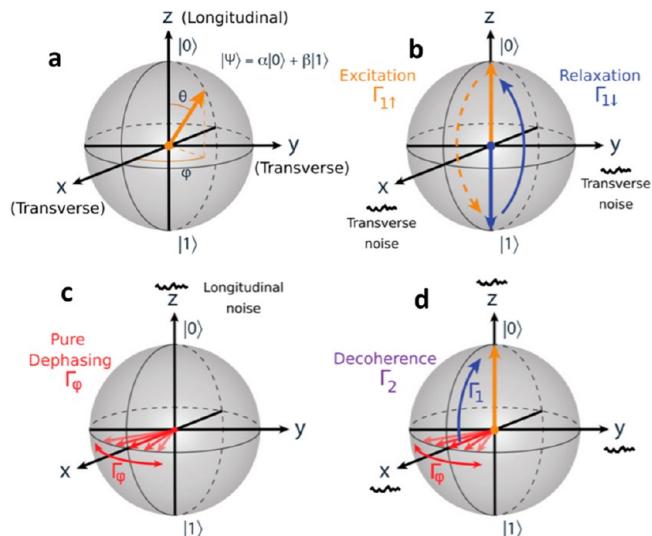


Figure 5. Bloch sphere (a) with a qubit state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$. Longitudinal relaxation rate Γ_1 (b), pure dephasing rate Γ_2 (c), and transverse relaxation rate Γ_2 (d) in the Bloch sphere. The states $|1\rangle$ and $|0\rangle$ correspond to the qubit's excited state $|e\rangle$ and the ground state $|g\rangle$, respectively. Γ_1 is the rate for energy relaxation from or the loss of polarization of the qubits. Up and down arrows represent qubit excitation and de-excitation. Γ_2 is the rate of dephasing in the transverse plane due to the adiabatic perturbation, which does not result in qubit excitation but randomizes the phase, introducing computing errors. $\Gamma_2 = \frac{\Gamma_1}{2} + \Gamma_\varphi$ is the rate due to combination of energy relaxation and pure dephasing. Reprinted with permission from ref 114. Copyright 2019 American Institute of Physics.

computing industry has not currently settled on any preferred physical implementation. As listed in Tables 2 and 3, currently, the leading contenders of physical implementations (and examples of companies developing that technology) are as follows: superconducting qubits (IBM, Google, Rigetti); trapped ion (IonQ, Honeywell); quantum photonics (Xanadu, PsiQuantum); Majorana (topological) qubit (Microsoft); and silicon spin qubit (Intel). Here, we discuss superconducting qubits systems used for physical realizations of quantum computation.

2.4.1. Superconducting Qubits. Superconducting qubits are collective excitations in a circuit made of superconductors. Currently, superconducting qubits are leading systems for realizing the logic elements in quantum computers due to their coherent interactions with high controllability and scalability. They suffer from a relatively low level of noise compared with other qubit systems. Although trapped ions are less noisy, they are less scalable. In superconducting circuits, qubits are realized in various forms; transmon is one such variant that reduces sensitivity to charge noise. Designed in 2007, transmon refers to transmission line shunted plasma oscillating qubits. Other variants include phase qubit,¹²¹ rf-SQUID,¹²² three Josephson junction-flux (JJ-flux) qubit,¹²³ fluxonium qubit,¹²⁴ c-shunt flux qubit,¹²⁵ charge qubit,¹²⁶ quantronium,¹²⁷ Xmon,¹¹⁵ Gate-mon,¹²⁸ and Majorana qubit.^{129,130} A detailed review on the variants of qubit and their design are presented in ref 131.

Figure 7a shows an energy spectrum of a quantum harmonic oscillator with equal energy spacing by $\hbar\omega_c$. The resonant LC circuit has the frequency $\omega_c = \frac{1}{\sqrt{LC}}$. An excellent review of the available design and engineering of such superconducting circuits is given in ref 114.

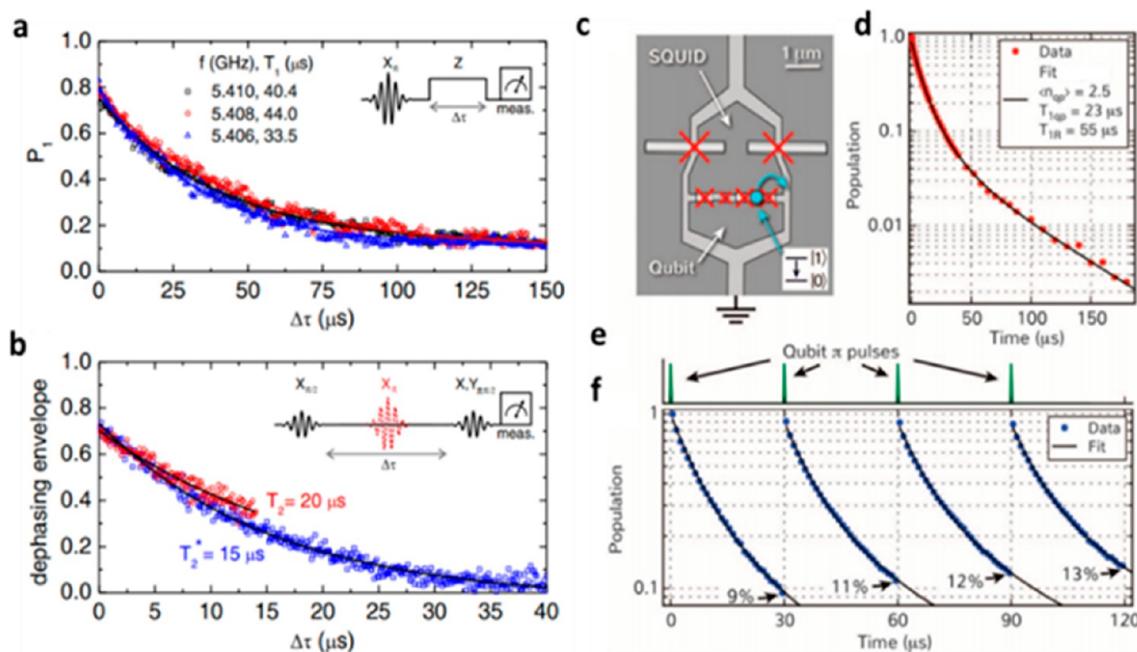


Figure 6. Energy decay of qubits at three nearby frequencies (a). The qubit frequency is adjusted by applying a rectangular pulse with length $\Delta\tau$. Ramsey T_2^* and spin–echo T_2 dephasing envelopes measured by phase tomography. Spin–echo measurements are limited by electronics to 14 μs (b). Reprinted with permission from ref 115. Copyright 2013 American Physical Society. A device consisting of a flux qubit (lower loop) coupled to a dc superconducting quantum interference device (SQUID) for qubit readout (outer loop) (c). Red crosses are the Josephson junctions. Qubit decay as measured by applying a π -pulse (a pulse that flips the qubit state) (d). The data were fitted to the theoretical qubit decay population $p(t) = e^{\langle n_{qp} \rangle (\exp[-t/T_{lqp}] - 1)} e^{-t/T_{IR}}$, where $\langle n_{qp} \rangle$ is the average number of quasiparticles (unpaired electrons), t is the time after qubit excitation, T_{lqp} is the relaxation time induced by a single quasiparticle, and T_{IR} is the residual relaxation time. With the application of qubit π -pulses (e), the non-exponential population decay are fitted with the data points (f). Reprinted with permission from ref 120. Copyright 2016 American Association for the Advancement of Science.

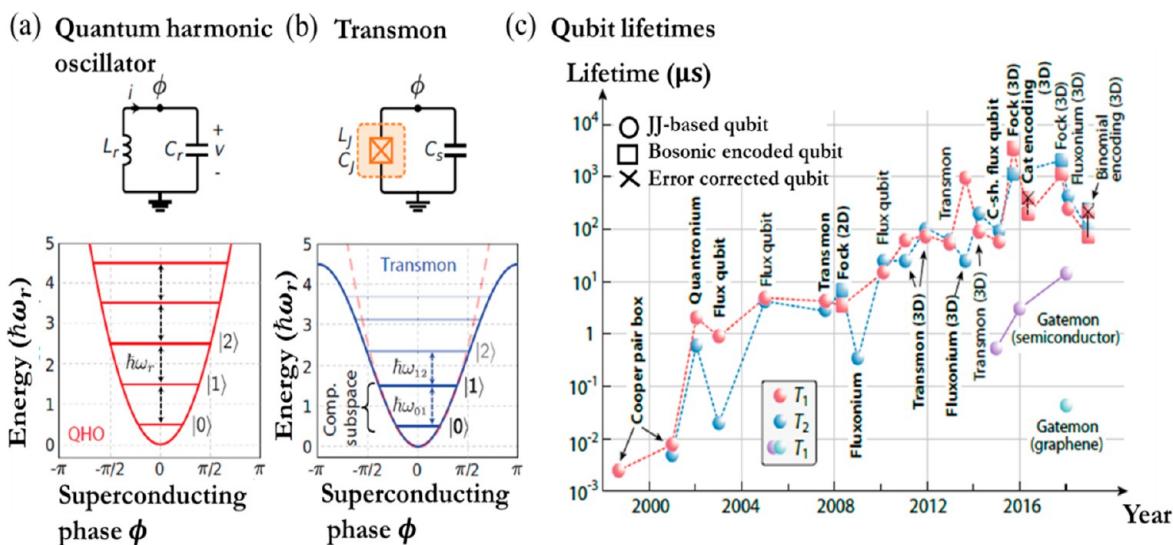


Figure 7. (a) Energy spectrum of a quantum harmonic oscillator with equal energy spacing of $\hbar\omega_c$ between two levels for LC (inductor–capacitor) circuit. (b) Energy spectrum for transmon with an unequal energy spacing of $\hbar\omega_{i,i+1}$, obtained after the quantum harmonic oscillator is placed in the nonlinear Josephson junction (b). Reprinted with permission from ref 114. Copyright 2019 American Institute of Physics. (c) Timeline of coherence times for variants of superconducting qubits (circles) including bosonic encoded qubits (rectangles). Reprinted with permission from ref 132. Copyright 2020 Annual Review Inc.

The energy spectrum of such oscillators in the presence of a nonlinear Josephson junction is a spectrum with unequal energy spacing $\hbar\omega_{i,i+1}$, as shown in Figure 7b. This represents the energy spectrum of transmon qubits. Figure 7c shows the evolution of coherence times from the 1990s to present. Note

that the qubit coherence time has significantly increased in recent years. JJ-based qubits carry information in excited states in superconducting circuits containing Josephson junctions. Bosonic encoded qubits carry information in superpositions of multiphoton states in a quantum harmonic oscillator, and a

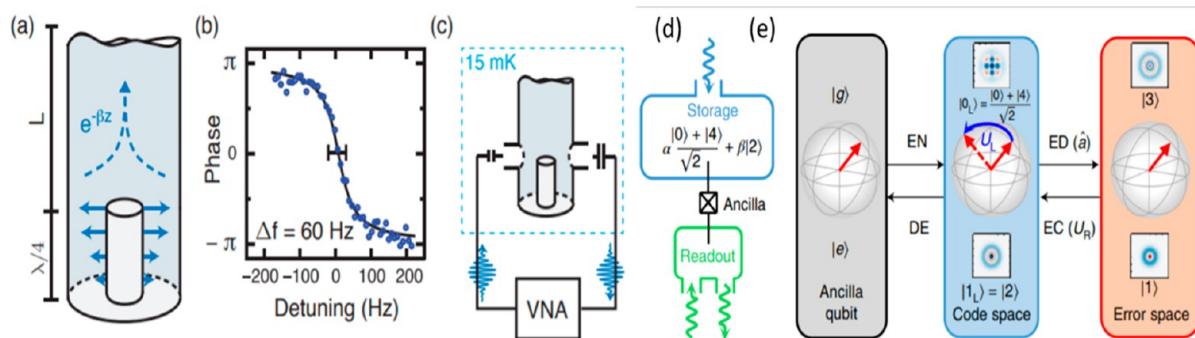


Figure 8. High Q -factor coaxial microwave cavity (a). The inner and outer conductors are formed with a piece of aluminum. A quality factor of $Q = 7 \times 10^7$ is recorded in a transmission line at single-photon excitation levels corresponding to a 60 GHz line width (b). A vector network analyzer at 15 mK for sample characterization (c). (a–c) Reprinted with permission from ref 139. Copyright 2016 American Physical Society. The experimental schematic for bosonic logical qubits (d,e), consisting of a quantum harmonic oscillator as an information storage cavity, ancilla transmon qubits for operation, and a readout cavity for measurement (d). Single logical qubit operation for information to encode and decode from the code space of the oscillator. A photon loss changes the even parity of code space to the odd parity of error space. A high-fidelity and parity measurement can detect the parity change, leaving encoded quantum information undisturbed. (d,e) Reprinted with permission from ref 134. Copyright 2019 Springer Nature.

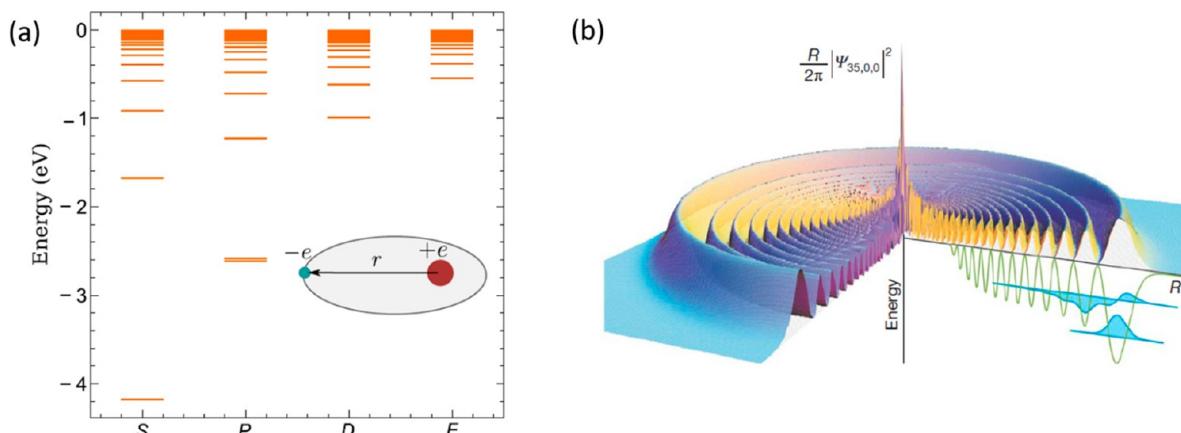


Figure 9. Electronic levels and the probability density of a ^{87}Rb atom. (a) Electron probability density and molecular potential for the $3S$ molecular state of rubidium dimer molecule. Reprinted with permission from ref 143. Copyright 2021 Chinese Physical Society. (b) Surface plot shows the spherically symmetric density distribution of the Rydberg electron in the $R-\Phi$ plane, $(R/2\pi)|\Psi_{35,0,0}(R)|^2$. The molecular potential for the state ${}^3\Sigma(\text{Ss} - 3\text{Ss})$ (green) is modeled for a polarizability $\alpha = 319$ au and a scattering length $a_{\text{rb}} = -18.5a_0$. The potential supports two vibrational bound states (wave functions given in blue) in the outermost potential wells at $R = 1900a_0$ with binding energies (in frequency units) of $E_B(v=0) = -23.4$ MHz and $E_B(v=1) = -10.6$ MHz. Reprinted with permission from ref 144. Copyright 2019 Springer Nature.

superconducting circuit mediates qubit operation, including the process of quantum information readout. A layer of active error correction is implemented to increase qubit lifetime. Qubits carrying error corrected information are called error corrected qubits. The T_1 and T_2 times shown are for the non-error corrected version of logical qubits.^{133,134} When a qubit, which behaves as a two-level artificial atom, is coupled to a single-mode harmonic oscillator, the Hamiltonian can be written as

$$H = H_q + H_{qr} + H_r \quad (1)$$

where $H_q = -\frac{1}{2}e\sigma_z$, $H_{qr} = g\sigma_x(a + a^\dagger)$, and $H_r = \hbar\omega(a^\dagger a + 1)$ are the qubit, qubit oscillator coupling, and oscillator energies, respectively. The Hamiltonian given by eq 1 is completely general and describes most of the qubit circuit models. H_{qr} can also be written in Jaynes–Cummings terms as

$$H_{qr} = g(\sigma^+a + \sigma^-a^\dagger) + g(\sigma^+a^\dagger + \sigma^-a) \quad (2)$$

Expressions 1 and 2 can be used to engineer the qubits in superconducting circuits for gate-based quantum computations.

2.4.2. Current State-of-the-Art Qubit Modalities.

Currently, transmons are the most widely used qubits in gate-operated quantum computation. In 2014, a controlled qubit–qubit interaction was realized in a multiqubit system with a fidelity of 0.99 using transmons.⁵⁹ The ability of superconducting circuits to enable quantum devices capable of performing computations with high fidelity in a multiqubit environment was demonstrated.¹³⁵ In addition, these systems are well-suited for the NISQ systems that are envisioned for use in the near future.^{136,137}

In quantum annealing architectures, rf-SQUID flux qubits are widely used; the commercial platform D-Wave computing is one example.¹³⁸ Due to the tunable structure of Hamiltonian and persistent current, these qubits are used for Hamiltonian emulation and in gate-based computing. Rf-SQUID flux qubits

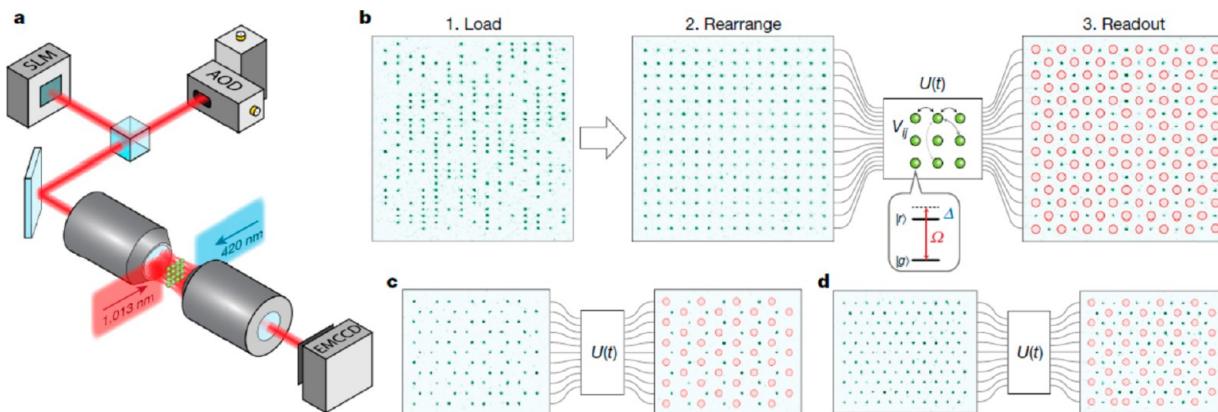


Figure 10. Programmable 2D arrays of strongly interacting Rydberg atoms. (a) Atoms are loaded into a 2D array of optical tweezer traps and rearranged into defect-free patterns by a second set of moving tweezers. Lasers at 420 and 1013 nm drive a coherent two-photon transition in each atom between ground state $|g\rangle$ and Rydberg state $|r\rangle$. (b) Fluorescence image of the initial random loading of atoms, followed by rearrangement to a defect-free 15×15 (225 atoms) square array. After this initialization, the atoms evolve coherently under laser excitation according to the Hamiltonian with Rabi frequency $\Omega(t)$, detuning $\Delta(t)$, and long-range interactions V_{ij} , realizing a many-body unitary $U(t)$. Finally, the state of each atom is read out, with atoms excited to $|r\rangle|l\rangle$ detected as loss and marked with red circles. Shown on the far right is an example measurement following quasi-adiabatic evolution into the checkerboard phase. (c,d) Similar evolution on honeycomb and triangular lattices result in analogous ordered phases of Rydberg excitations with filling 1/2 and 1/3, respectively. Reprinted with permission from ref 151. Copyright 2021 Springer Nature.

show high reproducibility, long coherence times, and a moderate level of anharmonicity.

Bosonic encoded qubits encode information in the infinite dimensional Hilbert space of a quantum harmonic oscillator.¹³⁴ Figure 8 shows the implementation of bosonic qubits in a high-quality factor microwave cavity.¹³⁹ Such qubits use superposition of multiphotonic states whose modes are described by bosonic statistics. The circuit model consists of a quantum harmonic oscillator that encodes information, which is coupled to a transmon that assists in control and the readout process. Harmonic oscillator space is used to encode information and is coupled to ancilla transmon qubits, as shown in Figure 8d,e. Qubit operations are performed in the code space, and error corrections are made in the error space by detecting parity change due to photon loss. In this implementation, controlling the individual energy level is not possible. As a result, qubit manipulation is a challenging task. Nevertheless, microwave irradiation can be used for universal manipulation and control of coupling with the transmons. A quantum harmonic oscillator is realized in a lithographically engineered transmission line on a 2D chip or a 3D microcavity. This implementation can take advantage of the long lifetimes of microcavities enabling hardware with efficient error correction architectures.

2.4.3. Rydberg Atoms. Neutral Rydberg atoms and molecules are an exciting platform for strong light–matter interactions, fundamental quantum chemistry research, and such exotic applications as anti-hydrogen trapping.^{140–142} Rydberg atoms in a high excited state of $n > 50$ are promising candidates for scalable implementation of quantum computing.

Atomic transition wavelength for an atomic system is given by the general formula

$$\frac{1}{\lambda} = R_h \left(\frac{1}{n^2} - \frac{1}{m^2} \right) \quad (3)$$

where R_h is Rydberg constant and n and m are integers (Figure 9 a). Large n number leads to dramatically enhanced properties compared to regular atoms. In particular, the size of the atom due to the delocalized nature of the Rydberg electron scales as

$\sim n^2$, atomic polarizability as $\sim n^7$, and coherence time $\sim n^3$ (Figure 9b). Because of their exaggerated sizes, Rydberg atoms experience large van der Waals or dipole–dipole interactions required for scalable many-qubit quantum systems. The qubits in Rydberg atom implementation are normally formed in hyperfine ground state manifolds.

From an experimental point of view, the loading of multiple atoms is an inherently nondeterministic process; however, it can be optimized by sequential sorting of the atoms in optical tweezer setups.¹⁴⁵ The readout can be realized in both high-fidelity destructive measurements where atoms are lost¹⁴⁶ and selective fluorescent measurements using a gradient of magnetic fields.¹⁴⁷ One qubit gate can also be performed using a gradient of magnetic fields or, alternatively, Stark shifts using focused laser beams.¹⁴⁸ Two qubit operations are implemented using Rydberg blockade¹⁴⁹ along with π and 2π sequences on control and target qubits.¹⁵⁰

Rydberg atoms are currently on the forefront of the race for a viable universal quantum computer along with superconducting qubits and trapped ions. Recently, a record number of qubits for a physical system ($N = 256$) was implemented using Rydberg atoms on 2D lattice (Figure 10), which may pave the way for simulation of 2D quantum phenomena as well as scalable quantum computing systems.¹⁵¹

2.5. Quantum Annealing

An initial approach for universal quantum computation was based upon the adiabatic evolution of the time-dependent Hamiltonian in the ground state.^{152,153} Adiabatic quantum evolution of the given Hamiltonian toward the global minimum of the potential energy landscape is translated to a problem that must be solved. In the quantum annealing approach, transitions between two states of the Hamiltonian are caused by quantum fluctuations rather than thermal fluctuations. This leads to an efficient convergence of some ground state problems.^{154–156}

Quantum annealing computation has been designed mainly to solve combinatorial optimization problems.^{154,157} These problems can be from a number of different domains including

computer science,¹⁵⁸ quantum chemistry,¹⁵⁹ machine learning,¹⁶⁰ protein folding,¹⁶¹ and search engine ranking.¹⁶²

Optimization problems require the minimization of a cost function. Such problems can be represented by a classical Ising Hamiltonian, in which the problems are reduced to finding the ground state of the Ising Hamiltonian. The cost functions corresponding to the Ising Hamiltonian have a number of local minima reminiscent of spin glasses eigenvalues.¹⁶³ Finding the global minimum is a formidable task for classical algorithms. Quantum annealing is thought to be an alternative solver for such problems, translating classical Ising Hamiltonians to a collection of interacting qubits. It is expected that many important optimization problems in science can be formulated as Ising models.^{161,164–f66}

Canada-based D-Wave Systems is one of the early players in implementing the quantum annealing approach for quantum computation. D-Wave Systems manufactured a device with more than 2000 superconducting flux qubits. At the device core are unit cells consisting of intercoupled frequency-tuned qubits. Each qubit is longitudinally coupled to four neighboring qubits that define a pattern called Chimera graph,¹⁶⁷ as shown in Figure 11. For efficient computation, the

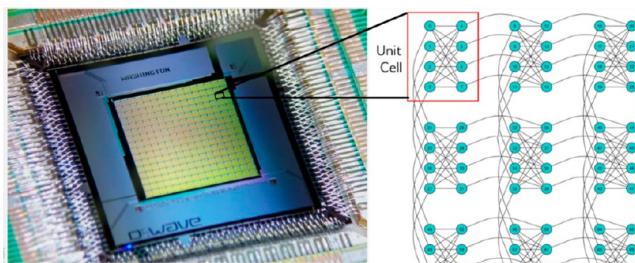


Figure 11. D-Wave 2000Q Washington chip (left) consisting of 2048 qubits patterned in a Chimera graph.¹⁶⁹

study of any logical optimization problem is required to match the connectivity graph currently available in the quantum annealers. Implementation in the Chimera graph structure of the D-Wave chip requires embedding the physical problem in one of the available graph structures.¹⁶⁸ Currently, the available structures are limited and embedding in this way requires significant overhead. Approximately 30 logical spin variables in a fully connected graph requires 2000 variables to embed in a D-Wave 200Q annealer. This severely limits the analysis of the asymptotic scaling behavior.¹⁶⁷

In a recent experiment,¹⁶⁷ quantum annealing was applied to simulate a spin glass problem from condensed matter physics. Interacting spins were considered in a cubic lattice with dimensions of $8 \times 8 \times 8$ and were simulated on a D-Wave processor to map the magnetic phase transition of the spin glass. Frustrated Ising model¹⁷⁰ and prime factorization¹⁷¹ problems were also studied using quantum annealing. Using D-Wave, prime factorization of up to a seven-digit number was achieved in an 89 qubit D-Wave machine.

2.5.1. Adiabatic Quantum Optimization. Quantum annealing aims to solve combinatorial problems using adiabatic quantum optimization (AQO) to gain decisive speed up over classical machines. AQO is performed at near-zero temperatures where thermal fluctuations are insignificant. In this approach, we consider a time evolution of $|\psi(t)\rangle = \hat{U}(t,0)|\psi(0)\rangle$ as an eigenfunction of the Hamiltonian:¹⁰⁵

$$\hat{H}(t) = [1 - s(t)]\hat{H}_0 + s(t)\hat{H}_T \quad (4)$$

where $s(t)$ is a scalar function with time between 0 and 1 and controls the switch on and off. \hat{H}_0 is a Hamiltonian at time $t = 0$, and \hat{H}_T is a target Hamiltonian. \hat{H}_T is often defined as an Ising-type Hamiltonian and encodes the problem under consideration. Now, the task is to search for the global minimum, if possible, that represents the final state function $|\psi(t_f)\rangle$, which is an eigenfunction of the Hamiltonian \hat{H}_T .

2.6. Noisy Intermediate-Scale Quantum Computers

The so-called noisy intermediate scale quantum (NISQ) computers can provide near- to intermediate-term quantum computing opportunities.⁶⁴ Here, “noisy” refers to the fact that the qubits are not error-corrected. Noise will pose a serious limitation on what quantum computers can deliver in the near future. The size of such quantum computers will be of “intermediate scale”, meaning they will range in size from 50 to 100 qubits.¹⁰⁷ An excellent review on NISQ requirements and challenges is given by John Preskill.¹⁷²

In several studies, superconducting qubits are engineered and manipulated to achieve a scalable architecture that functions in a multiqubit environment. Architectures based on multiqubit systems on the order of 10–20 qubits have been demonstrated,^{173–177} and more recently, larger systems up to 53 qubits have been developed.¹² Such multiqubit architectures still suffer a significant level of quantum errors as the number of qubits grows. Nevertheless, such architectures are suitable for the NISQ approach that aims to perform quantum algorithms and quantum simulations before the advent of fault-tolerant quantum computation. Recently, a Google team¹² developed a NISQ capable of achieving quantum supremacy,¹⁷⁸ which was an immediate goal in quantum computing.

Error correction in quantum computation is a major hurdle. Several studies have been performed for error correction in multiqubit systems based on NMR^{179,180} and superconducting circuits.^{181,182} Developing a qubit system that is robust against inherent environmental errors is a challenging task. Figure 12a,b shows a scheme in which a quantum nondemolition (QND) parity measurement technique is implemented using a repetition code and a 1D variant of the surface code.¹⁷⁴ Errors can be tracked repeatedly by performing projective QND parity measurements, as shown in Figure 12c,d. In this scheme, qubits are arranged in a checkerboard pattern with blue and green square patterns corresponding to data and measurement qubits, respectively. Ancilla qubits are used to perform the parity measurements to detect bit- and phase-flip errors. The interaction graph of the Ising model corresponding to the 6×6 , 7×6 , and 7×7 qubits circuit as a function of the circuit depth is shown in Figure 12e.

2.7. Quantum Logic Gates and Operations

While performing quantum information processing, classical data are mapped to the Hilbert space of the quantum circuit. We write the appropriate Hamiltonian whose eigenfunctions can be written as superpositions of states in that Hilbert space and let the problem evolve with time before performing readout measurements of the quantum registers. The time-dependent Hamiltonian of the many-body system consists of terms for the intrinsic system plus the control pulse; $H(t) = H_{\text{syst}} + H_{\text{ctrl}}(t)$. The first part is time-independent, and the second part is time-dependent describing the microwave photon interaction with the transmon. In general, for the transmon system, H_{syst} and $H_{\text{ctrl}}(t)$ are written as¹⁰⁵

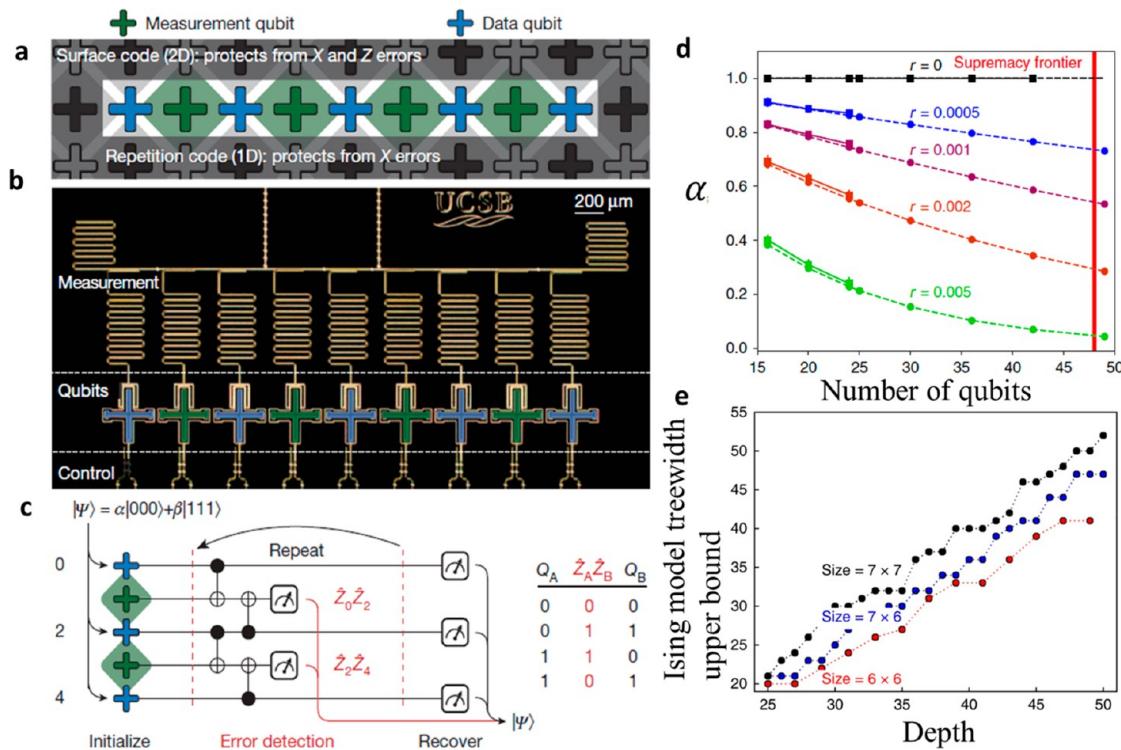


Figure 12. Schematic for the protection of states from environmental bit-flip errors and suppression of these errors with increasing system size using a repetition code, a 1D variant of surface code (a). Optical micrograph of the nine Xmon transmon qubits with individually addressed control unit (b). Tracking of errors as they occur by repeatedly performing projective QND parity measurements (c). Reprinted with permission from ref 174. Copyright 2018 Springer Nature. The fidelity α of complex multiqubit dynamics as a function of the number of qubits. Different colors correspond to different Pauli error rates, r (d).¹⁰⁷ This study predicts that quantum supremacy can be achieved with circuits in a 2D lattice of 7×7 qubits and around 40 clock cycle. The interaction graph of the Ising model that corresponds to circuits with 6×6 , 7×6 , and 7×7 qubits as a function of the circuit depth (e). Reprinted with permission from ref 107. Copyright 2018 Springer Nature.

$$H_{\text{syst}} = -\frac{1}{2} \sum_i \epsilon_i \sigma_{zi} + \sum_i g_i (\sigma_i^+ a + \sigma_i^- a^\dagger) + \hbar \omega a^\dagger a + \frac{1}{2} \sum_{i,j;v} \lambda_{v,ij} (\sigma_i^+ \sigma_j^- + \sigma_i^- \sigma_j^+) \quad (5)$$

and

$$H_{\text{ctrl}}(t) = \sum_{iv} f_{vi}(t) \sigma_{vi} + \frac{1}{2} \sum_{i,j;v} h_{v,ij}(t) \sigma_{vi} \sigma_{vj} + k(t) a^\dagger a \quad (6)$$

where f_{vi} , $h_{v,ij}$, and $k(t)$ are the control parameters. $H_{\text{ctrl}}(t)$ can be turned on or off. The important features of the control Hamiltonian (5) are that it describes the single qubit gate (first term) and the qubit–qubit coupling explicitly in the presence of a driving field (second term). In addition, it also allows for tuning the oscillator frequency (third term). The time evolution of each qubit is obtained by applying a unitary operator with time dynamics controlled by $H(t)$, which is written as $U(t) = e^{-\frac{i}{\hbar}H(t)}$.

Qubits are first initialized to a certain state, for example, all spin up corresponding to zero in the Bloch sphere. A microwave pulse is illuminated on the individual qubit to rotate its phase and bring it into any state in the Bloch sphere, as shown in Figure 13. The state position depends on the pulse's amplitude and duration. As an example, a $\pi/2$ -pulse creates a superposition state with a unit that normally lies in the equatorial plane. The frequency of this pulse is $\omega = \pi/2t$, and it is usually in the range of a few GHz for superconducting

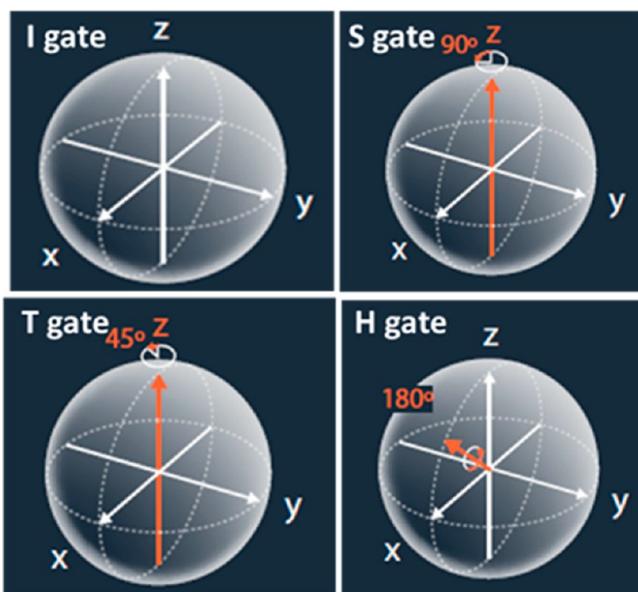


Figure 13. Rotation of Bloch vectors for single-qubit I, S, T, and H quantum logic gates in the Bloch sphere. Reprinted with permission from ref 114. Copyright 2019 American Institute of Physics.

qubits. Computationally, qubit rotation is performed using quantum logic gates.

Table 4 shows the different quantum logic gates, their circuit and matrix representations, and truth table obtained by

Table 4. Quantum Logic Gates and Operations

Gates and rotations in Bloch sphere	Circuit representation	Matrix representation	Truth table	
<i>I</i> gate: no rotation is performed.		$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	Input	Output
<i>X</i> gate: rotates the qubit state by π about the x-axis.		$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	0>	1>
<i>Y</i> gate: rotates the qubit state by π about the y-axis.		$Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$	0>	$i 1\rangle$
<i>Z</i> gate: rotates the qubit state by π about the z-axis.		$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	0>	0>
<i>S</i> gate: rotates the qubit state by $\pi/2$ about the z-axis.		$S = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/2} \end{pmatrix}$	0>	0>
<i>T</i> gate: rotates the qubit state by $\pi/4$ about the z-axis.		$T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$	0>	0>
<i>H</i> gate: rotates the qubit state by π about an axis diagonal in the x-z plane. This is equivalent to an X-gate followed by a $\frac{\pi}{2}$ rotation about the y-axis.		$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$	0>	$\frac{ 0\rangle + 1\rangle}{\sqrt{2}}$
<i>CNOT</i> gate: applies an X-gate to the target qubit if the control qubit is in state $ 1\rangle$.		$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	00>	00>
			01>	01>
			10>	11>
			11>	10>
<i>CPHASE</i> gate: apply a Z-gate to the target qubit if the control qubit is in state $ 1\rangle$.		$CPHASE = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$	00>	00>
			01>	01>
			10>	10>
			11>	$- 11\rangle$

applying each of these gates. A single-qubit operation is understood as moving an arbitrary quantum state from one point in the Bloch sphere to another point by rotating the Bloch vector around a particular axis. Examples of single-qubit quantum logic gates are identity (*I*), Pauli-X, -Y, and -Z, phase (*S*), and Hadamard (*H*) (see Table 4), whose operations in the computational basis are represented by the eigenvectors of the Pauli *z*matrix, σ_z . As an example, an *I* gate brings no rotation on the single-qubit state, while an *S* gate brings a $\frac{\pi}{2}$

rotation about the *z*-axis, as shown in Figure 13. Similarly, *T* and *H* gates each bring a rotation of the single-qubit state by $\frac{\pi}{4}$ and π rotation about an axis diagonal in the *x*-*z* plane. Two qubit gates are usually conditional gates, consisting of control and target qubits. Depending upon the state of the control qubit, a unitary operation is performed on the target qubit. As an example, a *CNOT* gate applies an *X* gate and flips the state of the target qubit if the control qubit is in $|1\rangle$. Similarly, a control phase (*CPHASE*) gate applies a *Z* gate with a

Table 5. Summary of Popular Quantum Algorithms with Brief Descriptions on Their Basic Functionalities and Applications

algorithms	(a) Generalized Quantum Algorithms for Universal Quantum Computers	functionality	applications
Deutsch–Jozsa algorithm	more efficient to determine whether a function is constant or balanced when executed on quantum computers than classical algorithms		foundational oracle-based quantum algorithm; the first example of a quantum algorithm that performs better than the best classical algorithm
Bernstein–Vazirani algorithm	extension of the Deutsch–Jozsa algorithm as the algorithm tries to learn a string encoded in a function		foundational oracle-based quantum algorithm
Simon's algorithm	quantum algorithm with exponential speed up on a quantum computer versus a classical computer for Simon's problem		foundational oracle-based quantum algorithm
Shor's algorithm	given an integer N , finds its prime factors		public-key cryptography (e.g., RSA)
Grover's algorithm	algorithm for speeding up unstructured searches that finds with high probability the unique input to a black box function that produces a particular output value		cryptography
Harrow, Hassidim, and Lloyd algorithm for solving for linear systems of equations	estimates the result of a scalar measurement on the solution vector to a given linear system of equations		linear differential equation solving, machine learning, and data analysis
quantum approximate optimization algorithm	iteratively applied unitary operators on a state that is an equal-weighted quantum superposition of all the possible states in the computational basis for solving optimization problems		combinatorial optimization problems solving; maximum cut problems
variational quantum eigensolver	combine classical optimization with efficient cost function evaluations on quantum computers to minimize the energy expectation of an ansatz state		quantum chemistry
quantum walks	quantum analogues of classical random walks with exponential speed ups for some black-box problems		element distinctness problem, the triangle finding problem, and NAND tree evaluation
(b) Algorithms Directly Implemented on a Physical System			
quantum annealing	finding the global minimum of a given objective function over a given set of candidate solutions, by a process using quantum fluctuations		model and find ground state of a spin glass; solve for “traveling salesman” problem
Boson sampling	sampling from the output distribution of indistinguishable bosons in a linear interferometer		linear optical quantum computing, determine molecular vibronic spectra, molecular docking, graph problems

condition that the control qubit is in $|1\rangle$. Many other quantum logic gates can be constructed using the fundamental gates above. An iSWAP gate, for example, can be constructed using CNOT and single-qubit gates. For further reading, excellent reviews and text materials on gate constructions and operation can be found in refs 114 and 183.

2.8. Quantum Algorithms

A fundamental aspect of developing quantum computation is to overcome the apparent exponential overhead in computing quantum mechanical problems on a classical computer. In addition to the progress on quantum computer hardware, quantum algorithms also must be developed, which is a research area of significant activity. A key goal designed to benchmark the quantum computer is to achieve quantum supremacy, or solving problems intractable on classical computers. Therefore, computational complexity theory (a theory that classifies problem such as integer factorization into P and NP classes) is always at the center of theoretical and experimental studies performed to benchmark the quantum computer. A list of popular quantum algorithms with brief description on their basic functionalities and applications is summarized in Table 5.

Table 6 shows the level of difficulty of different algorithms designed for quantum computers en route to achieving quantum supremacy. The most recent proposals include Boson sampling,¹⁸⁴ a constant-depth circuit¹⁸⁵ in which a single photon passes through a linear optical network, instantaneous quantum polynomial (IQP) time¹⁸⁶ random quantum circuits¹⁰⁷ containing commuting gates, and circuits that do not commute. Quantum circuits on many qubits with only a few layers of quantum gates are called low-depth circuits.¹⁸⁷ Adiabatic optimization¹⁵⁷ and quantum approximate optimization algorithm (QAOA)¹⁸⁸ are quantum algorithms designed to increase efficiency in solving

Table 6. Quantum Algorithms and Level of Difficulty¹⁷⁸

algorithm	difficulty for quantum computers	easy to verify	useful
factoring	hard	yes	yes
Boson sampling	easy	no	no
low-depth circuits	moderate	cannot fully verify	no
IQP	moderate	sometimes	no
QAOA	moderate	cannot fully verify	maybe
random circuits	moderate	no	no
adiabatic optimization	easy	cannot fully verify	maybe
analog simulation	easy	no	often

optimization problems. Column 2 in Table 6 shows the level of difficulty. The validity of the algorithms is indicated with “yes” or “no”, indicating whether their validity is easy to verify. Here, we present a brief discussion on the three major types of quantum algorithms: factorization, search and optimization, and quantum walks.

2.8.1. Integer Factorization Algorithm. One of the early applications of quantum computation was Shor's factorization algorithm.⁶² Simply stated, Shor's factorization algorithm is described as follows: given an integer $N = p \times q$ for some prime numbers p and q , find the numbers p and q . The best known classical algorithm runs in order of $\exp(O(\log N)^{1/3} (\log \log N)^{2/3})^{1/2}$ in time. Shor's algorithm solves this problem in the order of $O(\log N)^3$ in time. This is a substantial speed up. In 2010, Kleinjung et al.¹⁸⁹ studied classical factorization of a 768-bit number using hundreds of modern computers over a period of 2 years that went over 10^{21} operations. An estimate using a gate-based fault-tolerant quantum computation suggests that 2000-bit number could be factorized using 10^{11} gates running over 1 day at a clock rate of 10 MHz.¹⁹⁰ The

795-bit number (RSA-240) was factored in November 2019 using 2.1 GHz Intel Xeon Gold 6130 CPU, which utilized approximately 900 CPU core years.¹⁹¹ This calculation was performed using a number field sieve (NFS) algorithm. The above facts demonstrate a notion of speed up using quantum computation. Shor's algorithm relies upon shortening the calculation task of special types of problems called hidden subgroup problems (HSP) and gives an efficient quantum algorithm to solve that type of problem. Some HSP-type problems, such as dihedral,¹⁹² that give an efficient algorithm for finding the shortest vectors in lattices are not currently well-known.

2.8.2. Search and Optimization Algorithms. Classically, to evaluate a search function $f: \{0,1\}^n \rightarrow \{0,1\}$, the algorithm performs $O(N)$ evaluations, where $N = 2^n$. The same problem can be solved with quantum computation, using Grover's algorithm, by performing $O(\sqrt{N})$ evaluations.¹⁹³ Grover's algorithm assumes the internal structure of f as an oracle or black box, meaning it does not depend on the internal structure of f . A deterministic classical computer can check the solutions to these problems in polynomial time. An important feature of Grover's algorithm is its quadratic speed up over classical Monte Carlo type algorithms. Given a problem of NP class, Grover's searching algorithm uses the order $O(\sqrt{N})$, whereas the classical algorithm uses $O(N)$. This indicates that the quantum computation would be quadratically faster than the classical computation. Grover's algorithm can speed up more complicated classical problems. Amplitude amplification algorithms based on Brassard, Hoyer, Mosca, and Tapp¹⁹⁴ can be applied to achieve a speed up of $O(1/\sqrt{\epsilon})$ evaluations, compared to an average classical speed up of $O(\frac{1}{\epsilon})$. In recent years, Grover's algorithm has also been applied in combinatorial optimization problem and has achieved a significant speed up over the classical algorithm.¹⁹⁵

2.8.3. Quantum Walks. The Markovian chain, or random walk, is a powerful approach for searching and sampling in classical computers. In this approach, the motion of a randomly moving particle is simulated on a graph structure. Quantum walk algorithms can also be applied to simulate the coherent motion of a randomly moving particle in a graph structure, and this approach outperforms random walk algorithms in the following features: (i) the time taken to find a target vertex from a source vertex and (ii) the time taken to reach all vertices after starting from one source vertex. In both features, significant speed up is achieved (exponential speed up with the feature (i) in some cases,^{196,197} and quadratic speed up with the feature (ii) compared to classical machines).¹⁹⁸ A number of algorithms based on the quantum walk offer a quadratic improvement on spectral gap, δ , from $1/\delta$ to $1/\sqrt{\delta}$. Varieties of problems including determining whether a list of integers are all distinct¹⁹⁹ and finding triangles in a graph²⁰⁰ have been solved where such improvements are observed.

In one recent study,²⁰¹ a hybrid approach of adiabatic and quantum walks was proposed that resulted in a wealth of information on how different computational mechanisms are balanced in different computing scenarios. Figure 14 shows the types of graphs where quantum speed up is achieved. In the left two graphs, the exit can be quickly reached from the entrance using a simple classical algorithm. However, the classical algorithm stumbles once the middle part of the third graph is

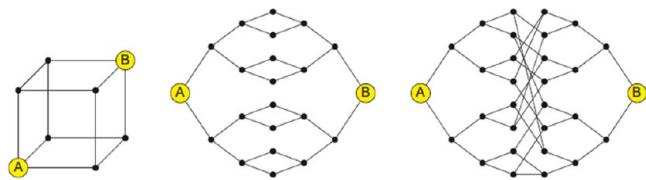


Figure 14. In the first two graphs, exit (B) can be quickly achieved from the entrance (A) using a simple classical algorithm. In the third graph, the quantum algorithm achieves a quadratic improvement as the classical algorithm stumbles within the randomness in the middle section. Reprinted from ref 190 under the terms of the Creative Commons (CC BY) license. Copyright 2016 Springer Nature.

reached. In this case, a quadratic speed up is achieved using an algorithm based on quantum walks. The classical algorithm requires $1/N^6$ order in time while the quantum algorithm takes $1/\text{poly}(\log N)$ to reach the exit.¹⁹⁰

Quantum speed up by quadratic improvement over classical counterparts has already been realized in many practical applications.^{85,87} One of the fundamental tasks in mathematics, physics and engineering is to solve sets of linear equations. A simple linear algebraic equation of the type $Ax = b$, where A is a $N \times N$ matrix and b is a vector; $b \in \mathbb{R}^N$ can be solved using the Gaussian elimination method. An impressive solution is to implement a quantum algorithm, given by Harrow, Hassidim and Lloyd,²⁰² which creates a state vector $|b\rangle = \sum_i^N b_i |i\rangle$ and access the matrix A . The algorithm also generates states proportional to $|x\rangle = \sum_i^N x_i |i\rangle$ and stores in $O(\log N)$ qubits.

3. QUANTUM SIMULATIONS

3.1. Overview of Quantum Simulations

Advanced fossil fuel and other energy technology development depend upon several categories of novel materials: catalysts for fuel conversion and syngas utilization, sorbents for CO₂ capture, anode and cathode materials for fuel cells, and high-entropy alloys for use in extreme environments are all notable examples.¹⁷ To accelerate the discovery of new materials, it is essential to have the capability to calculate material properties and to elucidate reaction mechanisms of materials not yet synthesized. These capabilities require a first-principles calculation involving quantum chemistry, which is intractable today because it is impossible to precisely represent quantum mechanical states of even moderately sized molecules on classical computers. This is because the number of parameters required to specify quantum mechanical states, and the number of operations required to evolve those states, both grow exponentially with the number of simulated particles. For example, the quantum mechanical states of 55 electrons requires 2^{55} bits of information or 4096 TB of memory in a classical computer, which far exceeds the memory available in the Summit supercomputer (2765 TB) at Oak Ridge National Laboratory, which is currently the world's second fastest supercomputer. More importantly, technology is not the only limitation of the current state-of-the-art in classical computers; rather, the limitation is fundamental and cannot be overcome. That is, the number of bits required to represent the quantum mechanical states of even a small number of electrons, 300, far exceeds 4×10^{80} , the total number of particles in the observable universe.²⁰³ This "exponentially explosive growth in the size of the simulating computer" led Feynman¹⁹ to exhort: "Let the computer itself be made of quantum mechanical elements which obey quantum mechanical laws." This is

because quantum systems can contain an exponentially large amount of information without using an exponentially large number of physical resources. The 300-particle system, for example, can be simulated with a practically achievable 300 qubit register of a quantum computer, highlighting the increasing interest and advances in the field of quantum computation over the past quarter century.

Two routes may be used for conducting a quantum chemistry simulation, both of which require representing the Hamiltonian or the total energy of the particles in a system: (1) analog quantum simulation, which directly realizes the Hamiltonian of a quantum system of interest by engineering another, controllable quantum system²⁰⁴ or (2) digital quantum simulation, which constructs the Hamiltonian out of elementary quantum logic gates.

Digital quantum simulation is also called “universal quantum simulation.”²⁰⁵ In fact, a digital quantum simulator is simply a universal quantum computer when used for simulating a quantum system. For example, Lanyon et al.³⁷ calculated the energy spectrum of a hydrogen molecule by encoding qubits into the polarization of single photons and by implementing a quantum algorithm using photonic quantum logic gates. Table 7 summarizes the similarities and differences between analog and digital quantum simulations.

3.2. Analog Quantum Simulation

This subsection focuses on analog quantum simulations, which are also known as physical (rather than numerical) simulations, dedicated quantum simulations, quantum emulations, or quantum simulation experiments. Analog quantum simulators are likely to become practicable before quantum computers because they are easier to construct for certain problems. Analog quantum simulators are reviewed by Lu et al.,²⁰⁶ Georgescu,¹³ Johnson et al.,²⁰⁷ and Zagoskin.²⁰⁸

3.2.1. Overview of Analog Quantum Simulation.

Analog quantum simulation involves using a “controllable quantum system to study another less controllable or accessible quantum system”.¹³ For example, the electrons in a crystal could be simulated by neutral atoms that can be manipulated in optical lattices. “Although these two systems have vastly different energy densities, they can in many cases be described by equivalent Hamiltonians, which give rise to equivalent physics.”²⁰⁹ The Hamiltonian of the electrons in a crystal (the quantum system of interest) is directly mapped onto the Hamiltonian of the neutral atoms in optical lattices (a controllable quantum system), to reproduce a property of interest. The system of neutral atoms can evolve, enabling direct measurement of physical quantities of interest pertaining to the electrons in a crystal.

In an analog quantum simulation, the first step is to encode the quantum information and prepare the simulator’s initial quantum state.²⁰⁶ Subsequent steps include evolving the initial quantum state with the system Hamiltonian and measuring the desired properties from the final state. The initial state can be prepared with either the first or the second quantization method. In the first quantization method, the number of gates required scales as $O(Q^2)$ for a Q -particle system and as $O(P^5)$ in the second quantization approach, where P denotes the size of the basis set. The first quantization scheme is more efficient for simulating reactions of more than four atoms.²⁰⁶ Despite the great advances made in preparing and controlling qubits, preparation of the initial state and measurement of the final state are challenges that must be overcome to make analog

Table 7. Similarities and Difference between Analog and Digital Quantum Simulation

analog quantum simulation	digital quantum simulation
1. Analog quantum simulation directly implements the Hamiltonian of a quantum system of interest by engineering another, controllable quantum system in an experimental device.	1. Digital quantum simulation constructs the Hamiltonian out of elementary quantum logic gates. A Hamiltonian of interest is first expressed in the second quantized form and is then simulated using a standard implementation protocol.
2. The Hamiltonian of the system of interest could be very different from the Hamiltonian of the controllable system. For example, the electrons in a crystal are simulated using neutral atoms that can be manipulated in optical lattices.	2. Since this type of simulator implements standard quantum circuits constructed using quantum gates, it has the same level of technical difficulty as the quantum computer.
3. Analog quantum simulators have been mostly useful for simulating condensed matter systems which are relevant problems in chemistry.	3. In principle, any quantum system can be simulated using digital quantum simulation. Therefore, it is also called universal quantum simulation.
4. Analog quantum simulators are relatively easy to implement and are likely to become practicable before universal quantum computers become available because such simulators are easier to construct for certain problems than digital quantum simulators.	4. The simulator is bound by decoherence, fidelities of state preparation, gate errors, and measurement. In practice, realization of digital quantum simulation is highly limited due to growing error as the number of qubits increases.
5. Simulators in analog quantum simulations are constructed specific to problems of interest and use fewer gates. These simulators must be validated to verify the faithful execution of the Hamiltonian.	5. The number of elementary gates to execute in each step, while simulating at a given second quantized Hamiltonian of interest, rapidly increases the depth of simulators, resulting in an exponential growth in error.

quantum simulators practicable. Also, the accuracy of the analog quantum simulation is hardware-dependent and cannot be arbitrarily increased.²⁰⁸

3.2.2. Realization of Analog Quantum Simulation.

Analog quantum simulators have been mostly used for simulating condensed matter systems.²⁰⁵ Garreau²¹⁰ reviews experiments conducted with cesium atoms laser-cooled to around 2 μK in a magneto-optical trap for the quantum simulation of disordered systems. The cold atoms interact with a standing wave formed by a laser beam, which is periodically turned on and off to simulate the physics of a disordered system that is difficult to study experimentally. The quantum simulation experiments most relevant to fossil energy and carbon management are those used for calculating molecular properties or for the study of chemical reactions. Kassal et al.²⁰⁵ and Lu et al.²⁰⁶ have reviewed the work in simulating chemistry using quantum computers.

Smirnov et al.²¹¹ proposed modeling chemical reactions using semiconductor quantum dots. The electrons within the quantum dot shells occupy discrete energy levels like electrons within atoms. Thus, quantum dots can act like artificial atoms and coupled quantum dots can act like artificial molecules. For example, a quantum dot with one electron can be considered an artificial hydrogen atom and a quantum dot with four electrons can be considered an artificial oxygen atom. An artificial water molecule can be simulated by coupling two one-electron dots with one four-electron dot. The control parameters for the quantum dots—such as gate voltages, barrier heights, distances between dots, and magnetic fields—are selected to map the energy spectrum of the real molecules to the energy spectrum of the quantum dots. To study a chemical reaction, only a part of the potential energy surface that characterizes the reaction needs to be mapped. Then, by varying the speed of voltage changes applied to the gates that form the quantum dots, an artificial chemical reaction can be simulated and directed along a desired pathway. As an illustration, Smirnov et al.²¹¹ discuss the reaction $\text{H} + \text{H}_2 \rightarrow \text{H}_2 + \text{H}$: the scattering of a hydrogen atom from a hydrogen molecule, which is a chemical reaction that requires quantum-level modeling to fully reveal the various reaction pathways. They describe how the necessary initial state can be obtained and what voltage pulses should be applied to simulate a desired final product.

Torrontegui et al.²¹² explored the analogy between collinear three-body chemical reactions and the motion of a single cold atom on a potential energy surface designed by a magnetic or optical waveguide. They work out the experimental parameters required for simulating the reaction $\text{F} + \text{H}_2 \rightarrow \text{FH} + \text{H}$ with ultracold ^7Li atoms in wave guides. Although time-dependent 2D Schrodinger equations for this system are solvable with classical computers, the analog quantum simulation could reduce the time from “several days to weeks on a supercomputer” to “milliseconds.” Another proof-of-principle analog quantum simulation of chemistry is the study of a one-dimensional isomerization chemical reaction in NMR.²⁰⁶

Gorman et al.²¹³ used an analog quantum simulator to study vibrationally assisted energy transfer, a step in many biochemical processes such as photosynthetic energy-harvesting. The efficiency of energy transfer is strongly dependent upon the noisy thermal environment of the system. Even moderately sized systems are intractable to theoretical modeling and cannot be experimentally probed because the underlying mechanisms cannot be isolated. These limitations

are overcome in an analog quantum simulation for the system developed by Gorman et al.,²¹³ who experimentally demonstrated a simple model of vibrationally assisted energy transfer consisting of a donor and an acceptor site. They used two trapped $^{40}\text{Ca}^+$ ions, one to simulate the donor site and the other to simulate the acceptor site, and then isolated the ions from the environment and engineered interactions between the sites according to the Hamiltonian of their simple model. A laser beam illuminating both ions generated site–site coupling with strength J . A localized beam generated the coupling to the environment with strength κ and controlled the energy barrier Δ between the sites. The Hamiltonian for the simple model for various parameter settings $[J, \kappa, \Delta]$ is realized by adjusting the strength and frequency of various laser tones. The laser beams are applied for a simulation time of around 1 ms, and the combined electronic state of both ions is measured by recording the fluorescence with a charge-coupled device. The simulations are repeated for each parameter setting 100–500 times to calculate the conditional probability that the system has transitioned from donor to acceptor state, which is the final result of the analog quantum simulation.

3.3. Digital Quantum Simulation

While the development of a scalable universal quantum computer remains a long-term goal, recent progress indicates that computing devices capable of outperforming their classical counterparts will soon be available.²¹⁴ One of the most important applications of quantum computers is simulating quantum dynamics.¹⁹ While quantum computers are expected to simulate a variety of problems such as fermionic lattice models, quantum chemistry and quantum field theories, simulation of spin systems with local interactions has less overhead and is likely to be an early candidate for realizing quantum simulations.^{215,216} The digital quantum simulation uses standard quantum circuits based on quantum gates and involves the same level of technical difficulty as the quantum computer. Therefore, the digital quantum simulator is bound by decoherence, fidelities of state preparation, gate errors, and measurement. They can be improved by implementing the usual techniques of quantum error correction and fault tolerance. In recent years, a significant improvement has been made on accurately simulating the time evolution of quantum systems.^{217,218}

3.3.1. Digital Simulations of Dynamical System. To understand the concept of digital quantum simulations, consider a simple example of the Heisenberg spin model.²⁷ The model Hamiltonian for this example can be expressed as $H = \sum_{k=1}^N H_k$, where

$$H_k = -\frac{1}{2} \sum_{j=1}^N (J_x \sigma_j^x \sigma_{j+1}^x + J_y \sigma_j^y \sigma_{j+1}^y + J_z \sigma_j^z \sigma_{j+1}^z - h \sigma_j^z) \quad (7)$$

where $J_{x,y,z}$ are coupling constants, h is the external magnetic field, and $\sigma_j^{x,y,z}$ are Pauli matrices on qubit j . Simulations of the time evolutions of H can be made by slicing it into n sequence of operations as

$$e^{\frac{i}{\hbar} H t} \approx (e^{\frac{i}{\hbar} H_1 t/n} e^{\frac{i}{\hbar} H_2 t/n} \dots e^{\frac{i}{\hbar} H_N t/n})^n \quad (8)$$

where error can be minimized by taking a sufficiently large number of steps n . Writing the time evolution in the form of eq 7 makes it easier to simulate the dynamics for each H_k because it acts on the reduced Hilbert space. Simulation of the time

evolution operator $e^{\frac{i}{\hbar}H_k t/n}$ is given by the number of elements in the matrix; for example, 4 for a single qubit term and 16 for a 2 qubit term. The error can be reduced by taking a sufficiently large n . This contrasts with the classical simulation where simulating $e^{\frac{i}{\hbar}H_k t/n}$ requires a matrix of size $2^N \times 2^N$.

In principle, this type of calculation can be realized using superconducting circuits. Currently, circuits and gates required for digital quantum simulations of the type given above are already demonstrated to work with superconducting resonators (transmons).^{219–221} Protocols that demonstrate digital quantum simulations using superconducting circuits for the Heisenberg model with two qubits (a), Heisenberg model with three qubits (b), and Ising model with three qubits (c) are shown in Figure 15. The work demonstrates the possibility of

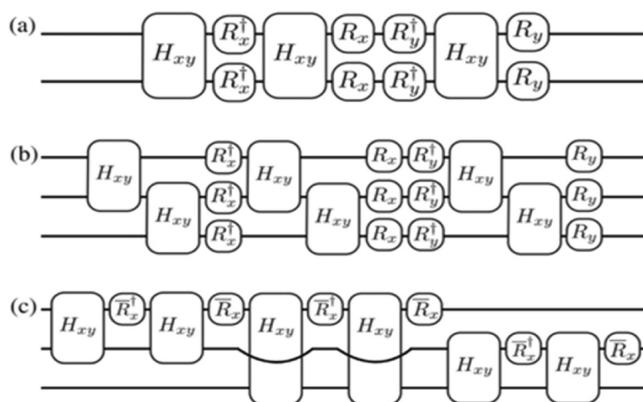


Figure 15. Protocols demonstrating digital quantum simulations using superconducting circuits for (a) Heisenberg model with two qubits, (b) Heisenberg model with three qubits, and (c) Ising model with three qubits. R_{xy} are the qubit rotation matrices with their adjoints R^\dagger . Reprinted with permission from ref 222. Copyright 2014 American Physical Society.

digital decomposition in a generic quantum simulator for a variety of spin dynamics models and unravels the capabilities of emulating general many qubit spin Hamiltonians.²²² A high level of error correction requires exceptionally large amounts of computational resources. Nevertheless, this type of quantum digital simulation outperforms classical computers even if it is not required to be highly precise.

The quantum simulation of simple spin models can be useful to get insight on a variety of open problems including quantum phase transitions, correlated 1D systems and high T_c superconductivity. In ref 223, trapped ions were used to efficiently simulate the full-time evolution of interacting spin-1/2 particles. The simulator was based on a string of electrically trapped and laser-cooled calcium ions. Qubit information was encoded in states split by the Zeeman effect. Simulated quantum states were encoded in the qubit and manipulated by laser pulses. The laser pulses implemented a set of operations under which the Hamiltonian adiabatically evolved from one magnetic phase to another. The full dynamics of a range of spin systems with sequences of up to 100 gates and 6 qubits were simulated. This demonstrated the feasibility of building a controllable full-scale simulator for certain complex spin-1/2 systems.

3.3.2. Steps for Digital Quantum Simulation. By implementing quantum gates, in principle, it is possible to simulate any quantum system. Any unitary operation can be

efficiently simulated using digital quantum simulation. However, not all Hamiltonians can be efficiently simulated in this way. Finding universal gates can be challenging by itself and the decomposition of unitary operations into 1 and 2 qubit levels generally involves an ever-increasing number of gates. Despite these facts, simulating any finite-dimensional local Hamiltonian, such as the Ising model, is possible using digital quantum simulation. For an efficient quantum simulation initial state preparation, unitary evolution, and final measurement are the three major steps.

(i) *Initial State Preparation.* The first simulation step is to initialize a state $|\psi(0)\rangle$ in a quantum register. For example, it is possible to initialize unsymmetrized states to prepare a many-body antisymmetrized state that contains the quantum characteristics for fermionic systems.²²⁴ In quantum chemistry, studies performed on the algorithm development for atomic and molecular systems focus on state preparation.^{225–227} The algorithm proposed by Wang et al.²²⁷ simulates the time evolution of the quantum system using auxiliary qubits that absorb a specified amounts of energy from the system and prepares the desired energy eigenstate.

(ii) *Unitary Operation.* The next step is to decompose the unitary operator that evolves with time into a number of time-steps, each of which corresponds to a standard quantum gate. When two Hamiltonians at different sites, say l and l' , in the unitary operator $U = \prod_l e^{-\{i\hbar H_l t\}}$ do not commute, decomposing the unitary operator using classical methods is highly inefficient. In such cases, it is possible to decompose U into smaller time steps, $U(\Delta t) = e^{-\{i\hbar \Delta t\}}$, and implement each operation into a local gate. Aspuru-Guzik et al.²²⁸ suggested a procedure for atomic and molecular systems using the recursive phase-estimation method presented in Figure 16.

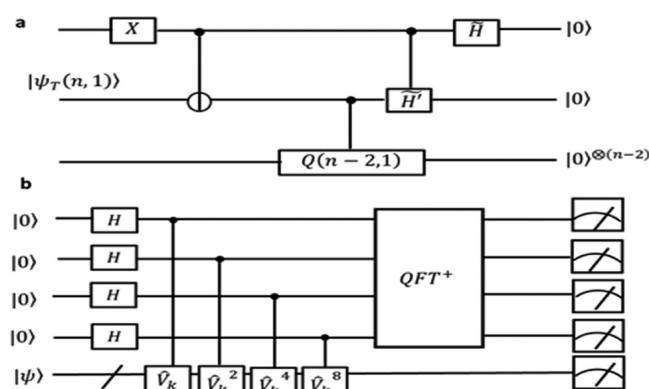


Figure 16. (a) Quantum circuit for initial state preparation for finding the target state $\psi_T(n,1)$ of an electron occupying n orbital. Reprinted with permission from ref 226. Copyright 2009 American Physical Society. (b) Quantum circuit implementing recursive phase estimation algorithm for molecular energy calculations.²²⁸ H and QFT^+ denote, respectively, the Hadamard gate and the inverse quantum Fourier transform, and $V_k = [e^{-i2\pi\varphi_{k-1}}V_{k-1}]^2$. Reprinted with permission from ref 228. Copyright 2005 American Association for the Advancement of Science.

The accuracy of this procedure increases as the number of iterations increases, the first being highly inaccurate, the second being relatively more accurate and so on until the desired accuracy is met.

(iii) *Measurement.* After the time evolution of $|\psi(0)\rangle$ under the unitary operation, a measurement is performed to extract information about the simulated system. One early technique

used for the measurement is quantum state tomography (QST).²²⁹ However, QST requires exponentially large resources as the system size increases. Therefore, in more recent years, a technique to measure physical quantities such as the correlation function or spectra of operators was developed to avoid the measurement's large resource requirement.²³⁰

3.3.3. Physical Realization. A physical realization of a quantum simulator requires a controllable quantum mechanical system. The time evolution of the operator is simplified and is mapped out to 1 and 2 qubit gates.²⁵ Here, we discuss the major systems used so far to realize digital quantum simulation in practice.

Experimentally, atoms and ions in optical lattices can be used to realize digital quantum simulation. In 2003, Jane et al.²³¹ proposed atomic ensembles subjected to two optical lattice potentials, one for each of the atomic states and each represented by the qubit. Interactions between the atoms were realized by replacing one of the optical lattices with respect to the other. The neutral atomic ensemble weakly interacts with the environment.

The high-fidelity gates were also realized to simulate an open quantum system with up to five qubits implemented in trapped ions for an engineered digital quantum simulator as shown in Figure 17.²³² This experiment demonstrated the possibility of

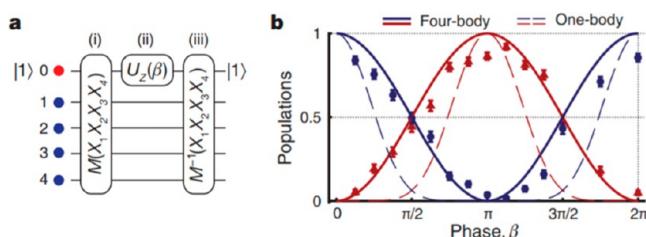


Figure 17. (a) Elementary building blocks used to simulate the operator U for four-body Hamiltonian. (b) Periodic variations in populations in the state $|0000\rangle$ (triangles) and $|1111\rangle$ (circles) are shown as a function of phase angle β as measured in the experiment. Details are presented in ref 232. Reprinted with permission from ref 232. Copyright 2011 Springer Nature.

engineering open quantum systems through the dissipative preparation of entangled quantum states and simulations of coherent many-body spin interactions.

Nuclear spins can be another test bed for small-system digital quantum simulations.^{228,233,234} Nuclear spins can be manipulated using NMR for implementation in simulations and algorithm problems. Nuclear spins are characterized with an ultralong coherence time (>1 s), which enables the development of high-fidelity quantum gates and coherent control over many qubits.

Superconducting qubits have a coherence time of several microseconds. State-of-the art superconducting circuits can be used as a digital quantum simulator and have advantages over real atoms in that these circuits can be designed and tailored to manipulate interactions and frequencies.²³⁵ Frequency can be tuned using an externally applied magnetic field, and the interaction between two near neighbor qubits can be turned off and on as desired. In addition, superconducting circuits can be easily integrated with cavities and other optoelectronic circuits. One great advantage of these circuit models is scalability. A chip containing over 512 qubits was fabricated in 2012 by R. Harris et al.²³⁶ However, coherence was a major challenge because the number of qubits increased significantly.

3.3.4. Simulating Systems with Many Spins. Generally, quantum computers are two-level qubit systems. A three-level system is called a qutrit. It is possible to have a system consisting of d -levels called qudits that are useful for simplifying specific quantum computation problems. Consider a spin s with basis $[s, m]$, where m has $2s + 1$ values given by $-s, -s + 1, \dots, s$. This requires a Hilbert space of the dimension $2s + 1$. To emulate this system, multilevel artificial atoms can be implemented. For example, a spin-1/2 can be emulated using a two-level system, a spin 1 using a three-level system, and a spin-3/2 using a four-level system. Thus, many spin systems can be efficiently emulated and studied based upon their geometric phases as such systems that naturally call for qudits with $d > 2$ ^{237,238}

In ref 238, a qudit system was used to emulate the dynamics of single spins with principal quantum numbers $s = 1/2, 1$, and $3/2$, which allowed the measurement of the Berry's phase and the parity of spins under rotation by 2π , as shown in Figure 18.

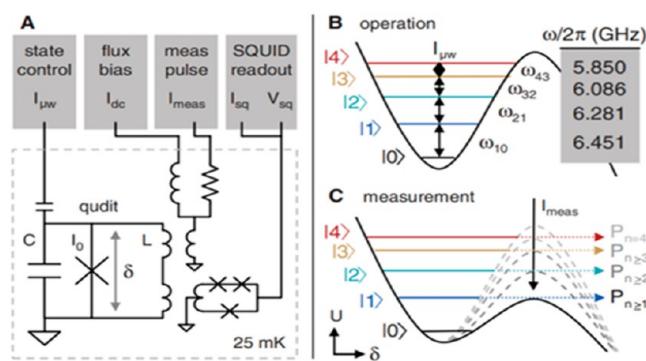


Figure 18. Demonstration for emulating a spin system with a superconducting phase qudit.²³⁸ Schematic for the qudit circuit (A). Potential energy as a function of superconducting junction phase (B). Current pulses are applied to reduce the potential energy barrier so that quantum states tunnel through it (C). Reprinted with permission from ref 238. Copyright 2009 American Association for the Advancement of Science.

Superconducting phase qubits were shown to operate as qudits up to five levels. Qubits could be used to model spin-1/2 system, but for $s \geq 1$, qudits are natural candidates for emulation in d -dimensional Hilbert space.

4. QUANTUM COMPUTING AND SIMULATIONS FOR ENERGY APPLICATIONS

While quantum computing is considered as a paradigm shift in our basic understanding of physical computation, effective implementation of quantum computing in energy applications also depends on progresses and development in the dimensions of both quantum computing hardware and quantum computing algorithms. In the perspectives of quantum computing hardware, the availability of the number of qubits and the noise level of the qubits should be weighed in, whereas in the perspective of quantum computing algorithms, error tolerance capability in the algorithm and gain of speed up relative to classical computing should be considered. In addition, current quantum processing devices and computing algorithms may also require pre- and postprocessing by classical computers for its basic operation within realistic architecture.

Based on projected advances in quantum computing hardware and algorithms, five simulation areas that can be impacted by quantum computing and their expected time frame are summarized in Figure 19. These five basic simulation

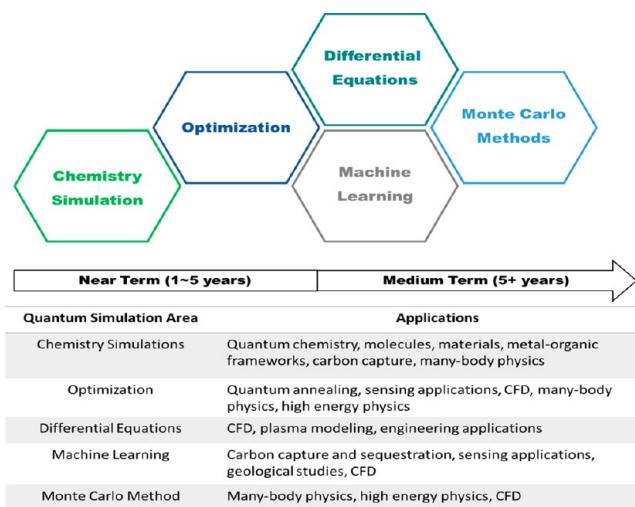


Figure 19. Quantum simulation areas along with projected time frame.

areas can be further adopted in numerous energy related fields including materials sciences, fossil energy specific applications, as well as physics, chemistry, and engineering applications, as discussed in the subsections below.

4.1. Quantum Computing in Material Sciences

The use of quantum computation in material sciences is rapidly growing as quantum computers technologically mature.^{65–67} With the appearance of higher qubit number quantum computers, the number of research articles related to material science is rapidly growing, highlighting the importance of quantum computation to the fields of physics and chemistry.^{37,42,66,205,239–241} Variational algorithms that utilize hybrid approaches where both the quantum and classical computer are working in tandem are becoming useful, because such algorithms partly avoid the shortcomings of current hardware limitations in quantum computers. Such computational approaches, known as hybrid quantum-classical (HQC) algorithms, are more practical frameworks in simulating heuristics models in NISQ. Variational algorithms have attracted considerable attention in the QIS community both theoretically^{242–244} and experimentally.^{82,173} Many problems in quantum physics, chemistry, and biophysics/biochemistry are still unresolved despite decades of efforts for finding solutions. These include (but are not limited to) finding the correct functions in density functional theory (DFT), 3D Ising problems, and Hubbard models. Lloyd²⁷ and Zalka²³⁹ independently introduced quantum simulation schemes for single many-body systems.

To solve classically intractable quantum chemistry problems with a quantum computer, the first step is state preparation. Some examples of state preparation are Hartree–Fock states and states obtained after solving the coupled cluster methods. In a seminal work, Zalka²³⁹ proposed discretizing the wave function and initializing the simulation using a series of controlled reactions. Conceptually, discretizing a many-body Hamiltonian using the second quantization while preparing the quantum states, which will eventually be formulated in terms of

qubits, is easier and less mathematically involved.^{245–247} Before making the choice of quantization, one must have a scheme for mapping a Hamiltonian to the qubits. Because nuclei have masses that are 3 orders of magnitude higher than electrons, nuclei are treated as stationary point charges relative to the electronic motions. This approximation is called Born–Oppenheimer approximation (BOA). Most of the time, the BOA is implemented to separate the nuclear motion from electronic motion while developing quantum algorithms.

Figure 20 shows a flowchart for a hybrid type of calculation where a quantum computer augments a classical computer

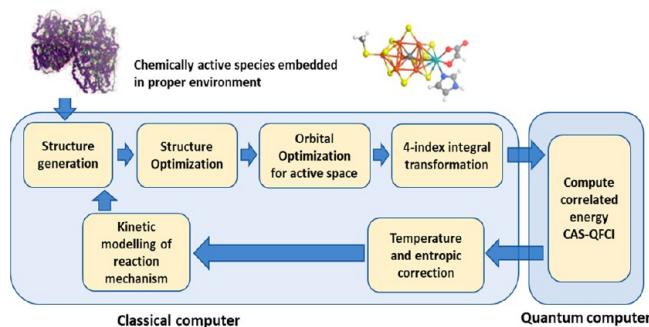


Figure 20. Flowchart showing a computational reaction mechanism with a quantum computer where a full configuration interaction energy is performed in a complete active orbital space (CAS). The steps of structure generation, structure and orbital optimization and transformation are completed classically to obtain a second quantized Hamiltonian. A quantum computer uses that Hamiltonian to calculate ground state energy, and then temperature and entropic corrections are applied using standard models such as DFT. The corrected energy is then used for kinetic modeling of the reaction mechanism. Reproduced with permission from ref 66 under the terms of the Creative Commons (CC BY-NC-ND or CC BY) license. Copyright 2017 National Academy of Science.

calculating the classically intractable problem of correlation energy under CAS. Reiher et al.⁶⁶ used this scheme to show the resource requirements, including error correction, for the simulations of the cofactor FeMoco of nitrogenase (an enzyme that catalyzes the conversion of atmospheric nitrogen molecules into ammonia through a process known as nitrogen fixation) using physical gates operating at 100 MHz with an error target of 0.1 mH (milli Hartree). Several published articles report the study of small molecules and ions simulated by applying quantum algorithms. Using an early stage quantum computer, Whitefield et al.²⁴⁹ implemented a Jordan–Wigner transformation on a second quantized Hamiltonian and developed a quantum algorithm that was applied to a H₂ molecule by decomposing the operation into elementary gates. Jones et al.²⁵⁰ also applied a similar scheme to calculate the ground state energy of LiH. Lanyon et al.³⁷ used a photonic quantum computer to calculate the complete energy spectrum of a H₂ molecule in a minimal basis set by implementing an iterative phase estimation algorithm.^{228,251} Using a trapped-ion simulator, Hempel et al. experimentally realized the digital quantum simulations of H₂ and LiH and compared that with the results from variational algorithms.²⁵² Very recently, Vera von Burg et al. implemented a quantum computing protocol (Figure 21) in the qubitization framework, which exploits a double-factorized electronic structure representation to reduce the runtime, and obtained sufficiently accurate results for intermediate and transition state structures of a catalytic cycle

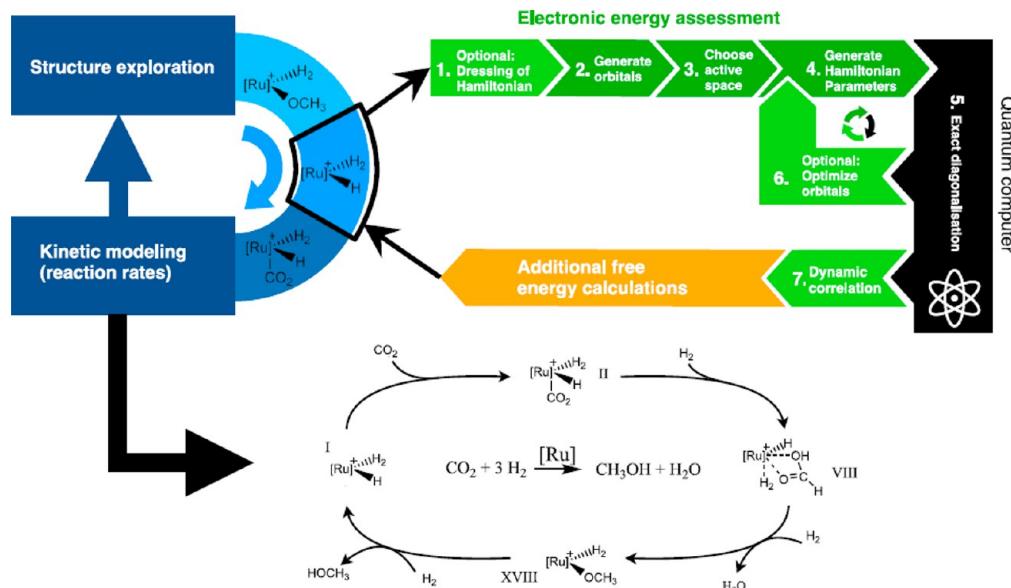


Figure 21. Quantum computing protocol for computational catalysis. A key step of quantum computing is embedded in this protocol (presented by the black box) and usually performed with traditional methods such as complete active space self-consistent field, density matrix renormalization group, or full configuration interaction quantum Monte Carlo. Reprinted with permission from ref 248 under the terms of the Creative Commons Attribution 4.0 International license. Copyright 2021 American Physical Society.

on a synthetic catalyst used for the conversion of carbon dioxide to methanol.²⁴⁸ These studies show the possibility of using quantum computation to solve a variety of problems that belong to quantum chemistry and material sciences.

4.2. Quantum Computing: Fossil Energy Specific Applications

Worldwide, a significant portion of total energy consumption comes from fossil energy, and this trend is expected to continue for decades to come. Improving and enhancing the performance of existing technologies and equipment is necessary to circumvent the growing challenges of safe and secure production, processing, and consumption of energy. Quantum computation is expected to overcome some of the specific near- to intermediate-term challenges related to fossil energy by leveraging (i) quantum many-body computation of material properties to an unprecedented level of accuracy at a lower cost, (ii) a better understanding of downstream, midstream, and upstream fluid flows, and (iii) machine learning and artificial intelligence for (a) evaluating optimum materials in carbon capture technology that outperform existing materials and (b) studying deep geological data for oil, gas, and mineral explorations. Since quantum computing is in its early stage, more avenues are expected to arise in energy sectors with the implementation of NISQ¹⁷² computing as short- or intermediate-term opportunities. Here, we discuss aspects of quantum computing for fossil energy applications.

4.2.1. Quantum Computation of Material Properties for Fossil Energy Applications. One priority area in fossil energy is the technological development of materials with a high gas separation factor and permeability that yield an upper bound in the logarithmic relationship of trade-off parameters (separation factor vs permeability). To achieve optimal material performance with a high upper bound and to overcome the problem of low selectivity and permeability with polymeric compounds, membranes made of zeolites or combinations of zeolites with polymeric systems must be developed. At the current time, the properties that arise due to

multimaterial compositions are too computationally intensive to study using quantum mechanical calculations. Despite the development of advanced supercomputing facilities, studying porous candidate gas capture and separation materials such as metal–organic frameworks (MOFs) is a challenge. Computational modeling of MOFs such as ZIF-8 (that has a total of 276 atoms: C-96, H-120, N-48, and Zn-12) using quantum mechanical solutions just by taking a $2 \times 2 \times 2$ supercell of its crystal in a periodic calculation is already a formidable endeavor. Increasing the system size by a factor of N increases the computational effort by N^3 (i.e., a cubic scaling exists even with today's reliable DFT approach).²⁵³ Classical approaches such as molecular dynamics, which is an order of magnitude faster, can be implemented to calculate certain bulk properties such as gas diffusivities if the interaction of the electronic system is weak.^{254,255} However, a major shortcoming of classical approaches is that, because they cannot provide insights into the electronic charge rearrangements between gas molecules and absorbent, they largely fail to account for interactions other than the van der Waals type. A possible solution, which is frequently used in carbon capture and catalysis, is the so-called QM/MM (quantum mechanics/molecular mechanics)^{256,257} approach, where only the active site is treated at a highly accurate ab initio level and the environment is handled using classical force fields. This type of approach is seemingly useful to study the reactions between gas molecules and aqueous organic compounds used to capture CO₂ prior to storage, reuse, or sequestration.²⁵⁶ For example, in ref 258, QM/MM is applied to investigate the structure and dynamics of aqueous CO₂ and to provide the associated hydration free energy from first principles. Unfortunately, a problem at the interface between QM and MM exists due to over polarization if the covalent bonds are cut.²⁵⁹ Quantum computation may provide a path for modeling carbon capture systems that are too computationally expensive to easily model using classical approaches.²⁶⁰

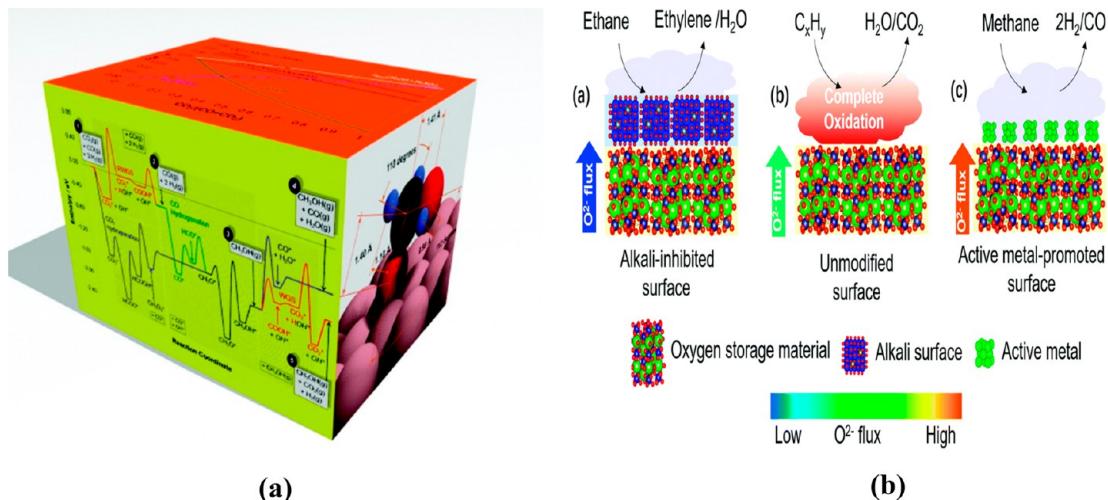


Figure 22. Examples of low-hanging fruits of fossil-energy-related technologies by a quantum computing approach. (a) Conversion of CH_4/CO_2 into CH_3OH . Reprinted from ref 283. Copyright 2011 American Chemical Society. (b) Schematic illustration of surface modifications of redox catalysts to improve product selectivity by changing the relative rates of surface oxygen removal and bulk O^{2-} flux. The arrows in the three cases (a–c) correspond to the O^{2-} fluxes, and the colors correspond to the relative intensities of the O^{2-} fluxes. Reprinted with permission from ref 285 under a Creative Commons Attribution-Noncommercial 3.0 unported license. Copyright 2020 Royal Society of Chemistry.

In addition to modeling carbon capture, quantum computation may also be helpful in modeling complex catalytic reactions. For example, the conversion of CO_2 into useful chemical products has been postulated as an economically viable way to mitigate greenhouse gas emissions.^{261,262} Yet, modeling CO_2 interactions with large, complex structures such as nanoparticle catalysts is a challenge for classical computational simulations.²⁶³ The use of quantum computers to model reaction mechanisms may aid significantly in the development of new catalytic materials.^{66,67} Indeed, quantum computers are already being used to model chemical reactions^{264,265} and are expected to facilitate material design and discovery in the coming decades.²⁶⁶ In addition, functional materials useful for applications such as energy harvesting and storage, memory chips and communication require proper optimization of the electronic, optical, and chemical properties to maximize the materials' stability. To simulate such material systems requires more efficient quantum algorithms to be built up on many-body electronic simulation models.²⁶⁷ Density matrix embedding techniques provides a method to solve a complex atomic and molecular system by fragmenting the chemically active region from the rest of the structure and solving the active region with a high level quantum mechanical theory.²⁶⁸ Such techniques could be useful if implemented in quantum algorithm techniques to solve more challenging chemical systems.

The design of materials capable of chelating high-value metals is another pressing issue in the fossil energy sector. Specifically, coal utilization byproducts including coal refuse,²⁶⁹ acid mine drainage,²⁷⁰ and fly ash²⁷¹ all are rich in high-value elements including rare earths. The design of highly selective chelating agents is crucial both for the recovery and separation²⁷² of rare earths and other metals, as well as the development of high performance, low-cost sensors.²⁷³ Candidate sensing materials such as MOFs^{274,275} and biomolecules²⁷⁶ are computationally expensive to screen due to their complexity and size. Quantum computers may therefore supplement ongoing efforts to computationally design and screen potential metal extraction agents.^{277,278}

Studies currently underway apply quantum computers for material design^{279,280} and modeling binding site interactions,²⁸¹ and similar techniques may be applied to develop highly selective chelation agents.

Recently, the conversion of methane into an easily transportable liquid fuel (e.g., CH_3OH) or chemicals has become a highly sought-after goal spurred by the increasing availability of cheap and abundant natural gas. While utilization of CH_4 for the production of syngas and its subsequent conversion via an indirect route is typical, it is cost-intensive. Hence recently, alternative direct conversion routes have been investigated actively. Among them, one of the most promising directions is the low-temperature partial oxidation of methane to methanol over a metal-loaded zeolite, which mimics facile enzymatic chemistry of methane oxidation.^{282,283} Currently, the most important catalyst for CH_4 conversion is $\text{Cu}/\text{ZnO}/\text{Al}_2\text{O}_3$ and Cu-zeolites. Cu is also an excellent water–gas shift catalyst, facilitating the conversion of CO to CO_2 and vice versa; the controversy about the carbon source in methanol synthesis still lives on, but the majority of researchers nowadays are in favor of CO_2 hydrogenation mechanisms (Figure 22a).²⁸³ Obviously, catalysis for methane conversion to methanol is low-hanging fruit for catalyst design and quantum computing. Identifying these materials and step-changing catalysts would be game changing.¹⁷ Chemical looping combustion is presently considered as a cutting-edge combustion technology that enables capturing CO_2 without a major energy penalty for its separation. The technology involves the use of solid metal oxides, so-called oxygen carriers, which are alternately subjected to the redox reactions.²⁸⁴ Although chemical looping beyond combustion (CLBC) has attracted increasing attentions over the past 5–10 years, such an emerging research area is far from being adequately explored particularly considering its significant complexity and excellent potential, as demonstrated in Figure 22b.²⁸⁵ As the redox catalysts can undergo significant changes in its surface and bulk properties within a CLBC cycle that exceeds complexities typically observed in heterogeneous catalysts,

such complexities should be addressed through continued research via interdisciplinary efforts.

4.2.2. Quantum Machine Learning for Carbon Capture, Geological Studies, and Sensing Applications.

The concept of quantum algorithms can be readily applied in machine learning approaches for carbon capture technologies.^{286–288} Evaluating promising materials for gas separation can be daunting, given the pool of tens of thousands of complex chemical compounds that must be screened based on their inherent molecular properties while demonstrating critical features of CO₂ capture capabilities.^{289–291} Machine learning approaches can aid in the search for materials with optimal properties for capturing CO₂ and other toxic gases. This approach is not only economical but also drastically reduces time in the laboratory conducting repetitive tests on multiple candidate chemical compounds that would potentially have suitable diffusivity and selectivity. In a recent study,²⁹² a multiscale approach combined DFT, grand canonical Monte Carlo, and machine learning to investigate the role of various pore chemical and topological features in enhancing the CO₂ capture metrics of MOFs. However, the multitude of features that can be simultaneously altered within the MOF space (i.e., thousands of different chemical compounds may be used; linkers may be functionalized with a range of species such as hydroxyl, thiol, amino, or nitro groups; various metal centers may be used, etc.) creates significant scaling challenges that are intractable using existing machine learning approaches for finding optimized structures. Algorithms based on quantum computation avoid the statistical complexity involved as a result of the large sample space. In addition, such algorithms have access to a wider computational space, which allows for a higher number of permutations and combinations during the search process. Quantum machine learning and artificial intelligence combined with a deep learning approach can also be useful in geological surveying for oil and gas exploration and carbon sequestration.^{293,294}

High-performance sensors are also required throughout the energy sector, for applications such as pipeline integrity, greenhouse gas monitoring, resource discovery, and grid monitoring, among others.^{15,295–298} One emerging application of quantum computational techniques is the optimization of sensing platforms.^{299,300} Quantum simulation may also be used to improve the performance of quantum sensing technologies; for example, a quantum simulator has been used to gain new insights into the entanglement between nitrogen vacancy centers in diamond,³⁰¹ which is a widely used material for quantum sensing applications.^{15,302,303} Additionally, quantum machine learning techniques have shown promise for image classification in remote sensing applications.^{300,304} Simulating material properties and performance is also crucial for sensor design; for example, complex systems such as MOFs are widely used for the sensitive detection of gases and ions.³⁰⁵ Thus, the design and optimization of next-generation sensing technologies and materials is an additional area in which quantum computers can significantly benefit the energy sector.

4.2.3. Developing Advanced Materials for Energy Storage.

Development of next-generation energy storage materials is one of the hottest research topics in the materials science field. These materials can be used for H₂ storage, as a rechargeable secondary battery, a redox-flow battery, a supercapacitor, etc. to store chemical, thermal, or electric energies.^{306–308} Hybrid analog and digital simulations are powerful tools to tackle such materials development. Recently,

by employing variational quantum algorithms for near-term quantum devices, Rice et al.³⁰⁹ explored the stability of Li_xS in Li–S batteries. Using the hardware-efficient R_y Ansatz with five qubits linearly connected (Figure 23a–c), the ground-state

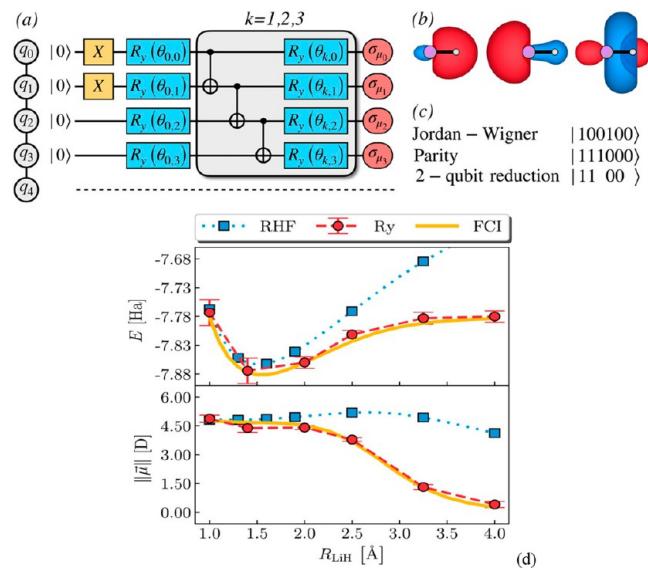


Figure 23. (a) Schematic representation of the five qubit linearly connected devices and of the quantum circuit used to simulate the ground-state energy and dipole moment of LiH. Orange symbols denote gate encoding of the Hartree–Fock state, blue symbols denote the y rotations defining the variational Ansatz, and red symbols denote the measurements of Pauli operators. (b) Molecular orbitals (MOs) encoded on the quantum hardware for LiH at equilibrium geometry [the highest occupied MO and the two virtual MOs in the A_1 irreducible representation of the $C_{\infty v}$ group (left to right)]. (c) Binary strings encoding the Hartree–Fock wave function under Jordan–Wigner and parity mappings, without and with removal of the two qubits related to the spin-up and spin-down particle number conservation in the parity mapping (top to bottom). (d) Hardware results of ground-state energy (top) and dipole moment (bottom) calculations for LiH on the five qubit devices accessed via IBM Quantum Experience. Reprinted with permission from ref 309. Copyright 2021 American Institute of Physics.

energy and dipole moment at representative values of R_{LiH} were obtained. The qualitative behavior of both energies and dipoles is correctly captured by the hardware experiments upon extrapolation (Figure 23d). This work provides a steppingstone on the way to larger quantum computing calculations on battery development.

4.3. Quantum Computation in Fluid Dynamics

Computational fluid dynamics (CFD) modeling is widely used for scaling up, optimizing and troubleshooting various reactors and devices used by the energy industry, such as fossil fuel powerplants, oil refineries, wind farms, and so on. CFD is required for calculating the turbulent flow around wind turbines, combustion in turbines and internal combustion engines, ocean flow around offshore drilling platforms, heat transfer to the particle receiver in a concentrating solar power system, and gas-particle dynamics in a fluidized bed reactor, to name a few energy related applications. A class of such problems can be solved with the basic set of equations well-known as the Navier–Stokes equations (NSE). Other classes of problems may require significant additions to or

Table 8. Quantum Computing Algorithms for Solving Flow Equations

flow problem description	maximum problem size	numerical method	quantum computing approach
steady-state inviscid, compressible flow through a convergent–divergent (de Laval) nozzle ^{31,4}	61 mesh points	finite difference	spatial discretization of NSE yields the nonlinear ordinary differential equation $dU/dt = f(U)$, where U is the vector of flow variables at discrete spatial locations, which is solved using the Kacewicz algorithm ^{31,5} based on the quantum amplitude estimation algorithm ¹⁹⁴
time evolution of the Burgers equation ^{31,6}	8192 mesh points	finite difference	quantum-classical hybrid approach, evaluating the cost function with a gate-based quantum computer and optimizing variational parameters on a classical computer
one-dimensional laminar flow in a channel ^{31,7}	10 mesh points	finite difference	discretized form of the flow equation is expressed as a linear equation set in binary variables using a fixed-point approximation. The equation set is then posed as a quadratic unconstrained binary optimization problem and solved using a quantum annealer
free-molecular flow: ^{31,8} •around a rectangular blunt body •out of a rectangular domain into vacuum	64 × 64 mesh points; 16 × 16 discrete velocities	discrete velocity method for the collisionless Boltzmann equation	high-dimensional solution is represented using a small number of qubits; convection and specular-reflection boundary condition are implemented with quantum circuits based on multiqubit controlled-NOT gates
two-dimensional cavity flow ^{31,9}	16 × 16 lattice	lattice Boltzmann method (LBM)	stream function–vorticity form of the flow equations is solved using a D2Q5 (two dimensions, five speeds) configuration of LBM represented with quantum circuits; velocity components are calculated from the stream function on a classical computer

- computational complexity of the algorithm depends upon q_f the Hölder class smoothness parameter of $f(U)$:
 - no speed up in the smooth limit ($q \gg 1$)
 - exponential speed up in the rough limit ($q \ll 1$)
 - exponential speed up in the strongly disordered regime, determined by a model parameter
 - exponential speed up is unlikely because the number of velocities that can be represented scales linearly with the number of qubits, each of which represents a single classical bit
 - memory required:
 - classical $O(N_v^d M^d)$
 - quantum $O(\log(N_v^d M^d))$
 - complexity of time evolution:
 - classical $O(T_d N_v^d M^d)$
 - quantum $O(T d N_v^d \log(M))$
- where N_v is the number of discrete velocities in each dimension, M is the number of mesh points in each dimension, d is the number of spatial dimensions, and T is the time interval quantum advantage of the IBM could be compromised by the encoding required every time step after calculating the velocity on a classical computer

modifications of NSE. For an incompressible fluid, the NSE consists of the three momentum equations

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = - \frac{\partial P}{\partial x_i} + \frac{1}{\text{Re}} \frac{\partial}{\partial x_i} \left(\frac{\partial u_i}{\partial x_j} \right) \quad (9)$$

and a continuity equation

$$\frac{\partial u_j}{\partial x_j} = 0 \quad (10)$$

where u_i is a velocity component, t is time, x_i is a spatial coordinate, P is pressure, Re is the Reynolds number, and repeated indices imply summation. Even this basic equation set cannot be solved for most flows of practical interest because the number of grid points required, and hence, the computational cost becomes prohibitively large as Reynolds number becomes large; for example, the computational cost is $O(\text{Re}^{37/14})$ for the direct numerical simulation of a certain type of flows.³¹⁰ For large values of Re , that is when the flow is turbulent, the NSE cannot be solved because the required computational capabilities are not available even on the fastest supercomputers. Therefore, approximate solutions of the NSE are used for practical applications. The computational challenge is further increased in energy applications because the NSE must be supplemented with other equations, such as equations of energy and species mass balance, equations for multiple phases, and so on. If the required computing resources were to scale logarithmically with the Reynolds number, many practical flow problems could become solvable. Quantum computing may offer that opportunity.

An investigation of quantum algorithms for the numerical solution of the NSE for incompressible flows at finite Reynolds numbers can be found in ref 311. A summary of key tools and algorithms and possible approaches of quantum computing in fluid dynamics can be found in refs 312–314. A summary of recently reported quantum computing algorithms for solving different simplified forms of the NSE is given in Table 8.

For modeling turbulent combustion, the flow equations must be augmented with evolution equations for describing the mixing of reactants.^{85,87,88,320} In this type of problem, it is possible to show a quadratic complexity improvement over the parameter estimation. Classically, parameter estimation is achieved within the precision of $1/\sqrt{N_r}$, where N_r is the number of computational steps. Using quantum computing, this problem is dramatically simplified and the parameter estimation is shown to be achieved within the precision of $1/N_r$. In the reactant conversion rate calculation, two reactants $F(x, t)$ and $O(x, t)$ are assumed to be segregated at time $t=0$. Their joint probability density function (PDF), $P(\Psi, t=0)$ where $\Psi: \psi_1 = F, \psi_2 = O$, at $t=0$ is given as

$$P(\Psi, t=0) = W_F \delta(\psi_1 - F_0) \delta(\psi_2) + W_O \delta(\psi_1) \delta(\psi_2 - O_0) \quad (11)$$

where W_F and W_O are weight factors of the two reactants: $W_F + W_O = 1$, and F_0 and O_0 are the initial mass functions. An evolution equation for the PDF is solved classically using MC technique under certain assumption to calculate the conversion rate. Details on the evolution equation are presented in ref 87. The MC technique solves for the reactant conversion rate as given by $\mathcal{L}(t) = 1 - \langle F(t) \rangle / \langle F(0) \rangle$. For the purpose of comparison, the important parameter to be noted with the

solution using quantum simulation is number of repetitions, N_r , of the MC method to provide the estimate within the same level of precision and confidence. Scaling of the error estimation with respect to the number of runs provides a sense of the computational cost to achieve certain accuracy in the calculation. In the MC simulation technique, the results show error estimation scales on the order of $1/\sqrt{N_r}$.

The authors in ref 87 solve above problem using a quantum simulation technique. N_r in the quantum simulation case is the total number that a unitary operation U must be implemented, as $U|0,0,\dots,0\rangle = \psi$, to prepare the initial state. Error estimation is calculated in a number of steps by evaluating a median value of the phase factor, θ , in the eigenvalue $e^{i\theta}$ of the unitary operator U using a phase estimation approximation (PEA) quantum algorithm. The number of steps L to arrive the median value of θ using $M = 2^m$, where m is the number of qubits, operation yields the parameter N_r : $N_r = L \times M$. The simulated error estimation is shown in Figure 24. Precision in the estimation of

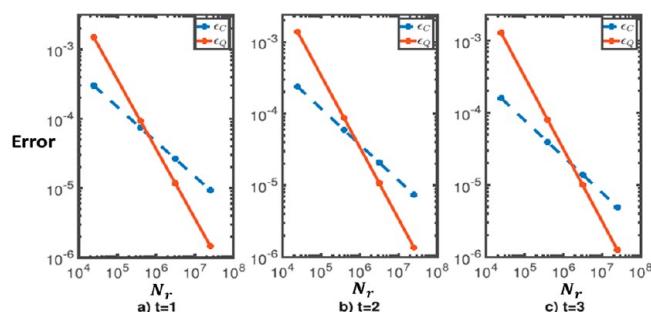


Figure 24. Error estimation, ϵ_C and ϵ_Q simulated using the classical MC and quantum algorithms for the Damköhler numbers (Da) equal 1 to estimate the rate of reactant conversion, $\mathcal{L}(t)$. Errors were calculated for the different $N_r = L \times M$. Reprinted with permission from ref 87. Copyright 2019 Taylor & Francis.

$\mathcal{L}(t)$ was found to scale as $1/N_r$, using the quantum algorithm. This showed a quadratic improvement over the complexity with quantum simulation on solving the reactant conversion rate. Similarly, efficient quantum simulation of the Vlasov equation for plasma modeling has been demonstrated.³²¹

For solving NSE and associated equations, the advantage quantum computing could offer is through the storage of discretized flow field variables as amplitudes of a quantum register, whose size scales logarithmically with the problem size.^{311,313,318,319} For example, the discretized spatial locations of a two-dimensional 32×32 mesh can be stored as the amplitudes of a 10 qubit register $|q_{x4}q_{x3}q_{x2}q_{x1}q_{x0}q_{y4}q_{y3}q_{y2}q_{y1}q_{y0}\rangle$, where the subscripts indicate the qubit's role. Now, to store the discretized values of a field variable, only one more qubit (q_u) need to be added to the quantum register $|q_{x4}q_{x3}q_{x2}q_{x1}q_{x0}q_{y4}q_{y3}q_{y2}q_{y1}q_{y0}q_u\rangle$.³¹⁸ Note that for this case the memory required in a classical computer would have doubled.

Griffin et al.³¹¹ discuss the upper bound on computational speed up. For a three-dimensional problem with M^3 mesh points the classical problem size is $O(M^3)$, whereas the quantum problem size is $O(\log(M))$ when the encoding shown in the last paragraph is used. The number of time steps scales like M for explicit time advancement. So, the lower bound on the cost of a classical simulation is $O(M^4)$, and a quantum simulation is $O(M \log(M))$. The number of time steps could be held constant as the mesh is refined, $O(1)$ scaling, when (1) an

implicit time advancement scheme is used, (2) only the steady solution is of interest, or (3) quasi-steady modes are present. In such cases the lower bound on the cost of a classical simulation is $O(M^3)$ and a quantum simulation is $O(\log(M))$, showing that exponential speed up may be possible. This analysis of quantum computing does not consider the number of required simulations or the gate depth and complexity, however.

The exponential speed up achieved by a quantum algorithm could be lost by the operations required for initializing the quantum register and extracting the solution. Initializing the quantum state could become prohibitively expensive because even the best-known algorithm for preparing an arbitrary m qubit quantum register requires up to $(2^{m+1} - 2m)$ controlled-NOT gates, which is only a factor of 4 larger than the theoretical lower bound.³²² So, the cost of initializing the quantum register scales as $O(M^3)$.

The field variables represented by the amplitudes of the quantum register cannot be read; they can only be estimated to a desired level of precision by repeatedly initializing the quantum register, doing the computations, and measuring the final state of the quantum register. This operation also scales as $O(M^3)$.³¹¹ Because of the enormous cost of input and output operations on a quantum computer, it may not be possible to fully and frequently read all flow field variables. This need not be a showstopper, however. It is often the case that the detailed flow field calculations are only a means for obtaining certain quantities of interest, for example, the pressure drop in a flow device or the mean composition of the products of a reactor. They could be calculated from the flow field with a few qubits, reducing the cost of measurement to $O(1)$.

Another casualty would be *checkpointing*, which is required for long CFD calculations on classical supercomputers. This refers to storing the entire flow field data at specified time intervals so that the calculation can be restarted in the event of a machine failure. There is no direct way to checkpoint quantum calculations because it is not possible to copy quantum states, which is known as the *no-cloning theorem*.²⁰ An alternative is to extract the flow field data into classical bits to a specified precision, which requires $O(M^3)$ memory, and reinitialize the quantum register, which may incur $O(M^3)$ in computational cost.

Finally, handling the nonlinearities in NSE could be problematic because "...nonlinear problems are intrinsically difficult to solve on a quantum computer due to the linear nature of the underlying framework of quantum mechanics".³¹⁶ An approach widely used in classical algorithms is to solve a linearized form of the equations. Another approach proposed by Lubasch et al.³¹⁶ based variational quantum computing requires exponentially fewer resources for storing information than classical computing. Treating nonlinearities in quantum computing is still an outstanding problem.³¹¹

4.4. Quantum Computing for Energy Grid Optimization

The growing complexities of electric grids and their vulnerability to security threats have created a need for transformational changes in the existing grid technologies. The new electric grids are increasingly dependent on renewable energy sources, intermittent loads, subject to extreme weather events, and, importantly, vulnerable to cyber attacks. Furthermore, the electric grid must serve a rapidly increasing number of electric vehicle charging stations. Thus, the reliable and resilient operation of the electric grid requires solving

complex combinatorial optimization problems linking sources of power supply with sinks of power consumption such as homes, industries, and charging stations. Current mathematical optimization algorithms face significant challenges as the number of parameters to be optimized grows. Quantum computing can be a promising alternate platform, which can solve discrete combinatorial optimization problems using algorithms such as adiabatic quantum computation (AQC). Reviews on several aspects of AQC implementation in space exploration problems and on future quantum-enhanced power grid are provided in refs 323 and 324. AQC could also be made more efficient by combining a machine learning approach. In ref 325, the authors present that the quantum behaviors could be integrated into a support vector regression method to improve the load forecasting accuracy. Quantum-behaved particle swarm optimization algorithms, which have been already applied for forecasting a financial market, could also be implemented for load forecasting in power grid problems.³²⁶ The quantum computing model used in CFD (see section 4.3) could also be implemented in designing wind turbines for wind power. Cybersecurity has become a new challenge because of the transition from a traditional to a smart grid in power systems. The data transfer and storage required for smart grid operations need to be protected from cyber-attacks. Quantum cryptography could be implemented to secure data transfer with the highest level of security.

4.5. Quantum Simulations in Areas of Physics, Chemistry, and Engineering

Several problems are either intractable to classical computers or are experimentally inaccessible. Problems including Hubbard models, quantum chemistry calculations, lattice gauge theories, and spin frustration and disorder are beyond the capability of current classical computers. Many of these problems are within the reach of quantum simulators using limited resources. Here, we discuss relevant applications of both analog and digital quantum simulators in different areas of physics, chemistry and engineering.

4.5.1. Condensed Matter Physics. A number of problems remain largely unsolved in condensed matter physics. Problems including the understanding of high- T_c superconducting and frustrated systems challenge current state-of-the-art computing and experimental approaches. Here, we briefly describe major problems in condensed matter physics where quantum simulation can be useful for their study. Solutions of these problems can greatly benefit energy applications by solving chemical properties of materials that would otherwise be either computationally expensive or impossible to probe.

(i) *Hubbard Model.* The first such problem is the Hubbard model, which is the simplest model of interacting many-particle systems in a lattice. The one-dimensional Hubbard model can be solved using classical computers, but higher dimensional Hubbard models quickly exceed the capabilities of classical computers. Using an analog simulation, Jakusch³²⁷ proposed a solution to the Bose-Hubbard model in optical lattices that was later implemented by Greiner et al.³²⁸ Somma et al. implemented the Hubbard model using a digital quantum simulator and demonstrated how to obtain the energy spectrum.²³⁰

(ii) *Spin Model.* Another important but classically intractable problem is the spin model, which also can be simulated using a quantum simulator.³²⁹ Under certain conditions, the

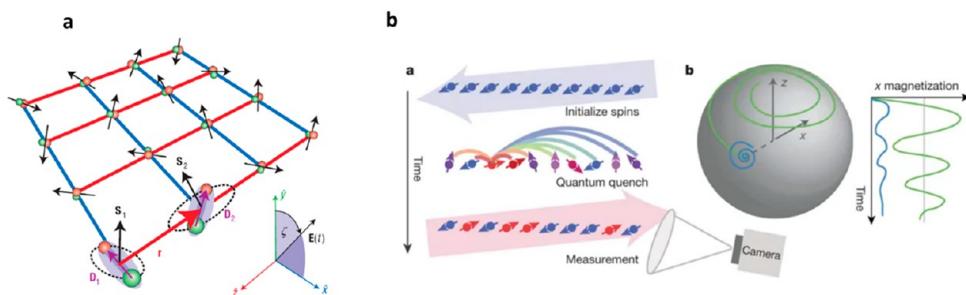


Figure 25. (a) Schematic of the anisotropic spin model for polar molecules trapped in an optical lattice (a 2D square lattice with nearest-neighbor orientation-dependent Ising interactions). Reprinted with permission from ref 332. Copyright 2006 Springer Nature. (b) Illustration for dynamical phase transitions in the Ising model with long-range interactions. Reprinted with permission from ref 42. Copyright 2017 Springer Nature.

Hubbard model reduces to the spin model. Therefore, the spin model can also be simulated using a digital quantum simulator as in the case of the Hubbard model. A digital quantum simulator was used in a trapped-ion experiment that demonstrated efficient simulation of the spin Hamiltonian using sequences of elementary gates.²²³ An array of gate-defined semiconductor quantum dots was also implemented recently to simulate the Hubbard model.^{330,331} Electrons excited in arrays of quantum dots can mimic a situation like many-particle systems in a lattice.

(iii) *Quantum Phase Transition.* Quantum phase transition occurs under certain limiting conditions at near zero temperatures when quantum fluctuations vanish. At low temperatures, materials show a variety of interesting properties entirely governed by quantum laws such as a phase transition from superfluidity to Mott insulator, and from a paramagnet to an antiferromagnet. Friedenauer et al. emulated the transition from a paramagnet to an antiferromagnet using two trapped calcium ions.³³³ Quantum simulation was also demonstrated in experiments for antiferromagnetic spin chains using neutral atoms in an optical lattice.³³⁴ Scientists have used a 53 qubit quantum simulator to study nonequilibrium dynamics in the Ising model with long-range interactions and observed a sudden phase change in a regime to which classical statistical mechanics do not apply. This is shown in Figure 25. In this experiment, spins are represented by trapped ions.⁴²

(iv) *Superconductivity.* Similarly, a high-temperature superconductor such as a compound containing copper-oxide (CuO_2) planes is another domain that can exploit analog quantum simulations.^{335,336} The study of the Bardeen–Cooper–Schrieffer (BCS) model of superconductivity can be conducted using digital quantum simulation. The BCS Hamiltonian was modeled using polynomial-time algorithms,³³⁷ and a version of this algorithm with 2 qubits was experimentally realized.³³⁸

In addition to the applications described above, a myriad of the problems in condensed matter physics, such as anyons in topological materials,³³⁹ tunable metamaterials,³⁴⁰ spin glasses,³⁴¹ and disordered and frustrated systems^{342,343} can be studied using quantum simulators. Of those, topological materials feature several properties that make them robust against certain impurities as well as the loss of coherence and are therefore considered as future candidate materials for quantum computing.

4.5.2. Quantum Chemistry. Quantum chemistry studies the electronic structure of molecules and materials, providing information on how they associate and dissociate, absorb light, and interact with other molecules and materials. As

demonstrated in Figure 19, realizing quantum chemistry on quantum computers is one of the near-term goals of quantum computing. Several recent reviews have addressed the developments of quantum algorithms and provide an overview of quantum computational chemistry and quantum materials science.^{65,67,248,344–347} A number of quantum chemistry problems including thermal rate constants, atomic and molecular energy eigenvalues and wave functions, and chemical reactions can be studied using quantum simulators. Digital quantum simulators are currently the most promising avenue for addressing quantum chemistry problems because most of the chemical proposals assume a universal quantum computer. To date, strongly correlated systems remain a challenge in electronic structure simulation. Quantum chemists have tried using the full configuration interaction (CI) method; however, when using the CI method, an accurate simulation is beyond the reach of classical computers.

Because an arbitrary unitary operation acting on a system with n spins has $2^n \times 2^n$ free parameters, such an operation would require an exponential number of elementary quantum gates to implement. However, natural systems can be solved in a finite dimensional Hilbert space. The interactions involved are local, which facilitates the efficient simulation of crucial parts of their structures. That means the Hamiltonian can be simply written as a sum: $H = \sum_i H_i$. This enables us to write the unitary operation into time-steps using the Lie-Trotter formula. The time it takes to perform the simulation scales as a polynomial in simulated time t .

There are two ways to describe quantum mechanical wave functions while preparing or initializing the states: first and second quantization.²⁰⁵ First quantization has better asymptotic scaling and requires fewer gates whereas second quantization has a compact wave function representation and requires fewer qubits. Second quantization is relatively easy to implement experimentally because this description is natural to represent the interaction. It should be noted that first quantization is a conventional way of presenting the Hamiltonian, whereas the second quantization is required to write interaction in the operator's form that creates and annihilates particles called creation (a^\dagger) and annihilation (a) operators. Quantum simulations of chemical processes can be realized using several different systems. Some of the major systems are explained here briefly.

(i) *Quantum Chemistry Simulation Using Trapped Ions and Ultracold Atoms.* Long-range hopping can be implemented by creating a wide trap potential and overlapping to all different optical lattice sites.^{348,349} In the NSF report for quantum information and computation in chemistry,¹⁷³ two

approaches were identified to build a fermionic simulator for the quantum simulation of electronic structure: (a) a potential-based approach and (b) an operation sequence approach. In the first approach, ultracold atoms in an optical lattice are used to directly emulate the behavior of molecules whereas in the second approach, operations performed over time are executed on ultracold atoms, which would allow for the simulation of molecular fermionic interaction terms. Figure 26 shows the

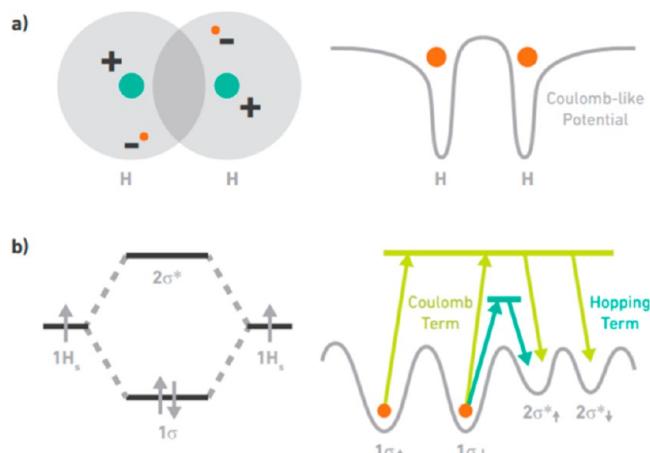


Figure 26. Example of the potential-based approach (a) and the operation sequence approach (b). See text in ref 352 for the details.

mapping of H_2 molecules in a minimal basis set to elements in an optical lattice. The potential landscape in the operational-based approach in the optical lattice mimics the Coulomb potential generated by nuclei, in which ultracold atoms play the role of electrons. The optical lattice sites in the operation sequence approach represent orbitals of the molecule.^{350,351}

Trapped ions and ultracold atoms are highly controllable technologies available today. Qubits can be encoded in the quantum states of cold trapped ions. In a recent study by Argüello-Luengo et al.,³⁵³ an analog approach has been implemented that combines state-of-the-art ultracold technology with cavity QED to engineer Coulomb interactions. Studying Coulomb interactions usually poses a significant challenge in quantum chemistry (Figure 27). In the study, Argüello-Luengo et al. also tested their approach using an H_2 molecule. Chemical reactions can also be simulated using ultracold atoms in a waveguide.²¹²

(ii) *Quantum Chemistry Simulation Using a Photonic System.* Alongside trapped ions and ultracold atoms, the photonic approach provides another excellent test bed for the study of material electronic properties. Not only does the photonic approach offer a variety of opportunities for the simulation of material properties, it also provides a natural platform for building a universal quantum computer. Photonic quantum architecture was first used by Lanyon et al. to study the H_2 molecule, which is a minimal basis-model.³⁷ Qubits were encoded in photon polarization. Two qubits were sufficient for the case of two spin-orbitals for each hydrogen atom. It demonstrated that the quantum phase estimation algorithm could produce accurate bonding and excitation energies.

Experimental efforts have focused on the variational quantum eigensolver (VQE) algorithm. Peruzzo et al.¹¹³ performed the first VQE experimental demonstration in 2014. This experiment used a 2 qubit photonic chip to

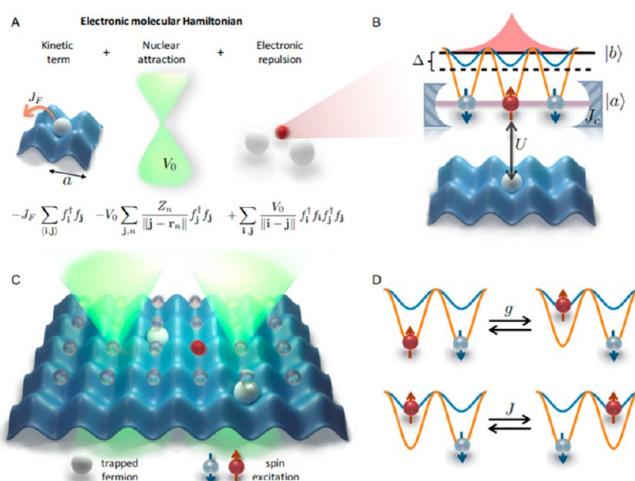


Figure 27. Illustration of an analog quantum simulator for quantum chemistry problems. Panels A, B, and D represent the Hamiltonian for the electronic structure, Coulomb repulsive interaction, and the exchange interaction, respectively. Panel C represents the model simulator for a H_2 molecule. Reprinted with permission from ref 353. Copyright 2019 Springer Nature.

variationally minimize the energy of a HeH^+ molecule. Since then, a number of experiments and algorithms have been developed as a proof-of-concept by implementing quantum architectures in simple molecular structures such as lithium hydride (LiH) and beryllium hydride (BeH_2).¹⁷³

(iii) *Quantum Chemistry Simulation Using NMR Techniques.* Nuclear spins can be used as qubits, and can be manipulated and read out using NMR techniques. Nuclear spin qubits can be employed to simulate electronic properties and chemical reaction dynamics in quantum chemistry.³⁵⁴ The first experimental simulation was performed using NMR for a harmonic oscillator.³⁵⁵ In numerous studies after that pioneering experiment, NMR has been employed to simulate atomic and molecular structures.^{338,356,357}

Du et al. reported an NMR implementation to simulate a H_2 molecule in a minimal basis to obtain its ground-state energy as shown in Figure 28.³⁵⁸ The research team used an iterative NMR interferometer to measure the phase shift. In the experiment, they achieved 45 bits of precision (i.e., 15 iterations of PEA with 3 bits per interaction). The proof-of-principle experiments on simulating the chemical dynamics of a laser-driven isomerization demonstrated the feasibility of using NMR as a quantum simulator that could easily outperform classical computers.^{359,360} NMR-based quantum simulators have also been used to probe photosynthesis pathways. Photosynthetic processes are challenging problems to understand because pigment–protein complexes are intrinsically open quantum systems where the system-bath couplings are comparable to the intrasystem couplings. Because quantum simulation has the power of probing the dynamics of 2^N states with N qubits, the NMR technique could be implemented for the complex photosynthetic Hamiltonian to verify theoretical predictions.³⁶¹ In 2018, a system with $\log_2 N$ qubits using an NMR technique could effectively simulate a system with an N -chromophore photosynthetic complex with arbitrary structure and bath spectral density. A 2 qubit NMR system was utilized to demonstrate the coherent oscillations in a short-time scale and the overall thermalization process in a long-time scale.³⁶²

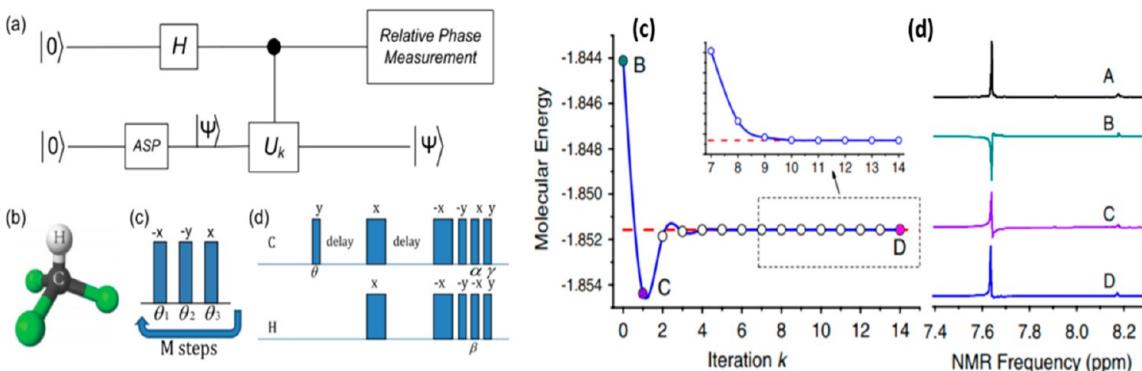


Figure 28. Schematic circuit for calculating molecular energies (a). A quantum register for CHCl_3 (b). Pulse sequences for the ^{13}C nucleus (c). Pulse sequence to implement the controlled- U_k operation (d). Energy values for 15 iterations (c,d). The blue line represents the spline fit of experimental values, and the dashed red line represents the theoretical D expectation (c). The reference spectrum A that denotes the initial state, and B–D represent iterations 0, 1, and 14 (d). Reprinted with permission from ref 358. Copyright 2010 American Physical Society.

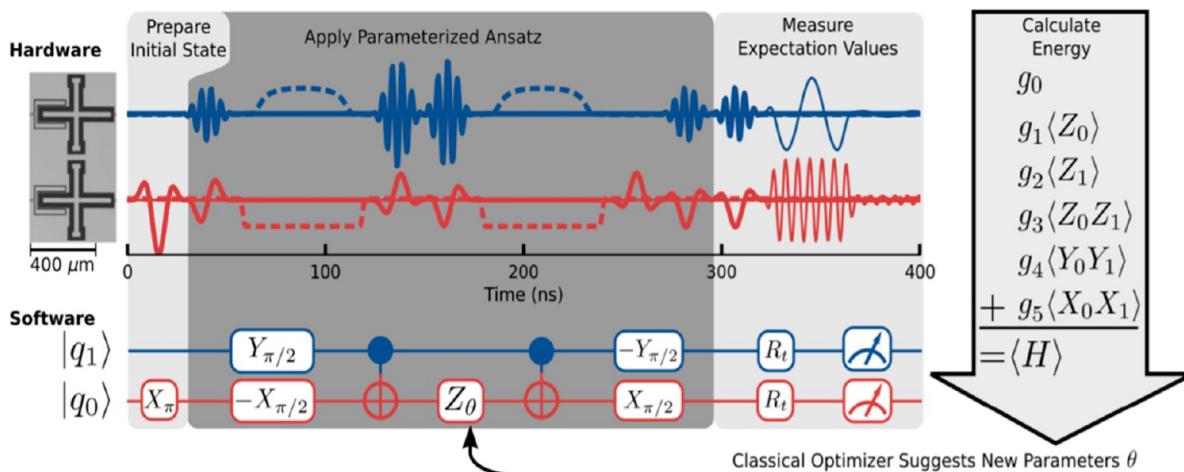


Figure 29. Schematic of the hardware and software for VQE implemented using a superconducting circuit. Reproduced from ref 363 under the terms of the Creative Commons Attribution 3.0 license. Copyright 2016 American Physical Society.

(iv) *Quantum Chemistry Simulation Using a Superconducting System.* Superconducting systems stand as top candidate systems for simulating complex chemical processes. A clockwise or counterclockwise circulating current in a submicrometer-sized loop of a superconducting material can be employed as a qubit. As demonstrated in Figure 29, Malley et al. used a programmable array of superconducting qubits to compute the energy surface of a H_2 molecule using two distinct quantum algorithms: VQE and canonical quantum algorithm.³⁶³

Scientists at IBM implemented VQE in a quantum processor that was combined with a compact encoding of a fermionic Hamiltonian and stochastic optimization routines to determine the ground state energy for molecules of a size up to BeH_2 .¹⁷³ They simulated up to a 6 qubit Hamiltonian, and further probed the problem of quantum magnetism. In section 3, we provide a detailed description of the quantum simulation approach for more relevant and advanced platforms that appear as quantum computers and could be applied to quantum chemistry.

4.5.3. Atomic and Nuclear Physics. Energy levels in neutral atoms are discrete and those levels can be manipulated using visible or microwave photons. They show a coherent oscillation between two levels. In this view, neutral atoms have quantum characteristics that overlap with artificial atoms such

as superconducting loops. Applied microwaves or voltages induce electric and magnetic fields across the Josephson junctions that control electron tunneling in the superconductor. This is analogous to the Stark and Zeeman effect under applied electric and magnetic fields, respectively, in neutral atoms. Neutral atoms offer the advantage of weak coupling with the environment,²³⁵ but their intrinsic properties cannot be tuned with respect to geometry by artificial means (using techniques such as lithography). One promising atomic physics model is the Jaynes–Cummings Hamiltonian that describes the interaction of a single mode of an electromagnetic field with a two-level system. This can be simulated using superconducting circuits.^{364,365}

Nuclear physics involves many-body problems with a large number of nucleons interacting with each other. The quantum simulation naturally exhibits long-range behavior and, hence, could potentially be engineered to yield nuclear potentials with intrinsic long-range components,^{41,42} such as those that occur, for example, in pion exchange. The Schwinger model for gauging degrees of freedom could also benefit from quantum simulation.³⁶⁶

4.5.4. High Energy Physics and Cosmology. Boghosian et al., in 1998, proposed a quantum simulator to study relativistic quantum systems.³⁶⁷ In 2007, Bermudez et al. suggested experimental mapping between a 2+1-dimensional

Table 9. Overview of National and Regional Investments into QIS-Related Research

country/ region	QIS investment(s)	source
United States	provided \$1.3 billion dollars from 2019 to 2023 for QIS research as part of the National Science and Technology Council's <i>The National Strategic Overview for Quantum Information Science</i>	381,382
United Kingdom	funded £385M for four multi-institution research "hubs" for QIS-related research, encompassing industry, academia, and government institutions as part of the UK National Quantum Technology Programme (NQTP)	383
Germany	provided €650M in funding from 2018 to 2022 to promote the development and commercialization of quantum technologies	384
European Union	announced in 2018 an investment of €1.3B over 10 years for QIS research in four main pillars: communication, sensors, simulation, and computers	385
China	provided \$987 million in QIS funding over the past 10 years, and announced the \$337 million "Quantum Control and Quantum Information" project, which led to the launch of the quantum science satellite Micius; the satellite that has three main missions: satellite-to-ground QKD, testing of satellite-based quantum nonlocality, and testing of ground-to-satellite quantum teleportation	386–388
Japan	announced Q-LEAP, a \$200 million initiative focused on the development of quantum computing, sensors, and pulsed lasers	389
Australia	contributed to an \$83M AUD investment for the production of a 10 qubit quantum integrated circuit, with an estimated completion date of 2022	390
Canada	created a National Quantum Strategy, investing \$360 million for QIS development over a 7 year period	391,392
Russia	announced the investment of \$790 million over 5 years for QIS research	393
India	budgeted \$1.12 billion over 5 years for quantum technology development	394
Brazil	created the Latin American Quantum Computer Center to develop the region's quantum workforce and use an in-house quantum simulator for chemical and biological research	395,396
Africa	established "Quantum Leap Africa", a research center focused on research and workforce development in the area of quantum information science	397,398
South Africa	announced in 2021 the establishment of "South Africa Quantum Technology Initiative" with a \$5 million annual budget for quantum research	397,398
South Korea	designated ~\$40 million over 5 years for quantum computing architectures	399,400
United Arab Emirates	announced construction of a quantum computer in 2021 in Abu Dhabi	401
Israel	allocated in 2021 \$60 million to build a quantum computer	402
France	established €1.8 billion to fund quantum computing, sensing, and communications research over a 5 year period	403
Singapore	established the Center for Quantum Technologies in 2007	404
Taiwan	announced \$282 million in funding over a 5 year term for quantum computing experimentation	405
Netherlands	announced the investment of €615 million over 7 years to bolster domestic quantum computing innovations	406

Dirac model and the Jaynes–Cummings model using a trapped ion experiment.³⁶⁸ Lamata et al. studied the Dirac equation in the 3+1 dimension for a spin-1/2 particle using a single trapped ion.³⁶⁹ This study demonstrated the possibility of studying effects such as Zitterbewegung and the Klein paradox. Zitterbewegung particles have never been observed in their relativistic form but have been simulated using trapped ions.³⁷⁰ The Klein paradox arises when the barrier energy is equivalent to a particle's mass, and the barrier becomes transparent. The Klein paradox has also been simulated using trapped ions.³⁷¹ The lattice gauge theory was simulated using a digital quantum simulation.³⁷² A chain of trapped ions was used to simulate the Schwinger model, highlighting the possibility of using quantum simulation where gauge symmetries play a prominent role.³⁷³ Semiao et al. proposed a quantum circuit for nucleon state simulation,³⁷⁴ which estimated the requisite computational resources using a photonic network design. Recently, a proposal for the analog simulation of simple lattice gauge theories was provided. The dynamics in lattice gauge theories could be mapped onto spin–spin interactions in 1 + 1D QED, 2 + 1D Abelian Chern–Simons theory that is coupled to fermions, and pure Z2 gauge theory.³⁷⁵

Similarly, cosmology problems such as Hawking radiations can also be simulated using the superconducting circuit model. Analogs of Hawking radiation were studied using atoms in superconducting circuits,³⁷⁶ exciton–polariton superfluid in semiconductors,³⁷⁷ and with ultrashort pulses of light in optical fibers.³⁷⁸ In a recent experiment, a 4 qubit NMR was used experimentally to simulate spin-network states by a space-time tetrahedral.³⁷⁹ This experiment served as a first step toward the

Feynman diagram vertex in the formulation of loop quantum gravity.

In addition to the aforementioned applications, several other applications can use quantum simulations to study system dynamics. One example is an open quantum system. Compared to a closed quantum system, simulating the dynamics of an open quantum system is a more formidable challenge. The Lindblad equation required to solve an open quantum system is quadratically more resource-consuming than solving the Schrödinger equation for the same physical system. In recent studies, trapped ions and linear optics were implemented to engineer the open quantum system using the dissipative preparation of entangled states.^{232,380} Quantum chaos and optical interferometry are also possible areas where quantum simulation can be implemented. An excellent review on quantum simulation for quantum chaos and optical interferometry is given in ref 13.

5. FURTHER CHALLENGES AND OUTLOOKS

5.1. Global Quantum Initiatives

A number of research centers and their physics, chemistry, engineering and material sciences departments around the world are pursuing QIS as a major research and development direction. This has significantly increased outcomes in the field and has also elicited, at a policy level, the continuous distribution of financial support to achieve realistic goals on implementing QIS successfully in high-priority areas like security and safety.

Global investments into QIS-related research have increased drastically over the past five years.¹⁵ Table 9 provides an overview of how nations around the globe have invested in

QIS research, whereas Figure 30 highlights the rapid growth of QIS research and development (R&D) funding from fiscal years 2019–2022.

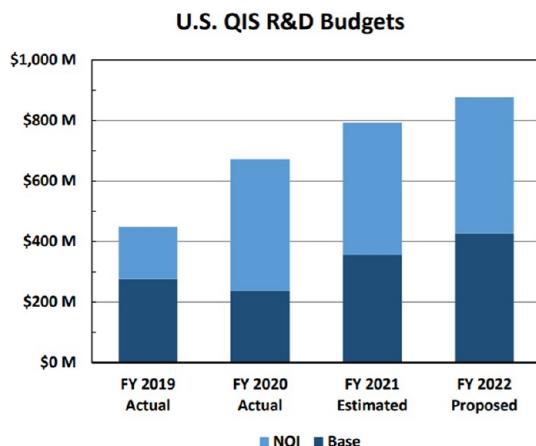


Figure 30. U.S. R&D budgets for QIS since the inception of the NQIA.⁴⁰⁷ The bar heights represent the total budget for each fiscal year. The portion of each bar marked “NQI” identifies funding allocated for NQIA-authorized activities; this funding is additional to the budgets for baseline QIS R&D activities. Increases reflect the Administration’s priority to grow QIS R&D.

Taken together, massive investments in quantum computing in every region of the world highlights the ever-increasing importance of QIS in the scientific strategies of nations across the globe. These investments are poised to create quantum computing infrastructure worldwide while also producing significant human capital in the areas of QIS. These investments will be particularly important in addressing challenges pertinent to energy applications, as outlined in next section.

5.2. Further Opportunities and Challenges

This review highlights the importance of QIS for future innovations within the energy sector, particularly through continued development of and increased access to quantum computers and simulators. Indeed, quantum computers have already been used to model chemical reactions, and as this technology continues to develop it may have transformative implications for material design and discovery. The ability to model large-scale systems and rapidly screen various material properties will have significant implications for the energy sector, where materials are continually being sought to improve greenhouse gas capture, catalyze new reactions, and selectively detect analytes of interest in harsh conditions. Once again, significant work is needed to not only improve performance of existing quantum computer designs, but also to lower production and operating costs and to increase accessibility in general.

Controlling the time evolution of complex dynamical systems characterized by the entangled quantum states in physical hardware registers is a decades-long challenge in QIS. Achieving quantum supremacy, and demonstrating quantum computations that outperform classical computations, has been a recent driving force for the QIS community. The near-term goal is to achieve a quantum device that simulates dynamic systems that classical devices cannot.¹⁰⁷

New developments in quantum platforms can be broadly categorized into directions of material science and quantum

devices. Qubits in superconducting platforms are typically fabricated by sandwiching aluminum and its oxide materials ($\text{Al}/\text{AlO}_x/\text{Al}$).^{408,409} These materials offer the advantage of low current leakage at the Josephson junction and simplicity of laboratory fabrications in the sandwich structure due to the low-temperature melting point of Al. Other common superconducting materials are niobium (Nb) and nitride based alloys (TiN and NbTiN). The substrate selection also requires attention. At the GHz frequency, ions and dipoles can absorb energy if the material has high dielectric loss and the absorbed energy is emitted as phonons. Such phonons could be detrimental to qubit operation. Despite promising attempts in the development of superconducting qubits, scaling qubits remains a major hurdle in reducing noise in quantum computer with several qubits. Temporal and spatial frequency variation can result in calibrating the quantum gates.^{410–413} In addition, noticeable changes in critical currents across the junction can cause a variation in the frequency.

Color centers such as the NV center in a nanodiamond are optically addressable qubits with coherence times of several milliseconds in room temperature.^{414,415} GHz pulses can be used to control the qubit states. Single- and double-qubit gates in color centers in nanodiamond have been shown to exhibit the highest fidelity (99.99% and 99.20%).⁴¹⁶ However, NV centers are difficult to fabricate due to the poor optical properties, such as hardness and low reactivity, incompatibility with the advanced communication fiber optics, and scalability. As a result, practical applications of color centers in quantum computing devices remain challenging. Defects and fluctuating nuclear spins in the background are additional sources of noise in the color centers. Alternate color centers are being explored, including nuclear spin free host material in rare earths and transition metals.^{417–419}

Topological materials offer another robust qubit-hosting platform that is immune to noises and dissipations. Topological photonic states are the surface states arising on the interface between two media with a different Chern number that occur, for instance, for materials with a broken time reversal symmetry.^{420,421} These types of states can be used to transmit quantum information over significant distances, such as in energy infrastructure, without suffering scattering losses due to material and surface imperfections. Topological designs using magneto-optic photonic crystals and coupled resonators have been experimentally demonstrated.^{422,423} Currently, this is an active field of research with many emerging approaches to realizing topological photonic states that are immune to scattering. The class of qubits realized in the topological materials are based on the non-Abelian anyons, as proposed by Kitaev.⁴²⁴ Anyons are neither fermion nor boson and obey non-Abelian statistics. Quantum computation using topological qubits are carried out by braiding the quantum processes, which are topologically protected from perturbations, back scatterings and phonons. Indeed, practical realization of such a quantum platform opens pathway to build long-sought fault-tolerant quantum computation. Several experiments have been conducted in an attempt to search for Majorana zero modes (MZMs) at the interface of topological/superconductor materials such as $\text{Bi}_2\text{Se}_3/\text{NbSe}_2$ ^{425,426} and Cr-doped $(\text{Bi},\text{Sb})_2\text{Te}_3/\text{Nb}$.⁴²⁷ MZM are zero energy modes that are believed to occur at the edge of nanowires. Non-Abelian anyons are supposed to be realized in systems with MZMs. Despite a number of attempts, the

observation of MZMs in experiments is still debated in condensed matter physics.

Rydberg atoms have been widely investigated and have been implemented in recent years in order to perform quantum simulation. Rydberg atoms are highly excited valence electrons with high electric dipoles and strongly interact with microscopic external fields.^{428,429} The interactions in Rydberg atoms can be easily controlled and tuned in the laboratory, which makes them candidate systems for future quantum simulation. Neutral atoms are of particular interest due to their uniformity, ease of scale up, long coherence time and tunable interactions mediated by Rydberg states. Such interactions can be mapped to the interaction between photons, which could open possibilities for photonic quantum computation and information processing that are carried out by remotely transmitting information encoded in photonic states. Neutral atoms with Rydberg interactions are also used to prepare highly entangled states. This has been shown in the recent work with 20 qubits GHZ state generation in quasi adiabatic driving.⁴³⁰ Despite these promising applications, an urgent need exists to circumvent limitations imposed by the small blockade of optical depth in the experiments. Development of novel methods to improve fidelity on optical depth offers great promise.^{431–433}

Cavity QED is an alternative quantum photonic subfield that carries great potential for future novel quantum phenomenon. By analogy with the Nong–Ou–Mandel effect, nonclassical cavity interactions with the environment can lead to new physics and applications that are highly applicable for energy purposes. As an example, we can mention the recently reported appearance of localized topological edge states in an array of coupled photonic resonators with interacting photon pairs,⁴³⁴ as well as quantum gates realized using hybrid cavity/photon and NV centers.⁴³⁵ Multiparticle entanglement required for scalable quantum computing can also be readily produced with cavity–QED interactions.⁴³⁶

Cluster state quantum computing is an alternative to the common direct cascaded quantum gate approach which has been gaining momentum recently.⁴³⁷ Cluster state is a special entangled many qubit state which is commonly prepared as a photonic state where qubits are encoded in a photon degree of freedom such as polarization or quadrature.^{438,439} A sequence of single qubit operations is applied and the state can be collapsed in a one-way fashion to produce a useful output. It has been shown that traditional quantum gates can be efficiently simulated in cluster states.⁴⁴⁰ Reports of very large cluster states capable of fault-tolerant quantum computation have been published recently.⁴⁴¹

As R&D on quantum computing hardware and software continues, engineers and scientists have begun to explore opportunities for the applications of quantum computing in the energy sector sector.^{17,442–444} Some examples of proposed applications of quantum computing in the energy industry are listed below:

(1) Materials for Energy Applications. A promising area of research is on materials for next generation batteries, the critical components of electric vehicles and energy storage systems. For example, the solid electrolyte interphase (SEI) that forms on the anode of a lithium-ion battery is a key determinant of the battery's long-term performance. Yet SEI formation is poorly understood because of the limitations of existing modeling techniques such as DFT and experimental techniques. Quantum computing holds promise in finely

resolving the complex reaction paths involved in SEI formation, enabling the industry to design better batteries.⁴⁴⁵ Daimler and Mitsubishi Chemical are independently partnering with IBM to advance battery technology using quantum computing, Daimler on lithium–Sulfur battery technology and Mitsubishi on lithium–air battery technology.⁴⁴⁶ ExxonMobil has been partnering with IBM to use quantum computing for materials simulations for eventually designing materials such as MOFs used for decarbonizing electricity generation.⁴⁴⁷

(2) Electric Grid Operation. The electric grid—a network of transmission lines, substations, transformers, and other components that deliver electricity from the power plant to homes and businesses—is being transformed by its growing number of renewable energy sources, such as solar and wind energy sources. Unlike fossil and nuclear power plants that steadily supply electricity to the grid, renewable energy sources are intermittent, supplying electricity only, for example, when the sun shines or wind blows. Thus, the reliable and efficient operation of the grid, requiring real time decision making, is becoming an increasingly complex task that could be aided by quantum computing.^{443,444,448}

Electric grid operators continually need to identify and deploy the best electricity generating units so that the total operational cost is the lowest for meeting the forecasted electric power demand, while also satisfying several other constraints.^{443,444} Quantum computing could be used to solve this unit commitment problem.^{449,450}

Electric grid operators need to rapidly respond to power outages caused by natural or man-made events. The operators must determine where and when to deploy equipment and personnel. This complex planning task that must be conducted in real time could be assisted by quantum computing. Commonwealth Edison Company, the electric utility in northern Illinois and Chicago, recently initiated an effort on the use of quantum computing for power systems modeling and decision-making.^{442,451}

(3) Energy Asset Optimization. Siting energy plants is a challenging computational task. For example, wind farms must be sited where the wind flow is high as well as where the electrical grid is readily accessible. Solar or wind farms need to be sited such that their startup costs are low. Quantum computing could help solve such location-allocation problems.^{450,452}

Heat exchanger network synthesis (HENS) is a challenging computational problem that could benefit from quantum computing.⁴⁵⁰ The goal of HENS is to reduce the energy consumption of an industrial plant, while also minimizing the total capital cost of the plant. This requires determining the optimal network of heat exchangers for transferring energy between process streams or between process streams and utility streams (e.g., steam, cooling water) to heat or cool the process streams.

(4) Logistics and Scheduling. ExxonMobil has been considering the use of quantum computing to solve maritime inventory routing problems for reducing the cost of supplying petroleum products from multiple ports to multiple customers within a certain time window.^{447,453}

The electric power company Enel has been considering the use of quantum computing to speed up dispatch management with the goal of reducing the traveling time of workers compared to their working time, when more than 32 million jobs are annually dispatched to tens of thousands of

fieldworkers and contractors in 13 distribution companies across the company.⁴⁴⁶

(5) **Customer Analytics.** Electric power companies have access to large amounts of data from smart homes that provide homeowners convenience and cost savings by allowing them to control appliances, thermostats, lights, and other devices remotely. The companies may use quantum computing to analyze this data and improve their operations.⁴⁴²

(6) **Expanding reservoir production.** Imaging subsurface and analyzing seismic data for oil and gas exploration could be amenable to quantum computing.⁴⁴⁷ Quantum computing may be used to better understand the flows in subsurface through reservoir simulations that consider molecular-scale physics in tight reservoirs.⁴⁵³ Quantum computing can be used for modeling the chemistry and buildup of various types of clay in hydrocarbon wells to help improve oil and gas production.⁴⁵⁴ Finding solutions to corrosion and solid formations in pipelines could improve safety and reduce costs in oil and gas production.⁴⁵⁵

Oil field development requires decisions about where to place oil wells in a sequence governed by the availability of drilling equipment. The objective is to increase the value at each well location, while reducing the drilling costs. This challenging optimization problem could be solved with the help of quantum computers.⁴⁵⁵

(7) **Fluid Dynamics.** Simulating the fluid flow is important in many energy applications such as chemical reactors used in oil refining, pipelines that transport various fluids (e.g., oil, gas, H₂, CO₂), ocean dynamics for offshore drilling platform design, and the airflow in wind farms.^{447,449,454} Qubit Engineering, for example, is using Microsoft Azure Quantum for simulating airflow around windmill rotors for providing wind farm developers with optimized turbine layout designs.⁴⁴⁹

6. CONCLUSIONS

The discovery, production, transportation, and consumption of energy impacts nearly every aspect of society, and an attempt to meet the world's ever-evolving energy needs has driven unprecedented levels of technological innovations. Hence, the energy sector will likely be among the first beneficiaries of the impending "quantum revolution", as emerging QIS-enhanced technologies may be applied to ensure the safe, secure, and efficient use of energy resources.

A variety of systems, such as trapped ions, atoms in optical lattices, polar molecules, quantum dots, nuclear spins, and superconducting circuits, have been shown as promising candidates for quantum simulation. A number of complex quantum systems from quantum chemistry and condensed matter physics have been simulated with the quantum computer, which would otherwise be unfeasible with classical computers. Quantum simulation may open avenues in solving specific problems that have a high impact in fossil energy but pose severe computational complexity, such as simulating Haber-Bosch catalytic processes.

Quantum computers, for example, may facilitate the rapid screening of new sorbents for CO₂ uptake or new catalysts for CO₂ conversion. Several material science studies have implemented the quantum computer to study the electronic, optical, and chemical properties of materials. Quantum chemistry is expected to be one of the early areas that can benefit from quantum computing. Quantum algorithms have shown promising results in terms of time and resources while solving several test-stage problems. Integration of quantum

computation to enhance sensor performance is another exciting direction with the potential to benefit the energy sector.^{298,300}

While progress in QIS continues, several challenges exist to its implementation in advancing energy technologies. In addition, a gap exists between the capability of current QIS stakeholders and the needs of the energy sector. A further collation between researchers working in QIS and energy communities will help in addressing specific energy sector needs with the possible quantum technologies. Hence, advances in QIS and energy sector performance are inextricably linked, where the multitude of potential benefits to the energy sector from QIS will drive additional QIS-related research.

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Notes

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REFERENCES

- (1) Rieffel, E.; Polak, W. *Quantum Computing: A Gentle Introduction*, 1st ed.; MIT Press: Cambridge, MA, 2011.
- (2) Benioff, P. The computer as a physical system - a microscopic quantum-mechanical hamiltonian model of computers as represented by turing-machines. *J. Stat. Phys.* **1980**, *22*, 563–591.
- (3) Benioff, P. Quantum-mechanical models of turing-machines that dissipate no energy. *Phys. Rev. Lett.* **1982**, *48*, 1581–1585.
- (4) Bennett, C. H.; Bernstein, E.; Brassard, G.; Vazirani, U. Strengths and weaknesses of quantum computing. *Siam Journal on Computing* **1997**, *26*, 1510–1523.
- (5) Das, A.; Chakrabarti, B. K. Colloquium: Quantum annealing and analog quantum computation. *Rev. Mod. Phys.* **2008**, *80*, 1061–1081.
- (6) Ekert, A.; Jozsa, R. Quantum computation and Shor's factoring algorithm. *Rev. Mod. Phys.* **1996**, *68*, 733–753.
- (7) Jaynes, E. T. Information theory and statistical mechanics. *Phys. Rev.* **1957**, *106*, 620–630.
- (8) Hayashi, M. *Quantum Information Theory: Mathematical Foundation*; Springer, 2017.
- (9) Shannon, C. E. A Mathematical Theory of Communication. *Bell Labs Technical Journal* **1948**, *27*, 379–423.
- (10) *Quantum Computing: Progress and Prospects*; The National Academies Press: Washington, DC, 2019; pp 1–272.
- (11) Report to Congressional Addressees: Quantum Computing and Communications—Status and Prospects. *United States Government Accountability Office*; <https://www.gao.gov/assets/gao-22-104422.pdf> (accessed 2022-01-05).
- (12) Arute, F.; Arya, K.; Babbush, R.; Bacon, D.; Bardin, J. C.; Barends, R.; Biswas, R.; Boixo, S.; Brandao, F. G. S. L.; Buell, D. A.; Burkett, B.; Chen, Y.; Chen, Z.; Chiaro, B.; Collins, R.; Courtney, W.; Dunsworth, A.; Farhi, E.; Foxen, B.; Fowler, A.; Gidney, C.; Giustina, M.; Graff, R.; Guerin, K.; Habegger, S.; Harrigan, M. P.; Hartmann, M. J.; Ho, A.; Hoffmann, M.; Huang, T.; Humble, T. S.; Isakov, S. V.; Jeffrey, E.; Jiang, Z.; Kafri, D.; Kechedzhi, K.; Kelly, J.; Klimov, P. V.; Knysh, S.; Korotkov, A.; Kostritsa, F.; Landhuis, D.; Lindmark, M.; Lucero, E.; Lyakh, D.; Mandrà, S.; McClean, J. R.; McEwen, M.; Megrant, A.; Mi, X.; Michelsen, K.; Mohseni, M.; Mutus, J.; Naaman, O.; Neeley, M.; Neill, C.; Niu, M. Y.; Ostby, E.; Petukhov, A.; Platt, J. C.; Quintana, C.; Rieffel, E. G.; Roushan, P.; Rubin, N. C.; Sank, D.; Satzinger, K. J.; Smelyanskiy, V.; Sung, K. J.; Trevithick, M. D.; Vainsencher, A.; Villalonga, B.; White, T.; Yao, Z. J.; Yeh, P.; Zalcman, A.; Neven, H.; Martinis, J. M. Quantum supremacy using a programmable superconducting processor. *Nature* **2019**, *574*, S05–S10.
- (13) Georgescu, I. M.; Ashhab, S.; Nori, F. Quantum simulation. *Rev. Mod. Phys.* **2014**, *86*, 153–185.
- (14) National Academy of Engineering. *Frontiers of Engineering: Reports on Leading-Edge Engineering from the 2018 Symposium*; The National Academies Press: Washington, DC, 2019; <https://doi.org/10.17226/25333> (accessed 2022-01-05).
- (15) Crawford, S. E.; Shugayev, R. A.; Paudel, H. P.; Lu, P.; Syamlal, M.; Ohodnicki, P. R.; Chorpeling, B.; Gentry, R.; Duan, Y. Quantum Sensing for Energy Applications: Review and Perspective. *Advanced Quantum Technologies* **2021**, *4*, 2100049.
- (16) Degen, C. L.; Reinhard, F.; Cappellaro, P. Quantum sensing. *Rev. Mod. Phys.* **2017**, *89*, 035002.
- (17) Bush, S.; Duan, Y.; Gilbert, B.; Hussy, A.; Levi, J.; Miller, D.; Pooser, R.; Syamlal, M. Fossil Energy Workshop on Quantum Information Science & Technology (QIST) Summary Report. *FE QIST Workshop Report*; DOE-NETL: Pittsburgh, PA, 2020; <https://netl.doe.gov/onsite-research/quest>. DOI: [10.2172/1639026](https://doi.org/10.2172/1639026).
- (18) Manin, Y. *Computable and Uncomputable (in Russian)*; Sovetskoye Radio: Moscow, 1980.
- (19) Feynman, R. P. Simulating physics with computers. *International Journal of Theoretical Physics* **1982**, *21*, 467–488.
- (20) Nielsen, M. A.; Chuang, I. L. *Quantum Computation and Quantum Information*; Cambridge University Press, 2000.
- (21) Deutsch, D. Quantum-theory, the church-turing principle and the universal quantum computer. *Proceedings of the Royal Society of London Series a-Mathematical Physical and Engineering Sciences* **1985**, *400*, 97–117.
- (22) Deutsch, D.; Jozsa, R. Rapid solution of problems by quantum computation. *Proceedings of the Royal Society of London Series a-Mathematical Physical and Engineering Sciences* **1992**, *439*, 553–558.
- (23) Bernstein, E.; Vazirani, U. Quantum complexity theory. *Siam Journal on Computing* **1997**, *26*, 1411–1473.
- (24) Shor, P. W. Algorithms for quantum computation - discrete logarithms and factoring. In *Proceedings of the 35th Annual Symposium on Foundations of Computer Science*; Goldwasser, S., Ed.; IEEE, 1994; pp 124–134.
- (25) Ladd, T. D.; Jelezko, F.; Laflamme, R.; Nakamura, Y.; Monroe, C.; O'Brien, J. L. Quantum computers. *Nature* **2010**, *464*, 45–53.
- (26) Grover, L. K. A Fast Quantum Mechanical Algorithm for Database Search. *Proceedings of the Twenty-Eighth Annual ACM Symposium on the Theory of Computing*; ACM: Philadelphia, PA, 1996; pp 212–219.
- (27) Lloyd, S. Universal quantum simulators. *Science* **1996**, *273*, 1073–1078.
- (28) Quantum Algorithm Zoo; <https://quantumalgorithmzoo.org/> (accessed on 2022-01-05).
- (29) Park, C.; Kim, U.; Ju, C. J.; Park, J. S.; Kim, Y. M.; Char, K. High mobility field effect transistor based on BaSnO₃ with Al₂O₃ gate oxide. *Appl. Phys. Lett.* **2014**, *105*, 203503.
- (30) Maurand, R.; Jehl, X.; Kotekar-Patil, D.; Corra, A.; Bohuslavskyi, H.; Lavieville, R.; Hutin, L.; Barraud, S.; Vinet, M.; Sanquer, M.; De Franceschi, S. A CMOS silicon spin qubit. *Nat. Commun.* **2016**, *7*, 13575.
- (31) Pla, J. J.; Tan, K. Y.; Dehollain, J. P.; Lim, W. H.; Morton, J. J. L.; Jamieson, D. N.; Dzurak, A. S.; Morello, A. A single-atom electron spin qubit in silicon. *Nature* **2012**, *489*, 541–545.
- (32) Kane, B. E. A silicon-based nuclear spin quantum computer. *Nature* **1998**, *393*, 133–137.

- (33) Jones, J. A.; Mosca, M.; Hansen, R. H. Implementation of a quantum search algorithm on a quantum computer. *Nature* **1998**, *393*, 344–346.
- (34) Du, J. F.; Wu, J. H.; Shi, M. J.; Han, L.; Zhou, X. Y.; Ye, B. J.; Weng, H. M.; Han, R. D. Implementation of quantum logic gates by nuclear magnetic resonance spectroscopy. *Chin. Phys. Lett.* **2000**, *17*, 64–66.
- (35) Kim, J. H.; Lee, J. S.; Hwang, T. S.; Lee, S. C. Experimental demonstration of a programmable quantum computer by NMR. *J. Magn. Reson.* **2004**, *166*, 35–38.
- (36) Hanneke, D.; Home, J. P.; Jost, J. D.; Amini, J. M.; Leibfried, D.; Wineland, D. J. Realization of a programmable two-qubit quantum processor. *Nat. Phys.* **2010**, *6*, 13–16.
- (37) Lanyon, B. P.; Whitfield, J. D.; Gillett, G. G.; Goggin, M. E.; Almeida, M. P.; Kassal, I.; Biamonte, J. D.; Mohseni, M.; Powell, B. J.; Barbieri, M.; Aspuru-Guzik, A.; White, A. G. Towards quantum chemistry on a quantum computer. *Nat. Chem.* **2010**, *2*, 106–111.
- (38) Richerme, P.; Gong, Z. X.; Lee, A.; Senko, C.; Smith, J.; Foss-Feig, M.; Michalakis, S.; Gorshkov, A. V.; Monroe, C. Non-local propagation of correlations in quantum systems with long-range interactions. *Nature* **2014**, *511*, 198–201.
- (39) Jurcevic, P.; Lanyon, B. P.; Hauke, P.; Hempel, C.; Zoller, P.; Blatt, R.; Roos, C. F. Quasiparticle engineering and entanglement propagation in a quantum many-body system. *Nature* **2014**, *511*, 202–205.
- (40) Barends, R.; Lamata, L.; Kelly, J.; Garcia-Alvarez, L.; Fowler, A. G.; Megrant, A.; Jeffrey, E.; White, T. C.; Sank, D.; Mutus, J. Y.; Campbell, B.; Chen, Y.; Chen, Z.; Chiaro, B.; Dunsworth, A.; Hoi, I. C.; Neill, C.; O’Malley, P. J. J.; Quintana, C.; Roushan, P.; Vainsencher, A.; Wenner, J.; Solano, E.; Martinis, J. M. Digital quantum simulation of fermionic models with a superconducting circuit. *Nat. Commun.* **2015**, *6*, 7654.
- (41) Martinez, E. A.; Muschik, C. A.; Schindler, P.; Nigg, D.; Erhard, A.; Heyl, M.; Hauke, P.; Dalmonte, M.; Monz, T.; Zoller, P.; Blatt, R. Real-time dynamics of lattice gauge theories with a few-qubit quantum computer. *Nature* **2016**, *534*, 516–519.
- (42) Zhang, J.; Pagano, G.; Hess, P. W.; Kyriyanidis, A.; Becker, P.; Kaplan, H.; Gorshkov, A. V.; Gong, Z.-X.; Monroe, C. Observation of a many-body dynamical phase transition with a 53-qubit quantum simulator. *Nature* **2017**, *551*, 601–604.
- (43) Debnath, S.; Linke, N. M.; Figgatt, C.; Landsman, K. A.; Wright, K.; Monroe, C. Demonstration of a small programmable quantum computer with atomic qubits. *Nature* **2016**, *536*, 63–66.
- (44) Watson, T. F.; Philips, S. G. J.; Kawakami, E.; Ward, D. R.; Scarlino, P.; Veldhorst, M.; Savage, D. E.; Lagally, M. G.; Friesen, M.; Coppersmith, S. N.; Eriksson, M. A.; Vandersypen, L. M. K. A programmable two-qubit quantum processor in silicon. *Nature* **2018**, *555*, 633–637.
- (45) Wright, K.; Beck, K. M.; Debnath, S.; Amini, J. M.; Nam, Y.; Grzesiak, N.; Chen, J. S.; Pisenti, N. C.; Chmielewski, M.; Collins, C.; Hudek, K. M.; Mizrahi, J.; Wong-Campos, J. D.; Allen, S.; Apisdorf, J.; Solomon, P.; Williams, M.; Ducore, A. M.; Blinov, A.; Kreikemeier, S. M.; Chaplin, V.; Keesan, M.; Monroe, C.; Kim, J. Benchmarking an 11-qubit quantum computer. *Nat. Commun.* **2019**, *10*, 5464.
- (46) Wu, Y.; Wang, Y.; Qin, X.; Rong, X.; Du, J. F. A programmable two-qubit solid-state quantum processor under ambient conditions. *Npj Quantum Information* **2019**, *5*, 9.
- (47) Wei, K. X.; Lauer, I.; Srinivasan, S.; Sundaresan, N.; McClure, D. T.; Toyli, D.; McKay, D. C.; Gambetta, J. M.; Sheldon, S. Verifying multipartite entangled Greenberger-Horne-Zeilinger states via multiple quantum coherences. *Phys. Rev. A* **2020**, *101*, 032343.
- (48) Hendrickx, N. W.; Lawrie, W. I. L.; Russ, M.; van Riggelen, F.; de Snoo, S. L.; Schouten, R. N.; Sammak, A.; Scappucci, G.; Veldhorst, M. A four-qubit germanium quantum processor. *Nature* **2021**, *591*, 580–585.
- (49) Bronn, N. T.; Abdo, B.; Inoue, K.; Lekuch, S.; Corcoles, A. D.; Hertzberg, J. B.; Takita, M.; Bishop, L. S.; Gambetta, J. M.; Chow, J. M. Iop, Fast, high-fidelity readout of multiple qubits. In *12th International Workshop on Low Temperature Electronics* **2017**, 834, 012003.
- (50) Tracy, L. A.; Luhman, D. R.; Carr, S. M.; Bishop, N. C.; Ten Eyck, G. A.; Pluym, T.; Wendt, J. R.; Lilly, M. P.; Carroll, M. S. Single shot spin readout using a cryogenic high-electron-mobility transistor amplifier at sub-Kelvin temperatures. *Appl. Phys. Lett.* **2016**, *108*, 063101.
- (51) Vandersypen, L. M. K.; Bluhm, H.; Clarke, J. S.; Dzurak, A. S.; Ishihara, R.; Morello, A.; Reilly, D. J.; Schreiber, L. R.; Veldhorst, M. Interfacing spin qubits in quantum dots and donors-hot, dense, and coherent. *Npj Quantum Information* **2017**, *3*, 34.
- (52) Hornibrook, J. M.; Colless, J. I.; Conway Lamb, I. D.; Pauka, S. J.; Lu, H.; Gossard, A. C.; Watson, J. D.; Gardner, G. C.; Fallahi, S.; Manfra, M. J.; Reilly, D. J. Cryogenic Control Architecture for Large-Scale Quantum Computing. *Physical Review Applied* **2015**, *3*, 024010.
- (53) Degenhardt, C.; Geck, L.; Kruth, A.; Vliex, P.; van Waes, S. CMOS based scalable cryogenic Control Electronics for Qubits. *IEEE* **2017**, 332–335.
- (54) Bardin, J. C.; Jeffrey, E.; Lucero, E.; Huang, T.; Naaman, O.; Barends, R.; White, T.; Giustina, M.; Sank, D.; Roushan, P.; Arya, K.; Chiaro, B.; Kelly, J.; Chen, J.; Burkett, B.; Chen, Y.; Dunsworth, A.; Fowler, A.; Foxen, B.; Gidney, C.; Graff, R.; Klimov, P.; Mutus, J.; McEwen, M.; Megrant, A.; Neeley, M.; Neill, C.; Quintana, C.; Vainsencher, A.; Neven, H.; Martinis, J. A 28nm Bulk-CMOS 4-to-8 GHz < 2mW Cryogenic Pulse Modulator for Scalable Quantum Computing. In *2019 IEEE International Solid-State Circuits Conference*; Fujino, L. C., Anderson, J. H., Belostotski, L., Dunwell, D., Gaudet, V., Gulak, G., Haslett, J. W., Halupka, D., Smith, K. C., Eds.; IEEE, 2019; Vol. 62, pp 456-U2006.
- (55) Pirandola, S.; Eisert, J.; Weedbrook, C.; Furusawa, A.; Braunstein, S. L. Advances in quantum teleportation. *Nat. Photonics* **2015**, *9*, 641–652.
- (56) Geiger, Z. A. An Apparatus for Dynamical Quantum Emulation Using Ultracold Lithium. Ph.D. Thesis, University of California, Santa Barbara, 2017.
- (57) Anderegg, L.; Cheuk, L. W.; Bao, Y. C.; Burchesky, S.; Ketterle, W.; Ni, K. K.; Doyle, J. M. An optical tweezer array of ultracold molecules. *Science* **2019**, *365*, 1156–1158.
- (58) Saffman, M.; Walker, T. G.; Molmer, K. Quantum information with Rydberg atoms. *Rev. Mod. Phys.* **2010**, *82*, 2313–2363.
- (59) Barends, R.; Kelly, J.; Megrant, A.; Veitia, A.; Sank, D.; Jeffrey, E.; White, T. C.; Mutus, J.; Fowler, A. G.; Campbell, B.; Chen, Y.; Chen, Z.; Chiaro, B.; Dunsworth, A.; Neill, C.; O’Malley, P.; Roushan, P.; Vainsencher, A.; Wenner, J.; Korotkov, A. N.; Cleland, A. N.; Martinis, J. M. Superconducting quantum circuits at the surface code threshold for fault tolerance. *Nature* **2014**, *508*, 500–503.
- (60) Veldhorst, M.; Yang, C. H.; Hwang, J. C. C.; Huang, W.; Dehollain, J. P.; Muñonen, J. T.; Simmons, S.; Laucht, A.; Hudson, F. E.; Itoh, K. M.; Morello, A.; Dzurak, A. S. A two-qubit logic gate in silicon. *Nature* **2015**, *526*, 410–414.
- (61) Phillip Kaye, R. L.; Mosca, M. *An Introduction to Quantum Computing*; Oxford University Press, 2007.
- (62) Shor, P. W. Polynomial-time algorithms for prime factorization and discrete logarithms on a quantum computer. *Siam Journal on Computing* **1997**, *26*, 1484–1509.
- (63) Rivest, R. L.; Shamir, A.; Adleman, L. Method for obtaining digital signatures and public-key cryptosystems. *Communications of the ACM* **1978**, *21*, 120–126.
- (64) Ian, C.; Cloët, M. R. D. Opportunities for Nuclear Physics & Quantum Information Science. *arXiv* **2021**; <https://arxiv.org/pdf/1903.05453.pdf> (accessed 2022-01-05).
- (65) Sugisaki, K.; Nakazawa, S.; Toyota, K.; Sato, K.; Shiomi, D.; Takui, T. Quantum Chemistry on Quantum Computers: A Method for Preparation of Multiconfigurational Wave Functions on Quantum Computers without Performing Post-Hartree-Fock Calculations. *ACS Central Science* **2019**, *5*, 167–175.
- (66) Reiher, M.; Wiebe, N.; Svore, K. M.; Wecker, D.; Troyer, M. Elucidating reaction mechanisms on quantum computers. *Proc. Natl. Acad. Sci. U.S.A.* **2017**, *114*, 7555–7560.

- (67) Cao, Y.; Romero, J.; Olson, J. P.; Degroote, M.; Johnson, P. D.; Kieferová, M.; Kivlichan, I. D.; Menke, T.; Peropadre, B.; Sawaya, N. P. D.; Sim, S.; Veis, L.; Aspuru-Guzik, A. Quantum Chemistry in the Age of Quantum Computing. *Chem. Rev.* **2019**, *119*, 10856–10915.
- (68) Crane, K. W.; Joneckis, L. G.; Acheson-Field, H.; Boyd, I. D.; Corbin, B. A.; Han, X.; Rozansky, R. N. *Assessment of the Future Economic Impact of Quantum Information Science*; IDA Science & Technology Policy Institute: Washington, DC, 2017.
- (69) Shubik, M. Quantum economics, uncertainty and the optimal grid size. *Economics Letters* **1999**, *64*, 277–278.
- (70) Wehner, S.; Elkouss, D.; Hanson, R. Quantum internet: A vision for the road ahead. *Science* **2018**, *362*, No. eaam9288.
- (71) Wiebe, N.; Braun, D.; Lloyd, S. Quantum Algorithm for Data Fitting. *Phys. Rev. Lett.* **2012**, *109*, 050505.
- (72) Poggiali, F.; Cappellaro, P.; Fabbri, N. Optimal Control for One-Qubit Quantum Sensing. *Physical Review X* **2018**, *8*, 021059.
- (73) Chakraborty, S.; Ito, T.; Senju, T.; Saber, A. Y. Intelligent Economic Operation of Smart-Grid Facilitating Fuzzy Advanced Quantum Evolutionary Method. *IEEE Transactions on Sustainable Energy* **2013**, *4*, 905–916.
- (74) Cui, C. T.; Li, X. G.; Sui, H.; Sun, J. S. Optimization of coal-based methanol distillation scheme using process superstructure method to maximize energy efficiency. *Energy* **2017**, *119*, 110–120.
- (75) Lee, U.; Mitsos, A.; Han, C. Optimal retrofit of a CO₂ capture pilot plant using superstructure and rate-based models. *International Journal of Greenhouse Gas Control* **2016**, *50*, 57–69.
- (76) Azeez, O. S.; Isafiade, A. J.; Fraser, D. M. Supply-based superstructure synthesis of heat and mass exchange networks. *Comput. Chem. Eng.* **2013**, *56*, 184–201.
- (77) Liu, L. L.; Du, J.; Yang, F. L. Combined mass and heat exchange network synthesis based on stage-wise superstructure model. *Chinese Journal of Chemical Engineering* **2015**, *23*, 1502–1508.
- (78) Kwon, S.; Won, W.; Kim, J. A superstructure model of an isolated power supply system using renewable energy: Development and application to Jeju Island, Korea. *Renewable Energy* **2016**, *97*, 177–188.
- (79) Toffolo, A.; Rech, S.; Lazzaretto, A. Generation of Complex Energy Systems by Combination of Elementary Processes. *Journal of Energy Resources Technology-Transactions of the Asme* **2018**, *140*, 112005.
- (80) Cappellaro, P.; Lukin, M. D. Quantum correlation in disordered spin systems: Applications to magnetic sensing. *Phys. Rev. A* **2009**, *80*, 032311.
- (81) Wiese, U. J. Ultracold quantum gases and lattice systems: quantum simulation of lattice gauge theories. *Annalen Der Physik* **2013**, *S25*, 777–796.
- (82) Dumitrescu, E. F.; McCaskey, A. J.; Hagen, G.; Jansen, G. R.; Morris, T. D.; Papenbrock, T.; Pooser, R. C.; Dean, D. J.; Lougovski, P. Cloud Quantum Computing of an Atomic Nucleus. *Phys. Rev. Lett.* **2018**, *120*, 210501.
- (83) Torlai, G.; Melko, R. G. Machine-Learning Quantum States in the NISQ Era. *Annual Review of Condensed Matter Physics* **2020**, *11*, 325–344.
- (84) Monroe, C.; Raymer, M. G.; Taylor, J. Quantum information—The US National Quantum Initiative: From Act to action. *Science* **2019**, *364*, 440–442.
- (85) Xu, G. L.; Daley, A. J.; Givi, P.; Somma, R. D. Turbulent Mixing Simulation via a Quantum Algorithm. *Aiaa Journal* **2018**, *56*, 687–699.
- (86) Hinton, A.; Perea-Ortiz, M.; Winch, J.; Briggs, J.; Freer, S.; Moustoukas, D.; Powell-Gill, S.; Squire, C.; Lamb, A.; Rammeloo, C.; Stray, B.; Voulazeris, G.; Zhu, L.; Kaushik, A.; Lien, Y. H.; Niggebaum, A.; Rodgers, A.; Stabrawa, A.; Boddice, D.; Plant, S. R.; Tuckwell, G. W.; Bongs, K.; Metje, N.; Holynski, M. A portable magneto-optical trap with prospects for atom interferometry in civil engineering. *Philosophical Transactions of the Royal Society a-Mathematical Physical and Engineering Sciences* **2017**, *375*, 20160238.
- (87) Xu, G. L.; Daley, A. J.; Givi, P.; Somma, R. D. Quantum algorithm for the computation of the reactant conversion rate in homogeneous turbulence. *Combustion Theory and Modelling* **2019**, *23*, 1090–1104.
- (88) Givi, P.; Daley, A. J.; Mavriplis, D.; Malik, M. Quantum Speedup for Aeroscience and Engineering. *AIAA J.* **2020**, *58*, 3715–3727.
- (89) Quantum computing systems; <https://www.ibm.com/quantum-computing/systems/> (accessed 2022-01-05).
- (90) Kuramata, M.; Katsuki, R.; Nakata, K. In Larger Sparse Quadratic Assignment Problem Optimization Using Quantum Annealing and a Bit-Flip Heuristic Algorithm. *IEEE 8th International Conference on Industrial Engineering and Applications (ICIEA)* **2021**, 556–565.
- (91) Chapman, P. *Introducing the World's Most Powerful Quantum Computer*; <https://ionq.com/posts/october-01-2020-introducing-most-powerful-quantum-computer> (accessed 2022-01-05).
- (92) Honeywell system Model H1; <https://www.honeywell.com/us/en/company/quantum/quantum-computer> (accessed 2021-01-05).
- (93) Quantum computers; <https://www.aqt.eu/qc-systems/#> (accessed 2022-01-05).
- (94) Hou, S.-Y.; Feng, G.; Wu, Z.; Zou, H.; Shi, W.; Zeng, J.; Cao, C.; Yu, S.; Sheng, Z.; Rao, X.; Ren, B.; Lu, D.; Zou, J.; Miao, G.; Xiang, J.; Zeng, B. SpinQ Gemini: a desktop quantum computer for education and research. *arXiv* **2021**; <https://arxiv.org/pdf/2101.10017.pdf> (accessed 2022-01-05).
- (95) PsiQuantum; <https://psiquantum.com/about> (accessed 2022-01-05).
- (96) Hilbert: ColdQuanta's Powerful Quantum Computer; <https://coldquanta.com/computing> (accessed 2022-01-05).
- (97) Can we build a million qubit quantum computer? <https://universalquantum.com/> (accessed 2021-01-05).
- (98) Aaronson, S. The limits of quantum computers. *Sci. Am.* **2008**, *298*, 62–69.
- (99) Aaronson, S. *Quantum Computing Since Democritus*; Cambridge University Press: Cambridge, U.K., 2013.
- (100) Adleman, L. M. Molecular computation of solutions to combinatorial problems. *Science* **1994**, *266*, 1021–1024.
- (101) Lipton, R. J. DNA solution of hard computational problems. *Science* **1995**, *268*, 542–545.
- (102) Siegelmann, H. T. Computation beyond the turing limit. *Science* **1995**, *268*, 545–548.
- (103) Copeland, B. J.; Shagrir, O. Do Accelerating Turing Machines Compute the Uncomputable? *Minds and Machines* **2011**, *21*, 221–239.
- (104) Cabessa, J.; Siegelmann, H. T. *Evolving Recurrent Neural Networks are Super-Turing*, *International Joint Conference on Neural Networks (IJCNN)* **2011**, 3200–3206.
- (105) Wendum, G. Quantum information processing with superconducting circuits: a review. *Rep. Prog. Phys.* **2017**, *80*, 106001.
- (106) Dewes, A.; Lauro, R.; Ong, F. R.; Schmitt, V.; Milman, P.; Bertet, P.; Vion, D.; Esteve, D. Quantum speeding-up of computation demonstrated in a superconducting two-qubit processor. *Phys. Rev. B* **2012**, *85*, 140503.
- (107) Boixo, S.; Isakov, S. V.; Smelyanskiy, V. N.; Babbush, R.; Ding, N.; Jiang, Z.; Bremner, M. J.; Martinis, J. M.; Neven, H. Characterizing quantum supremacy in near-term devices. *Nat. Phys.* **2018**, *14*, 595–600.
- (108) Preskill, J. In *Quantum computing and the entanglement frontier, The Theory of the Quantum World, 25th Solvay Conference on Physics*; Gross, D., Henneaux, M., Severin, A., Eds.; World Scientific, 2013; pp 63–69.
- (109) DiVincenzo, D. P. The physical implementation of quantum computation. *Fortschritte Der Physik-Progress of Physics* **2000**, *48*, 771–783.
- (110) Shor, P. W. Scheme for reducing decoherence in quantum computer memory. *Phys. Rev. A* **1995**, *52*, R2493–R2496.
- (111) Steane, A. M. Error correcting codes in quantum theory. *Phys. Rev. Lett.* **1996**, *77*, 793–797.

- (112) Knill, E.; Laflamme, R.; Zurek, W. H. Resilient quantum computation. *Science* **1998**, *279*, 342–345.
- (113) Peruzzo, A.; McClean, J.; Shadbolt, P.; Yung, M. H.; Zhou, X. Q.; Love, P. J.; Aspuru-Guzik, A.; O'Brien, J. L. A variational eigenvalue solver on a photonic quantum processor. *Nat. Commun.* **2014**, *5*, 4213.
- (114) Krantz, P.; Kjaergaard, M.; Yan, F.; Orlando, T. P.; Gustavsson, S.; Oliver, W. D. A quantum engineer's guide to superconducting qubits. *Applied Physics Reviews* **2019**, *6*, 021318.
- (115) Barends, R.; Kelly, J.; Megrant, A.; Sank, D.; Jeffrey, E.; Chen, Y.; Yin, Y.; Chiaro, B.; Mutus, J.; Neill, C.; O'Malley, P.; Roushan, P.; Wenner, J.; White, T. C.; Cleland, A. N.; Martinis, J. M. Coherent Josephson Qubit Suitable for Scalable Quantum Integrated Circuits. *Phys. Rev. Lett.* **2013**, *111*, 080502.
- (116) Riste, D.; Bultink, C. C.; Tiggelman, M. J.; Schouten, R. N.; Lehnert, K. W.; DiCarlo, L. Millisecond charge-parity fluctuations and induced decoherence in a superconducting transmon qubit. *Nat. Commun.* **2013**, *4*, 1913.
- (117) Grabovskij, G. J.; Peichl, T.; Lisenfeld, J.; Weiss, G.; Ustinov, A. V. Strain Tuning of Individual Atomic Tunneling Systems Detected by a Superconducting Qubit. *Science* **2012**, *338*, 232–234.
- (118) Shaw, M. D.; Lutchyn, R. M.; Delsing, P.; Echternach, P. M. Kinetics of nonequilibrium quasiparticle tunneling in superconducting charge qubits. *Phys. Rev. B* **2008**, *78*, 024503.
- (119) Paik, H.; Schuster, D. I.; Bishop, L. S.; Kirchmair, G.; Catelani, G.; Sears, A. P.; Johnson, B. R.; Reagor, M. J.; Frunzio, L.; Glazman, L. I.; Girvin, S. M.; Devoret, M. H.; Schoelkopf, R. J. Observation of High Coherence in Josephson Junction Qubits Measured in a Three-Dimensional Circuit QED Architecture. *Phys. Rev. Lett.* **2011**, *107*, 240501.
- (120) Gustavsson, S.; Yan, F.; Catelani, G.; Bylander, J.; Kamal, A.; Birenbaum, J.; Hover, D.; Rosenberg, D.; Samach, G.; Sears, A. P.; Weber, S. J.; Yoder, J. L.; Clarke, J.; Kerman, A. J.; Yoshihara, F.; Nakamura, Y.; Orlando, T. P.; Oliver, W. D. Suppressing relaxation in superconducting qubits by quasiparticle pumping. *Science* **2016**, *354*, 1573–1577.
- (121) Martinis, J. M.; Nam, S.; Aumentado, J.; Urbina, C. Rabi oscillations in a large Josephson-junction qubit. *Phys. Rev. Lett.* **2002**, *89*, 117901.
- (122) Friedman, J. R.; Patel, V.; Chen, W.; Tolpygo, S. K.; Lukens, J. E. Quantum superposition of distinct macroscopic states. *Nature* **2000**, *406*, 43–46.
- (123) Mooij, J. E.; Orlando, T. P.; Levitov, L.; Tian, L.; van der Wal, C. H.; Lloyd, S. Josephson persistent-current qubit. *Science* **1999**, *285*, 1036–1039.
- (124) Pop, I. M.; Geerlings, K.; Catelani, G.; Schoelkopf, R. J.; Glazman, L. I.; Devoret, M. H. Coherent suppression of electromagnetic dissipation due to superconducting quasiparticles. *Nature* **2014**, *508*, 369–372.
- (125) Yan, F.; Gustavsson, S.; Kamal, A.; Birenbaum, J.; Sears, A. P.; Hover, D.; Gudmundsen, T. J.; Rosenberg, D.; Samach, G.; Weber, S.; Yoder, J. L.; Orlando, T. P.; Clarke, J.; Kerman, A. J.; Oliver, W. D. The flux qubit revisited to enhance coherence and reproducibility. *Nat. Commun.* **2016**, *7*, 12964.
- (126) Nakamura, Y.; Pashkin, Y. A.; Tsai, J. S. Coherent control of macroscopic quantum states in a single-Cooper-pair box. *Nature* **1999**, *398*, 786–788.
- (127) Vion, D.; Aassime, A.; Cottet, A.; Joyez, P.; Pothier, H.; Urbina, C.; Esteve, D.; Devoret, M. H. Manipulating the quantum state of an electrical circuit. *Science* **2002**, *296*, 886–889.
- (128) Casparis, L.; Larsen, T. W.; Olsen, M. S.; Kuemmeth, F.; Krogstrup, P.; Nygård, J.; Petersson, K. D.; Marcus, C. M. Gateon Benchmarking and Two-Qubit Operations. *Phys. Rev. Lett.* **2016**, *116*, 150505.
- (129) Sato, M.; Ando, Y. Topological superconductors: a review. *Rep. Prog. Phys.* **2017**, *80*, 076501.
- (130) Sarma, S. D.; Freedman, M.; Nayak, C. Majorana zero modes and topological quantum computation. *Npj Quantum Information* **2015**, *1*, 15001.
- (131) Girvin, S. M. Circuit QED: superconducting qubits coupled to microwave photons. *Quantum Machines: Measurement and Control of Engineered Quantum Systems: Lecture Notes of the Les Houches Summer School*; Oxford Scholarship Online, 2014; Vol. 96.
- (132) Kjaergaard, M.; Schwartz, M. E.; Braumüller, J.; Krantz, P.; Wang, J. L.-J.; Gustavsson, S.; Oliver, W. D. Superconducting Qubits: Current State of Play. *Annual Review of Condensed Matter Physics* **2020**, *11*, 369–395.
- (133) Ofek, N.; Petrenko, A.; Heeres, R.; Reinhold, P.; Leghtas, Z.; Vlastakis, B.; Liu, Y. H.; Frunzio, L.; Girvin, S. M.; Jiang, L.; Mirrahimi, M.; Devoret, M. H.; Schoelkopf, R. J. Extending the lifetime of a quantum bit with error correction in superconducting circuits. *Nature* **2016**, *536*, 441–445.
- (134) Hu, L.; Ma, Y.; Cai, W.; Mu, X.; Xu, Y.; Wang, W.; Wu, Y.; Wang, H.; Song, Y. P.; Zou, C. L.; Girvin, S. M.; Duan, L. M.; Sun, L. Quantum error correction and universal gate set operation on a binomial bosonic logical qubit. *Nat. Phys.* **2019**, *15*, 503–508.
- (135) Sheldon, S.; Magesan, E.; Chow, J. M.; Gambetta, J. M. Procedure for systematically tuning up cross-talk in the cross-resonance gate. *Phys. Rev. A* **2016**, *93*, 060302.
- (136) Gambetta, J. M.; Chow, J. M.; Steffen, M. Building logical qubits in a superconducting quantum computing system. *Npj Quantum Information* **2017**, *3*, 2.
- (137) Devoret, M. H.; Schoelkopf, R. J. Superconducting Circuits for Quantum Information: An Outlook. *Science* **2013**, *339*, 1169–1174.
- (138) Johnson, M. W.; Amin, M. H. S.; Gildert, S.; Lanting, T.; Hamze, F.; Dickson, N.; Harris, R.; Berkley, A. J.; Johansson, J.; Bunyk, P.; Chapple, E. M.; Enderud, C.; Hilton, J. P.; Karimi, K.; Ladizinsky, E.; Ladizinsky, N.; Oh, T.; Perminov, I.; Rich, C.; Thom, M. C.; Tolkacheva, E.; Truncik, C. J. S.; Uchaikin, S.; Wang, J.; Wilson, B.; Rose, G. Quantum annealing with manufactured spins. *Nature* **2011**, *473*, 194–198.
- (139) Reagor, M.; Pfaff, W.; Axline, C.; Heeres, R. W.; Ofek, N.; Sliwa, K.; Holland, E.; Wang, C.; Blumoff, J.; Chou, K.; Hatridge, M. J.; Frunzio, L.; Devoret, M. H.; Jiang, L.; Schoelkopf, R. J. Quantum memory with millisecond coherence in circuit QED. *Phys. Rev. B* **2016**, *94*, 014506.
- (140) Peyronel, T.; Firstenberg, O.; Liang, Q. Y.; Hofferberth, S.; Gorshkov, A. V.; Pohl, T.; Lukin, M. D.; Vuletic, V. Quantum nonlinear optics with single photons enabled by strongly interacting atoms. *Nature* **2012**, *488*, 57–60.
- (141) Shaffer, J. P.; Rittenhouse, S. T.; Sadeghpour, H. R. Ultracold Rydberg molecules. *Nat. Commun.* **2018**, *9*, 1965.
- (142) Andresen, G.B.; Ashkezari, M.D.; Baquero-Ruiz, M.; Bertsche, W.; Bowe, P.D.; Bray, C.C.; Butler, E.; Cesar, C.L.; Chapman, S.; Charlton, M.; Fajans, J.; Friesen, T.; Fujiwara, M.C.; Gill, D.R.; Hangst, J.S.; Hardy, W.N.; Hayano, R.S.; Hayden, M.E.; Humphries, A.J.; Hydomako, R.; Jonsell, S.; Jørgensen, L.V.; Kurchaninov, L.; Lambo, R.; Madsen, N.; Menary, S.; Nolan, P.; Olchanski, K.; Olin, A.; Povilus, A.; Pusa, P.; Robicheaux, F.; Sarid, E.; Seif El Nasr, S.; Silveira, D.M.; So, C.; Storey, J.W.; Thompson, R.I.; van der Werf, D.P.; Wilding, D.; Wurtele, J.S.; Yamazaki, Y. Search for trapped antihydrogen. *Physics Letters B* **2011**, *695*, 95–104.
- (143) Wu, X. L.; Liang, X. H.; Tian, Y. Q.; Yang, F.; Chen, C.; Liu, Y. C.; Tey, M. K.; You, L. A concise review of Rydberg atom based quantum computation and quantum simulation. *Chinese Physics B* **2021**, *30*, 020305.
- (144) Bendkowsky, V.; Butscher, B.; Nipper, J.; Shaffer, J. P.; Low, R.; Pfau, T. Observation of ultralong-range Rydberg molecules. *Nature* **2009**, *458*, 1005–1008.
- (145) Kim, H.; Lee, W.; Lee, H. G.; Jo, H.; Song, Y.; Ahn, J. In situ single-atom array synthesis using dynamic holographic optical tweezers. *Nat. Commun.* **2016**, *7*, 13317.
- (146) Nelson, K. D.; Li, X.; Weiss, D. S. Imaging single atoms in a three-dimensional array. *Nat. Phys.* **2007**, *3*, 556–560.
- (147) Boll, M.; Hilker, T. A.; Salomon, G.; Omran, A.; Nespolo, J.; Pollet, L.; Bloch, I.; Gross, C. Spin- and density-resolved microscopy of antiferromagnetic correlations in Fermi-Hubbard chains. *Science* **2016**, *353*, 1257–1260.

- (148) Wang, Y.; Kumar, A.; Wu, T. Y.; Weiss, D. S. Quantum information - Single-qubit gates based on targeted phase shifts in a 3D neutral atom array. *Science* **2016**, *352*, 1562–1565.
- (149) Urban, E.; Johnson, T. A.; Henage, T.; Isenhower, L.; Yavuz, D. D.; Walker, T. G.; Saffman, M. Observation of Rydberg blockade between two atoms. *Nat. Phys.* **2009**, *5*, 110–114.
- (150) Jaksch, D.; Cirac, J. I.; Zoller, P.; Rolston, S. L.; Cote, R.; Lukin, M. D. Fast quantum gates for neutral atoms. *Phys. Rev. Lett.* **2000**, *85*, 2208–2211.
- (151) Ebadi, S.; Wang, T. T.; Levine, H.; Keesling, A.; Semeghini, G.; Omran, A.; Bluvstein, D.; Samajdar, R.; Pichler, H.; Ho, W. W.; Choi, S.; Sachdev, S.; Greiner, M.; Vuletic, V.; Lukin, M. D. Quantum phases of matter on a 256-atom programmable quantum simulator. *Nature* **2021**, *595*, 227–232.
- (152) Aharonov, D.; van Dam, W.; Kempe, J.; Landau, Z.; Lloyd, S.; Regev, O. Adiabatic Quantum Computation Is Equivalent to Standard Quantum Computation. *SIAM Review* **2008**, *50*, 755–787.
- (153) Vinci, W.; Lidar, D. A. Non-stoquastic Hamiltonians in quantum annealing via geometric phases. *Npj Quantum Information* **2017**, *3*, 38.
- (154) Kadowaki, T.; Nishimori, H. Quantum annealing in the transverse Ising model. *Phys. Rev. E* **1998**, *58*, 5355–5363.
- (155) Boixo, S.; Smelyanskiy, V. N.; Shabani, A.; Isakov, S. V.; Dykman, M.; Denchev, V. S.; Amin, M. H.; Smirnov, A. Y.; Mohseni, M.; Neven, H. Computational multiqubit tunnelling in programmable quantum annealers. *Nat. Commun.* **2016**, *7*, 10327.
- (156) Hauke, P.; Katzgraber, H. G.; Lechner, W.; Nishimori, H.; Oliver, W. D. Perspectives of quantum annealing: Methods and implementations. *Rep. Prog. Phys.* **2020**, *83*, 054401.
- (157) Farhi, E.; Goldstone, J. Quantum Computation by Adiabatic Evolution. Technical Report MIT-CTP-2936, MIT. *arXiv*, **2021**; <https://arxiv.org/pdf/quant-ph/0001106.pdf> (accessed 2022-01-05).
- (158) Date, P.; Potok, T. Adiabatic quantum linear regression. *Sci. Rep.* **2021**, *11*, 21905.
- (159) Babbush, R.; Love, P. J.; Aspuru-Guzik, A. Adiabatic Quantum Simulation of Quantum Chemistry. *Sci. Rep.* **2015**, *4*, 6603.
- (160) Bakibayev, N.; Kočiský, T.; Olteanu, D.; Závodný, J. Aggregation and Ordering in Factorised Databases. *Proceedings of the VLDB Endowment* **2013**, *6*, 1990–2001.
- (161) Perdomo-Ortiz, A.; Dickson, N.; Drew-Brook, M.; Rose, G.; Aspuru-Guzik, A. Finding low-energy conformations of lattice protein models by quantum annealing. *Sci. Rep.* **2012**, *2*, 571.
- (162) Garnerone, S.; Zanardi, P.; Lidar, D. A. Adiabatic Quantum Algorithm for Search Engine Ranking. *Phys. Rev. Lett.* **2012**, *108*, 230506.
- (163) Binder, K.; Young, A. P. Spin-glasses - experimental facts, theoretical concepts, and open questions. *Rev. Mod. Phys.* **1986**, *58*, 801–976.
- (164) Lucas, A. Ising formulations of many NP problems. *Frontiers in Physics* **2014**, *2*, 5.
- (165) Hen, I. Period finding with adiabatic quantum computation. *EPL* **2014**, *105*, 50005.
- (166) Bian, Z. B.; Chudak, F.; Macready, W. G.; Clark, L.; Gaitan, F. Experimental Determination of Ramsey Numbers. *Phys. Rev. Lett.* **2013**, *111*, 130505.
- (167) Harris, R.; Sato, Y.; Berkley, A. J.; Reis, M.; Altomare, F.; Amin, M. H.; Boothby, K.; Bunyk, P.; Deng, C.; Enderud, C.; Huang, S.; Hoskinson, E.; Johnson, M. W.; Ladizinsky, E.; Ladizinsky, N.; Lanting, T.; Li, R.; Medina, T.; Molavi, R.; Neufeld, R.; Oh, T.; Pavlov, I.; Perminov, I.; Poulin-Lamarre, G.; Rich, C.; Smirnov, A.; Swenson, L.; Tsai, N.; Volkmann, M.; Whittaker, J.; Yao, J. Phase transitions in a programmable quantum spin glass simulator. *Science* **2018**, *361*, 162–165.
- (168) Zaribafyan, A.; Marchand, D. J. J.; Changiz Rezaei, S. S. Systematic and deterministic graph minor embedding for Cartesian products of graphs. *Quantum Information Processing* **2017**, *16*, 1–26.
- (169) McGeoch, C.; Farre, P. The D-Wave Advantage System: An Overview; https://www.dwavesys.com/media/s3qbjp3s/14-1049a-a_.pdf (accessed 2022-01-05).
- (170) Jiang, S. X.; Britt, K. A.; McCaskey, A. J.; Humble, T. S.; Kais, S. Quantum Annealing for Prime Factorization. *Sci. Rep.* **2018**, *8*, 17667.
- (171) Peng, W. C.; Wang, B. N.; Hu, F.; Wang, Y. J.; Fang, X. J.; Chen, X. Y.; Wang, C. Factoring larger integers with fewer qubits via quantum annealing with optimized parameters. *Science China-Physics Mechanics & Astronomy* **2019**, *62*, 060311.
- (172) Preskill, J. Quantum Computing in the NISQ era and beyond. *Quantum* **2018**, *2*, 79.
- (173) Kandala, A.; Mezzacapo, A.; Temme, K.; Takita, M.; Brink, M.; Chow, J. M.; Gambetta, J. M. Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets. *Nature* **2017**, *549*, 242–246.
- (174) Kelly, J.; Barends, R.; Fowler, A. G.; Megrant, A.; Jeffrey, E.; White, T. C.; Sank, D.; Mutus, J. Y.; Campbell, B.; Chen, Y.; Chen, Z.; Chiaro, B.; Dunsworth, A.; Hoi, I. C.; Neill, C.; O’Malley, P. J. J.; Quintana, C.; Roushan, P.; Vainsencher, A.; Wenner, J.; Cleland, A. N.; Martinis, J. M. State preservation by repetitive error detection in a superconducting quantum circuit. *Nature* **2015**, *519*, 66–69.
- (175) Neill, C.; Roushan, P.; Kechedzhi, K.; Boixo, S.; Isakov, S. V.; Smelyanskiy, V.; Megrant, A.; Chiaro, B.; Dunsworth, A.; Arya, K.; Barends, R.; Burkett, B.; Chen, Y.; Chen, Z.; Fowler, A.; Foxen, B.; Giustina, M.; Graff, R.; Jeffrey, E.; Huang, T.; Kelly, J.; Klimov, P.; Lucero, E.; Mutus, J.; Neeley, M.; Quintana, C.; Sank, D.; Vainsencher, A.; Wenner, J.; White, T. C.; Neven, H.; Martinis, J. M. A blueprint for demonstrating quantum supremacy with superconducting qubits. *Science* **2018**, *360*, 195–198.
- (176) Wei, K. X.; Lauer, I.; Srinivasan, S.; Sundaresan, N.; McClure, D. T.; Toyli, D.; McKay, D. C.; Gambetta, J. M.; Sheldon, S. Verifying Multipartite Entangled GHZ States via Multiple Quantum Coherences. *Phys. Rev. A* **2020**, *101*, 032343.
- (177) Otterbach, J. S.; et al. Unsupervised Machine Learning on a Hybrid Quantum Computer. *arXiv* **2021**; <https://arxiv.org/pdf/1712.05771.pdf> (accessed 2022-01-05).
- (178) Harrow, A. W.; Montanaro, A. Quantum computational supremacy. *Nature* **2017**, *549*, 203–209.
- (179) Chiaverini, J.; Leibfried, D.; Schaetz, T.; Barrett, M. D.; Blakestad, R. B.; Britton, J.; Itano, W. M.; Jost, J. D.; Knill, E.; Langer, C.; Ozeri, R.; Wineland, D. J. Realization of quantum error correction. *Nature* **2004**, *432*, 602–605.
- (180) Knill, E.; Laflamme, R.; Martinez, R.; Negrevergne, C. Benchmarking quantum computers: The five-qubit error correcting code. *Phys. Rev. Lett.* **2001**, *86*, 5811–5814.
- (181) Corcoles, A. D.; Magesan, E.; Srinivasan, S. J.; Cross, A. W.; Steffen, M.; Gambetta, J. M.; Chow, J. M. Demonstration of a quantum error detection code using a square lattice of four superconducting qubits. *Nat. Commun.* **2015**, *6*, 6979.
- (182) Nigg, D.; Müller, M.; Martinez, E. A.; Schindler, P.; Hennrich, M.; Monz, T.; Martin-Delgado, M. A.; Blatt, R. Quantum computations on a topologically encoded qubit. *Science* **2014**, *345*, 302–305.
- (183) MIT xpro quantum curriculum; <https://learn-xpro.mit.edu/quantum-computing> (accessed 2022-01-21).
- (184) Aaronson, S.; Arkhipov, A.; ACM, S. The Computational Complexity of Linear Optics. In *STOC 11: Proceedings of the 43rd ACM Symposium on Theory of Computing*; Association for Computing Machinery: New York, 2011; pp 333–342.
- (185) Terhal, B. M.; DiVincenzo, D. P. Adaptive Quantum Computation, Constant Depth Quantum Circuits and Arthur-Merlin Games. *Quant. Inf. Comp.* **2004**, *4*, 134–145.
- (186) Shepherd, D.; Bremner, M. J. Temporally unstructured quantum computation. *Proceedings of the Royal Society a-Mathematical Physical and Engineering Sciences* **2009**, *465*, 1413–1439.
- (187) Bravyi, S.; Gosset, D.; Konig, R. Quantum advantage with shallow circuits. *Science* **2018**, *362*, 308–311.
- (188) Pagano, G.; Bapat, A.; Becker, P.; Collins, K. S.; De, A.; Hess, P. W.; Kaplan, H. B.; Kyriakis, A.; Tan, W. L.; Baldwin, C.; Brady,

- L. T.; Deshpande, A.; Liu, F. L.; Jordan, S.; Gorshkov, A. V.; Monroe, C. Quantum approximate optimization of the long-range Ising model with a trapped-ion quantum simulator. *Proc. Natl. Acad. Sci. U.S.A.* **2020**, *117*, 25396–25401.
- (189) Kleinjung, T.; Aoki, K.; Franke, J.; Lenstra, A. K.; Thomé, E.; Bos, J. W.; Gaudry, P.; Kruppa, A.; Montgomery, P. L.; Osvik, D. A.; Riele, H. T.; Timofeev, A.; Zimmermann, P., Factorization of a 768-Bit RSA Modulus. In *Advances in Cryptology - Crypto 2010*; Rabin, T., Ed.; Springer, 2010; Vol. 6223, pp 333–350.
- (190) Montanaro, A. Quantum algorithms: an overview. *Npj Quantum Information* **2016**, *2*, 15023.
- (191) Boudot, F.; Gaudry, P.; Guillevic, A.; Heninger, N.; Thomé, E.; Zimmermann, P., Comparing the difficulty of factorization and discrete logarithm: a 240-digit experiment. *arXiv* 2020; <https://arxiv.org/pdf/2006.06197.pdf> (accessed 2022-01-05).
- (192) Regev, O. Quantum computation and lattice problems. *Siam Journal on Computing* **2004**, *33*, 738–760.
- (193) Grover, L. K. Quantum mechanics helps in searching for a needle in a haystack. *Phys. Rev. Lett.* **1997**, *79*, 325–328.
- (194) Brassard, G.; Hoyer, P.; Mosca, M.; Tapp, A. Quantum Amplitude Amplification and Estimation. In *Quantum Computation and Quantum Information*; Samuel, J., Lomonaco, J., Brandt, H. E., Eds.; American Mathematical Society: Providence, RI, 2002; Vol. 305, pp 53–74.
- (195) Farhi, E.; Goldstone, J.; Gutmann, S. A quantum approximate optimization algorithm applied to a bounded occurrence constraint problem. *arXiv* 2015; <https://arxiv.org/pdf/1412.6062.pdf> (accessed 2022-01-05).
- (196) Kempe, J. Discrete quantum walks hit exponentially faster. *Probability Theory and Related Fields* **2005**, *133*, 215–235.
- (197) Childs, A. M.; Farhi, E.; Gutmann, S. An Example of the Difference Between Quantum and Classical Random Walks. *Quantum Information Processing* **2002**, *1*, 35–43.
- (198) Aharonov, D.; Ambainis, A.; Kempe, J.; Vazirani, U. Quantum walks on graphs. In *33rd Annual ACM Symposium on Theory of Computing*; Vitter, J. S., Spirakis, P., Yannakakis, M., Eds.; Association for Computing Machinery: New York, 2001; pp 50–59.
- (199) Ambainis, A.; Schulman, L. J.; Ta-Shma, A.; Vazirani, U.; Wigderson, A. The quantum communication complexity of sampling. *Siam Journal on Computing* **2003**, *32*, 1570–1585.
- (200) Gall, F. L. In *Improved Quantum Algorithm for Triangle Finding via Combinatorial Arguments*, 2014 IEEE Annual Symposium on Foundations of Computer Science, the IEEE Computer Society Philadelphia, Pennsylvania **2014**, 216–225.
- (201) Morley, J. G.; Chancellor, N.; Bose, S.; Kendon, V. Quantum search with hybrid adiabatic-quantum-walk algorithms and realistic noise. *Phys. Rev. A* **2019**, *99*, 022339.
- (202) Harrow, A. W.; Hassidim, A.; Lloyd, S. Quantum Algorithm for Linear Systems of Equations. *Phys. Rev. Lett.* **2009**, *103*, 150502.
- (203) Vopson, M. M. Estimation of the information contained in the visible matter of the universe. *AIP Advances* **2021**, *11*, 105317.
- (204) Sanchez-Palencia, L. Quantum simulation: From basic principles to applications Foreword. *Comptes Rendus Physique* **2018**, *19*, 357–364.
- (205) Kassal, I.; Whitfield, J. D.; Perdomo-Ortiz, A.; Yung, M.-H.; Aspuru-Guzik, A. Simulating Chemistry Using Quantum Computers. *Annu. Rev. Phys. Chem.* **2011**, *62*, 185–207.
- (206) Lu, D. W.; Xu, B. R.; Xu, N. Y.; Li, Z. K.; Chen, H. W.; Peng, X. H.; Xu, R. X.; Du, J. F. Quantum chemistry simulation on quantum computers: theories and experiments. *Phys. Chem. Chem. Phys.* **2012**, *14*, 9411–9420.
- (207) Johnson, T. H.; Clark, S. R.; Jaksch, D. What is a quantum simulator? *EPJ. Quantum Technology* **2014**, *1*, 10.
- (208) Zagorskin, A. M. Analogue simulation with the use of artificial quantum coherent structures. *Reviews in Physics* **2018**, *3*, 1–14.
- (209) Rajagopal, S. V.; Fujiwara, K. M.; Senaratne, R.; Singh, K.; Geiger, Z. A.; Weld, D. M. Quantum Emulation of Extreme Non-Equilibrium Phenomena with Trapped Atoms. *Annalen Der Physik* **2017**, *529*, 1700008.
- (210) Garreau, J. C. Quantum simulation of disordered systems with cold atoms. *Comptes Rendus Physique* **2017**, *18*, 31–46.
- (211) Smirnov, A. Y.; Savel'ev, S.; Mourokh, L. G.; Nori, F. Modelling chemical reactions using semiconductor quantum dots. *EPL* **2007**, *80*, 67008.
- (212) Torrontegui, E.; Ruschhaupt, A.; Guery-Odelin, D.; Muga, J. G. Simulation of quantum collinear chemical reactions with ultracold atoms. *Journal of Physics B-Atomic Molecular and Optical Physics* **2011**, *44*, 195302.
- (213) Gorman, D. J.; Hemmerling, B.; Megidish, E.; Moeller, S. A.; Schindler, P.; Sarovar, M.; Haeffner, H. Engineering vibrationally assisted energy transfer in a trapped-ion quantum simulator. *Physical Review X* **2018**, *8*, 011038.
- (214) Chen, Y.; Neill, C.; Roushan, P.; Leung, N.; Fang, M.; Barends, R.; Kelly, J.; Campbell, B.; Chen, Z.; Chiaro, B.; Dunsworth, A.; Jeffrey, E.; Megrant, A.; Mutus, J. Y.; O'Malley, P. J. J.; Quintana, C. M.; Sank, D.; Vainsencher, A.; Wenner, J.; White, T. C.; Geller, M. R.; Cleland, A. N.; Martinis, J. M. Qubit Architecture with High Coherence and Fast Tunable Coupling. *Phys. Rev. Lett.* **2014**, *113*, 220502.
- (215) Wecker, D.; Hastings, M. B.; Wiebe, N.; Clark, B. K.; Nayak, C.; Troyer, M. Solving strongly correlated electron models on a quantum computer. *Phys. Rev. A* **2015**, *92*, 062318.
- (216) Jordan, S. P.; Lee, K. S. M.; Preskill, J. Quantum Algorithms for Quantum Field Theories. *Science* **2012**, *336*, 1130–1133.
- (217) Berry, D. W.; Childs, A. M.; Cleve, R.; Kothari, R.; Somma, R. D. Simulating Hamiltonian Dynamics with a Truncated Taylor Series. *Phys. Rev. Lett.* **2015**, *114*, 090502.
- (218) Low, G. H.; Chuang, I. L. Optimal Hamiltonian Simulation by Quantum Signal Processing. *Phys. Rev. Lett.* **2017**, *118*, 010501.
- (219) Neeley, M.; Bialczak, R. C.; Lenander, M.; Lucero, E.; Mariantoni, M.; O'Connell, A. D.; Sank, D.; Wang, H.; Weides, M.; Wenner, J.; Yin, Y.; Yamamoto, T.; Cleland, A. N.; Martinis, J. M. Generation of three-qubit entangled states using superconducting phase qubits. *Nature* **2010**, *467*, 570–573.
- (220) Fedorov, A.; Steffen, L.; Baur, M.; da Silva, M. P.; Wallraff, A. Implementation of a Toffoli gate with superconducting circuits. *Nature* **2012**, *481*, 170–172.
- (221) Chow, J. M.; Gambetta, J. M.; Corcoles, A. D.; Merkel, S. T.; Smolin, J. A.; Rigetti, C.; Poletto, S.; Keefe, G. A.; Rothwell, M. B.; Rozen, J. R.; Ketchen, M. B.; Steffen, M. Universal Quantum Gate Set Approaching Fault-Tolerant Thresholds with Superconducting Qubits. *Phys. Rev. Lett.* **2012**, *109*, 060501.
- (222) Heras, U. L.; Mezzacapo, A.; Lamata, L.; Filipp, S.; Wallraff, A.; Solano, E. Digital Quantum Simulation of Spin Systems in Superconducting Circuits. *Phys. Rev. Lett.* **2014**, *112*, 200501.
- (223) Lanyon, B. P.; Hempel, C.; Nigg, D.; Müller, M.; Gerritsma, R.; Zahringer, F.; Schindler, P.; Barreiro, J. T.; Rambach, M.; Kirchmair, G.; Hennrich, M.; Zoller, P.; Blatt, R.; Roos, C. F. Universal Digital Quantum Simulation with Trapped Ions. *Science* **2011**, *334*, 57–61.
- (224) Abrams, D. S.; Lloyd, S. Simulations of many-body Fermi systems on a universal quantum computer. *Phys. Rev. Lett.* **1997**, *79*, 2586–2589.
- (225) Ward, N. J.; Kassal, I.; Aspuru-Guzik, A. Preparation of many-body states for quantum simulation. *J. Chem. Phys.* **2009**, *130*, 194105.
- (226) Wang, H. F.; Ashhab, S.; Nori, F. Efficient quantum algorithm for preparing molecular-system-like states on a quantum computer. *Phys. Rev. A* **2009**, *79*, 042335.
- (227) Wang, H. F.; Ashhab, S.; Nori, F. Quantum algorithm for simulating the dynamics of an open quantum system. *Phys. Rev. A* **2011**, *83*, 062317.
- (228) Aspuru-Guzik, A.; Dutoi, A. D.; Love, P. J.; Head-Gordon, M. Simulated quantum computation of molecular energies. *Science* **2005**, *309*, 1704–1707.
- (229) D'Ariano, G. M.; Paris, M. G. A.; Sacchi, M. F. Quantum tomography. In *Advances in Imaging and Electron Physics*; Hawkes, P. W., Ed.; Elsevier, 2003; Vol. 128, pp 205–308.

- (230) Somma, R.; Ortiz, G.; Gubernatis, J. E.; Knill, E.; Laflamme, R. Simulating physical phenomena by quantum networks. *Phys. Rev. A* **2002**, *65*, 042323.
- (231) Jane, E.; Vidal, G.; Dur, W.; Zoller, P.; Cirac, J. I. Simulation of quantum dynamics with quantum optical systems. *Quantum Information & Computation* **2003**, *3*, 15–37.
- (232) Barreiro, J. T.; Muller, M.; Schindler, P.; Nigg, D.; Monz, T.; Chwalla, M.; Hennrich, M.; Roos, C. F.; Zoller, P.; Blatt, R. An open-system quantum simulator with trapped ions. *Nature* **2011**, *470*, 486–491.
- (233) Li, Z. K.; Yung, M. H.; Chen, H. W.; Lu, D. W.; Whitfield, J. D.; Peng, X. H.; Aspuru-Guzik, A.; Du, J. F. Solving Quantum Ground-State Problems with Nuclear Magnetic Resonance. *Sci. Rep.* **2011**, *1*, 88.
- (234) Zhang, J. F.; Yung, M. H.; Laflamme, R.; Aspuru-Guzik, A.; Baugh, J. Digital quantum simulation of the statistical mechanics of a frustrated magnet. *Nat. Commun.* **2012**, *3*, 880.
- (235) You, J. Q.; Nori, F. Atomic physics and quantum optics using superconducting circuits. *Nature* **2011**, *474*, 589–597.
- (236) Harris, R.; Johnson, M. W.; Lanting, T.; Berkley, A. J.; Johansson, J.; Bunyk, P.; Tolkacheva, E.; Ladizinsky, E.; Ladizinsky, N.; Oh, T.; Cioata, F.; Perminov, I.; Spear, P.; Enderud, C.; Rich, C.; Uchaikin, S.; Thom, M. C.; Chapple, E. M.; Wang, J.; Wilson, B.; Amin, M. H. S.; Dickson, N.; Karimi, K.; Macready, B.; Truncik, C. J. S.; Rose, G. Experimental investigation of an eight-qubit unit cell in a superconducting optimization processor. *Phys. Rev. B* **2010**, *82*, 024511.
- (237) Abdumalikov, A. A.; Astafiev, O.; Zagorskin, A. M.; Pashkin, Y. A.; Nakamura, Y.; Tsai, J. S. Electromagnetically Induced Transparency on a Single Artificial Atom. *Phys. Rev. Lett.* **2010**, *104*, 193601.
- (238) Neeley, M.; Ansmann, M.; Bialczak, R. C.; Hofheinz, M.; Lucero, E.; O’Connell, A. D.; Sank, D.; Wang, H. H.; Wenner, J.; Cleland, A. N.; Geller, M. R.; Martinis, J. M. Emulation of a Quantum Spin with a Superconducting Phase Qudit. *Science* **2009**, *325*, 722–725.
- (239) Zalka, C. Simulating quantum systems on a quantum computer. *Proceedings of the Royal Society a-Mathematical Physical and Engineering Sciences* **1998**, *454*, 313–322.
- (240) Lidar, D. A.; Wang, H. B. Calculating the thermal rate constant with exponential speedup on a quantum computer. *Phys. Rev. E* **1999**, *59*, 2429–2438.
- (241) Wang, H.; Kais, S.; Aspuru-Guzik, A.; Hoffmann, M. R. Quantum algorithm for obtaining the energy spectrum of molecular systems. *Phys. Chem. Chem. Phys.* **2008**, *10*, 5388–5393.
- (242) Wecker, D.; Hastings, M. B.; Troyer, M. Progress towards practical quantum variational algorithms. *Phys. Rev. A* **2015**, *92*, 042303.
- (243) McClean, J. R.; Romero, J.; Babbush, R.; Aspuru-Guzik, A. The theory of variational hybrid quantum-classical algorithms. *New J. Phys.* **2016**, *18*, 023023.
- (244) Li, Y.; Benjamin, S. C. Efficient Variational Quantum Simulator Incorporating Active Error Minimization. *Physical Review X* **2017**, *7*, 021050.
- (245) Abrams, D. S.; Lloyd, S. Quantum algorithm providing exponential speed increase for finding eigenvalues and eigenvectors. *Phys. Rev. Lett.* **1999**, *83*, 5162–5165.
- (246) Berry, D. W.; Kieferova, M.; Scherer, A.; Sanders, Y. R.; Low, G. H.; Wiebe, N.; Gidney, C.; Babbush, R. Improved techniques for preparing eigenstates of fermionic Hamiltonians. *Npj Quantum Information* **2018**, *4*, 22.
- (247) Veis, L.; Visnak, J.; Nishizawa, H.; Nakai, H.; Pittner, J. Quantum Chemistry beyond Born-Oppenheimer Approximation on a Quantum Computer: A Simulated Phase Estimation Study. *Int. J. Quantum Chem.* **2016**, *116*, 1328–1336.
- (248) von Burg, V.; Low, G. H.; Häner, T.; Steiger, D. S.; Reiher, M.; Roetteler, M.; Troyer, M. Quantum computing enhanced computational catalysis. *Physical Review Research* **2021**, *3*, 033055.
- (249) Whitfield, J. D.; Biamonte, J.; Aspuru-Guzik, A. Simulation of electronic structure Hamiltonians using quantum computers. *Mol. Phys.* **2011**, *109*, 735–750.
- (250) Jones, N. C.; Whitfield, J. D.; McMahon, P. L.; Yung, M. H.; Van Meter, R.; Aspuru-Guzik, A.; Yamamoto, Y. Faster quantum chemistry simulation on fault-tolerant quantum computers. *New J. Phys.* **2012**, *14*, 115023.
- (251) Dobsicek, M.; Johansson, G.; Shumeiko, V.; Wendin, G. Arbitrary accuracy iterative quantum phase estimation algorithm using a single ancillary qubit: A two-qubit benchmark. *Phys. Rev. A* **2007**, *76*, 030306.
- (252) Hempel, C.; Maier, C.; Romero, J.; McClean, J.; Monz, T.; Shen, H.; Jurcevic, P.; Lanyon, B.; Love, P.; Babbush, R.; Aspuru-Guzik, A.; Blatt, R.; Roos, C. F. Quantum Chemistry Calculations on a Trapped-Ion Quantum Simulator. *Physical Review X* **2018**, *8*, 031022.
- (253) Ratcliff, L. E.; Mohr, S.; Huhs, G.; Deutsch, T.; Masella, M.; Genovese, L. Challenges in large scale quantum mechanical calculations. *Wiley Interdisciplinary Reviews-Computational Molecular Science* **2017**, *7*, No. e1290.
- (254) Zhang, L. L.; Wu, G.; Jiang, J. W. Adsorption and Diffusion of CO₂ and CH₄ in Zeolitic Imidazolate Framework-8: Effect of Structural Flexibility. *J. Phys. Chem. C* **2014**, *118*, 8788–8794.
- (255) Zheng, B.; Pan, Y. C.; Lai, Z. P.; Huang, K. W. Molecular Dynamics Simulations on Gate Opening in ZIF-8: Identification of Factors for Ethane and Propane Separation. *Langmuir* **2013**, *29*, 8285–8872.
- (256) Yang, X.; Rees, R. J.; Conway, W.; Puxty, G.; Yang, Q.; Winkler, D. A. Computational Modeling and Simulation of CO₂ Capture by Aqueous Amines. *Chem. Rev.* **2017**, *117*, 9524–9593.
- (257) Duarte, F.; Amrein, B. A.; Blaha-Nelson, D.; Kamerlin, S. C. L. Recent advances in QM/MM free energy calculations using reference potentials. *Biochimica Et Biophysica Acta-General Subjects* **2015**, *1850*, 954–965.
- (258) Prasetyo, N.; Hofer, T. S. Structure, Dynamics, and Hydration Free Energy of Carbon Dioxide in Aqueous Solution: A Quantum Mechanical/Molecular Mechanics Molecular Dynamics Thermodynamic Integration (QM/MM MD TI) Simulation Study. *J. Chem. Theory Comput.* **2018**, *14*, 6472–6483.
- (259) Senn, H. M.; Thiel, W. QM/MM Methods for Biomolecular Systems. *Angew. Chem., Int. Ed.* **2009**, *48*, 1198–1229.
- (260) Altintas, C.; Keskin, S. Role of partial charge assignment methods in high-throughput screening of MOF adsorbents and membranes for CO₂/CH₄ separation. *Molecular Systems Design & Engineering* **2020**, *5*, 532–543.
- (261) Roy, S. C.; Varghese, O. K.; Paulose, M.; Grimes, C. A. Toward solar fuels: photocatalytic conversion of carbon dioxide to hydrocarbons. *ACS Nano* **2010**, *4*, 1259–1278.
- (262) Liu, C.; Yang, B.; Tyo, E.; Seifert, S.; DeBartolo, J.; von Issendorff, B.; Zapol, P.; Vajda, S.; Curtiss, L. A. Carbon dioxide conversion to methanol over size-selected Cu₄ clusters at low pressures. *J. Am. Chem. Soc.* **2015**, *137*, 8676–8679.
- (263) Chen, Y.; Huang, Y.; Cheng, T.; Goddard III, W. A. Identifying Active Sites for CO₂ Reduction on Dealloyed Gold Surfaces by Combining Machine Learning with Multiscale Simulations. *J. Am. Chem. Soc.* **2019**, *141*, 11651–11657.
- (264) Raugei, S.; Seefeldt, L. C.; Hoffman, B. M. Critical computational analysis illuminates the reductive-elimination mechanism that activates nitrogenase for N₂ reduction. *Proc. Natl. Acad. Sci. U. S. A.* **2018**, *115*, E10521–E10530.
- (265) Cai, X.; Fang, W.-H.; Fan, H.; Li, Z. Quantum computation of molecular response properties. *Physical Review Research* **2020**, *2*, 033324.
- (266) Mohseni, M.; Read, P.; Neven, H.; Boixo, S.; Denchev, V.; Babbush, R.; Fowler, A.; Smelyanskiy, V.; Martinis, J. Commercialize quantum technologies in five years. *Nature* **2017**, *543*, 171–174.
- (267) Outeiral, C.; Strahm, M.; Shi, J.; Morris, G. M.; Benjamin, S. C.; Deane, C. M. The prospects of quantum computing in

- computational molecular biology. *WIREs Computational Molecular Science* **2021**, *11*, No. e1481.
- (268) Wouters, S.; Jimenez-Hoyos, C. A.; Sun, Q. M.; Chan, G. K. L. A Practical Guide to Density Matrix Embedding Theory in Quantum Chemistry. *J. Chem. Theory Comput.* **2016**, *12*, 2706–2719.
- (269) Singh, S.; Ram, L. C.; Masto, R. E.; Verma, S. K. A comparative evaluation of minerals and trace elements in the ashes from lignite, coal refuse, and biomass fired power plants. *International Journal of Coal Geology* **2011**, *87*, 112–120.
- (270) Hedin, B. C.; Hedin, R. S.; Capo, R. C.; Stewart, B. W. Critical metal recovery potential of Appalachian acid mine drainage treatment solids. *International Journal of Coal Geology* **2020**, *231*, 103610.
- (271) Lin, R. H.; Stuckman, M. L.; Howard, B. H.; Bank, T. L.; Roth, E. A.; Macala, M. K.; Lopano, C.; Soong, Y.; Granite, E. J. Application of sequential extraction and hydrothermal treatment for characterization and enrichment of rare earth elements from coal fly ash. *Fuel* **2018**, *232*, 124–133.
- (272) Wang, Q. M.; Kail, B. W.; Wilfong, W. C.; Shi, F.; Tarka, T. J.; Gray, M. L. Amine Sorbents for Selective Recovery of Heavy Rare-Earth Elements (Dysprosium, Ytterbium) from Aqueous Solution. *ChemPlusChem* **2020**, *85*, 130–136.
- (273) Crawford, S. E.; Ohodnicki, P. R.; Baltrus, J. P. Materials for the photoluminescent sensing of rare earth elements: challenges and opportunities. *Journal of Materials Chemistry C* **2020**, *8*, 7975–8006.
- (274) Crawford, S. E.; Gan, X. Y.; Lemaire, P. C. K.; Millstone, J. E.; Baltrus, J. P.; Ohodnicki, P. R. Zinc-Adeninate Metal-Organic Framework: A Versatile Photoluminescent Sensor for Rare Earth Elements in Aqueous Systems. *ACS Sensors* **2019**, *4*, 1986–1991.
- (275) Crawford, S. E.; Ellis, J. E.; Ohodnicki, P. R.; Baltrus, J. P. Influence of the Anionic Zinc-Adeninate Metal-Organic Framework Structure on the Luminescent Detection of Rare Earth Ions in Aqueous Streams. *ACS Appl. Mater. Interfaces* **2021**, *13*, 7268–7277.
- (276) Mattocks, J. A.; Ho, J. V.; Cotruvo, J. A. A Selective, Protein-Based Fluorescent Sensor with Picomolar Affinity for Rare Earth Elements. *J. Am. Chem. Soc.* **2019**, *141*, 2857–2861.
- (277) Vo, M. N.; Bryantsev, V. S.; Johnson, J. K.; Keith, J. A. Quantum chemistry benchmarking of binding and selectivity for lanthanide extractants. *Int. J. Quantum Chem.* **2018**, *118*, No. e25516.
- (278) McCarver, G. A.; Hinde, R. J.; Vogiatzis, K. D. Selecting Quantum-Chemical Methods for Lanthanide-Containing Molecules: A Balance between Accuracy and Efficiency. *Inorg. Chem.* **2020**, *59*, 10492–10500.
- (279) Barkoutsos, P. K.; Gkrtsis, F.; Ollitrault, P. J.; Sokolov, I. O.; Woerner, S.; Tavernelli, I. Quantum algorithm for alchemical optimization in material design. *Chemical Science* **2021**, *12*, 4345–4352.
- (280) Mulligan, V. K.; Melo, H.; Merritt, H. I.; Slocum, S.; Weitzner, B. D.; Watkins, A. M.; Renfrew, P. D.; Pelissier, C.; Arora, P. S.; Bonneau, R. Designing Peptides on a Quantum Computer. *BioRxiv* **2020**, 752485.
- (281) Sandeep, S.; Gupta, V.; Keenan, T., Utilizing Quantum Biological Techniques on a Quantum Processing Unit for Improved Protein Binding Site Determination. *BioRxiv* **2020**; <https://www.biorxiv.org/content/10.1101/2020.03.20.000950v3> (accessed 2022-01-05).
- (282) Park, M. B.; Park, E. D.; Ahn, W. S. Recent Progress in Direct Conversion of Methane to Methanol Over Copper-Exchanged Zeolites. *Frontiers in Chemistry* **2019**, *7*, 514.
- (283) Grabow, L. C.; Mavrikakis, M. Mechanism of Methanol Synthesis on Cu through CO₂ and CO Hydrogenation. *ACS Catal.* **2011**, *1*, 365–384.
- (284) Idziak, K.; Czakiert, T.; Krzywanski, J.; Zylka, A.; Kozlowska, M.; Nowak, W. Safety and environmental reasons for the use of Ni-, Co-, Cu-, Mn- and Fe-based oxygen carriers in CLC/CLOU applications: An overview. *Fuel* **2020**, *268*, 117245.
- (285) Zhu, X.; Imtiaz, Q.; Donat, F.; Muller, C. R.; Li, F. X. Chemical looping beyond combustion - a perspective. *Energy Environ. Sci.* **2020**, *13*, 772–804.
- (286) Haldoupis, E.; Borycz, J.; Shi, H. L.; Vogiatzis, K. D.; Bai, P.; Queen, W. L.; Gagliardi, L.; Siepmann, J. I. Ab Initio Derived Force Fields for Predicting CO₂ Adsorption and Accessibility of Metal Sites in the Metal-Organic Frameworks M-MOF-74 (M = Mn, Co, Ni, Cu). *J. Phys. Chem. C* **2015**, *119*, 16058–16071.
- (287) Boyd, P. G.; Moosavi, S. M.; Witman, M.; Smit, B. Force-Field Prediction of Materials Properties in Metal-Organic Frameworks. *J. Phys. Chem. Lett.* **2017**, *8*, 357–363.
- (288) Zhang, Z. H.; Schott, J. A.; Liu, M. M.; Chen, H.; Lu, X. Y.; Sumpter, B. G.; Fu, J.; Dai, S. Prediction of Carbon Dioxide Adsorption via Deep Learning. *Angew. Chem., Int. Ed.* **2019**, *58*, 259–263.
- (289) Borboudakis, G.; Stergiannakos, T.; Frysali, M.; Klontzas, E.; Tsamardinos, I.; Froudakis, G. E. Chemically intuited, large-scale screening of MOFs by machine learning techniques. *Npj Computational Materials* **2017**, *3*, 40.
- (290) Chung, Y. G.; Gomez-Gualdrón, D. A.; Li, P.; Leperi, K. T.; Deria, P.; Zhang, H. D.; Vermeulen, N. A.; Stoddart, J. F.; You, F. Q.; Hupp, J. T.; Farha, O. K.; Snurr, R. Q. In silico discovery of metal-organic frameworks for precombustion CO₂ capture using a genetic algorithm. *Science Advances* **2016**, *2*, No. e1600909.
- (291) Saal, J. E.; Kirklin, S.; Aykol, M.; Meredig, B.; Wolverton, C. Materials Design and Discovery with High-Throughput Density Functional Theory: The Open Quantum Materials Database (OQMD). *JOM* **2013**, *65*, 1501–1509.
- (292) Anderson, R.; Rodgers, J.; Argueta, E.; Biong, A.; Gómez-Gualdrón, D. A. Role of Pore Chemistry and Topology in the CO₂Capture Capabilities of MOFs: From Molecular Simulation to Machine Learning. *Chem. Mater.* **2018**, *30*, 6325–6337.
- (293) Sun, A. Y. Optimal carbon storage reservoir management through deep reinforcement learning. *Applied Energy* **2020**, *278*, 115660.
- (294) Wen, G. G.; Hay, C.; Benson, S. M. CCSNet: A deep learning modeling suite for CO₂ storage. *Advances in Water Resources* **2021**, *155*, 104009.
- (295) Wright, R. F.; Lu, P.; Devkota, J.; Lu, F.; Ziomek-Moroz, M.; Ohodnicki, P. R. Corrosion Sensors for Structural Health Monitoring of Oil and Natural Gas Infrastructure: A Review. *Sensors* **2019**, *19*, 3964.
- (296) Su, Y. D.; Preger, Y.; Burroughs, H.; Sun, C. H.; Ohodnicki, P. R. Fiber Optic Sensing Technologies for Battery Management Systems and Energy Storage Applications. *Sensors* **2021**, *21*, 1397.
- (297) Sun, C.; Ohodnicki, P. R.; Stewart, E. M. Chemical Sensing Strategies for Real-Time Monitoring of Transformer Oil: A Review. *IEEE Sensors Journal* **2017**, *17*, 5786–5806.
- (298) Venketeswaran, A.; Lalam, N.; Wuenschell, J.; Ohodnicki, P. R.; Badar, M.; Chen, K. P.; Lu, P.; Duan, Y.; Chorpeling, B.; Buric, M. Recent Advances in Machine Learning for Fiber Optic Sensor Applications. *Advanced Intelligent Systems* **2021**, 2100067.
- (299) Kaubruegger, R.; Vasilyev, D. V.; Schulte, M.; Hammerer, K.; Zoller, P. Quantum Variational Optimization of Ramsey Interferometry and Atomic Clocks. *Physical Review X* **2021**, *11*, 041045.
- (300) Zaidenberg, D. A.; Sebastianelli, A.; Spiller, D.; Saux, B. L.; Ullo, S. L. Advantages and Bottlenecks of Quantum Machine Learning for Remote Sensing. *2021 IEEE International Geoscience and Remote Sensing Symposium IGARSS*; IEEE: Brussels, Belgium, 2021.
- (301) Mahony, D.; Bhattacharyya, S. Evaluation of highly entangled states in asymmetrically coupled three NV centers by quantum simulator. *Appl. Phys. Lett.* **2021**, *118*, 204004.
- (302) Plakhotnik, T. Diamonds for quantum nano sensing. *Curr. Opin. Solid State Mater. Sci.* **2017**, *21*, 25–34.
- (303) Shugayev, R. A.; Crawford, S. E.; Baltrus, J. P.; Diemler, N. A.; Ellis, J. E.; Kim, K. J.; Cvetic, P. C. Synthesis and Quantum Metrology of Metal-Organic Framework-Coated Nanodiamonds Containing Nitrogen Vacancy Centers. *Chem. Mater.* **2021**, *33*, 6365–6373.
- (304) Sebastianelli, A.; Zaidenberg, D. A.; Spiller, D.; Le Saux, B.; Ullo, S. On Circuit-based Hybrid Quantum Neural Networks for

- Remote Sensing Imagery Classification. *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing* **2022**, *15*, 565.
- (305) Ellis, J. E.; Crawford, S. E.; Kim, K. J. Metal–organic framework thin films as versatile chemical sensing materials. *Materials Advances* **2021**, *2*, 6169–6196.
- (306) Miroshnikov, M.; Mahankali, K.; Thangavel, N. K.; Satapathy, S.; Arava, L. M. R.; Ajayan, P. M.; John, G. Biderived Molecular Electrodes for Next-Generation Energy-Storage Materials. *ChemSusChem* **2020**, *13*, 2186–2204.
- (307) Ye, R. J.; Henkensmeier, D.; Yoon, S. J.; Huang, Z. F.; Kim, D. K.; Chang, Z. J.; Kim, S.; Chen, R. Y. Redox Flow Batteries for Energy Storage: A Technology Review. *Journal of Electrochemical Energy Conversion and Storage* **2018**, *15*, 010801.
- (308) Zhang, G.; Duan, W. H. Advanced Materials for Heat Energy Transfer, Conversion, Storage and Utilization. *Adv. Funct. Mater.* **2020**, *30*, 1907882.
- (309) Rice, J. E.; Gujarati, T. P.; Motta, M.; Takeshita, T. Y.; Lee, E.; Latone, J. A.; Garcia, J. M. Quantum computation of dominant products in lithium–sulfur batteries. *J. Chem. Phys.* **2021**, *154*, 134115.
- (310) Choi, H.; Moin, P. Grid-point requirements for large eddy simulation: Chapman’s estimates revisited. *Phys. Fluids* **2012**, *24*, 011702.
- (311) Griffin, K. P.; Jain, S. S.; Flint, T. J.; Chan, W. H. R. Investigation of quantum algorithms for direct numerical simulation of the Navier-Stokes equations. *Center for Turbulence Research, Annual Research Briefs 2019* **2019**, 347–363.
- (312) Bharadwaj, S. S.; Sreenivasan, K. R. Quantum Computation of Fluid Dynamics. *arXiv* **2020**; <https://arxiv.org/pdf/2007.09147v1.pdf> (accessed 2022-01-05).
- (313) Gaitan, F. Finding Solutions of the Navier-Stokes Equations through Quantum Computing—Recent Progress, a Generalization, and Next Steps Forward. *Advanced Quantum Technologies* **2021**, *4*, 2100055.
- (314) Gaitan, F. Finding flows of a Navier-Stokes fluid through quantum computing. *Npj Quantum Information* **2020**, *6*, 61.
- (315) Kacewicz, B. Almost optimal solution of initial-value problems by randomized and quantum algorithms. *Journal of Complexity* **2006**, *22*, 676–690.
- (316) Lubasch, M.; Joo, J.; Moinier, P.; Kiffner, M.; Jaksch, D. Variational quantum algorithms for nonlinear problems. *Phys. Rev. A* **2020**, *101*, 010301.
- (317) Ray, N.; Banerjee, T.; Nadiga, B.; Karra, S. Towards Solving the Navier-Stokes Equation on Quantum Computers. *arXiv* **2019**; <https://arxiv.org/pdf/1904.09033.pdf> (accessed 2022-01-05).
- (318) Todorova, B. N.; Steijl, R. Quantum algorithm for the collisionless Boltzmann equation. *J. Comput. Phys.* **2020**, *409*, 109347.
- (319) Budinski, L. Quantum algorithm for the Navier-Stokes equations. *arXiv* **2021**; <https://arxiv.org/pdf/2103.03804.pdf> (accessed 2022-01-05).
- (320) Givi, P. Machine learning and quantum computing for reactive turbulence modeling and simulation. *Mechanics Research Communications* **2021**, *116*, 103759.
- (321) Engel, A.; Smith, G.; Parker, S. E. Quantum algorithm for the Vlasov equation. *Phys. Rev. A* **2019**, *100*, 062315.
- (322) Shende, V. V.; Bullock, S. S.; Markov, I. L. Synthesis of quantum-logic circuits. *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems* **2006**, *25*, 1000–1010.
- (323) Eskandarpour, R.; Bahadur Ghosh, K. J.; Khodaei, A.; Paaso, A.; Zhang, L. Quantum-Enhanced Grid of the Future: A Primer. *IEEE Access* **2020**, *8*, 188993–189002.
- (324) Smelyanskiy, V. N.; Rieffel, E. G.; Knyshev, S. I., A Near-Term Quantum Computing Approach for Hard Computational Problems in Space Exploration. *arXiv* **2012**; <https://arxiv.org/pdf/1204.2821.pdf> (accessed 2022-01-05).
- (325) Lee, C.-W.; Lin, B.-Y. Application of Hybrid Quantum Tabu Search with Support Vector Regression (SVR) for Load Forecasting. *Energies* **2016**, *9*, 873.
- (326) Lee, C.-W.; Lin, B.-Y. Applications of the Chaotic Quantum Genetic Algorithm with Support Vector Regression in Load Forecasting. *Energies* **2017**, *10*, 1832.
- (327) Jaksch, D.; Bruder, C.; Cirac, J. I.; Gardiner, C. W.; Zoller, P. Cold bosonic atoms in optical lattices. *Phys. Rev. Lett.* **1998**, *81*, 3108–3111.
- (328) Greiner, M.; Mandel, O.; Esslinger, T.; Hansch, T. W.; Bloch, I. Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms. *Nature* **2002**, *415*, 39–44.
- (329) Childs, A. M.; Maslov, D.; Nam, Y.; Ross, N. J.; Su, Y. Toward the first quantum simulation with quantum speedup. *Proc. Natl. Acad. Sci. U.S.A.* **2018**, *115*, 9456–9461.
- (330) Hensgens, T.; Fujita, T.; Janssen, L.; Li, X.; Van Diepen, C. J.; Reichl, C.; Wegscheider, W.; Das Sarma, S.; Vandersypen, L. M. K. Quantum simulation of a Fermi-Hubbard model using a semiconductor quantum dot array. *Nature* **2017**, *548*, 70–73.
- (331) Dallaire-Demers, P. L.; Wilhelm, F. K. Quantum gates and architecture for the quantum simulation of the Fermi-Hubbard model. *Phys. Rev. A* **2016**, *94*, 062304.
- (332) Micheli, A.; Brennen, G. K.; Zoller, P. A toolbox for lattice-spin models with polar molecules. *Nat. Phys.* **2006**, *2*, 341–347.
- (333) Friedenauer, A.; Schmitz, H.; Glueckert, J. T.; Porras, D.; Schaetz, T. Simulating a quantum magnet with trapped ions. *Nat. Phys.* **2008**, *4*, 757–761.
- (334) Simon, J.; Bakr, W. S.; Ma, R. C.; Tai, M. E.; Preiss, P. M.; Greiner, M. Quantum simulation of antiferromagnetic spin chains in an optical lattice. *Nature* **2011**, *472*, 307–U200.
- (335) Vinen, W. F.; Niemela, J. J. Quantum turbulence. *Journal of Low Temperature Physics* **2002**, *128*, 167–231.
- (336) Yamaguchi, F.; Yamamoto, Y. Quantum simulation of the t-J model. *Superlattices Microstruct.* **2002**, *32*, 343–345.
- (337) Wu, L. A.; Byrd, M. S.; Lidar, D. A. Polynomial-time simulation of pairing models on a quantum computer. *Phys. Rev. Lett.* **2002**, *89*, 057904.
- (338) Yang, X. D.; Wang, A. M.; Xu, F.; Du, J. F. Experimental simulation of a pairing Hamiltonian on an NMR quantum computer. *Chem. Phys. Lett.* **2006**, *422*, 20–24.
- (339) Han, Y. J.; Raussendorf, R.; Duan, L. M. Scheme for demonstration of fractional statistics of anyons in an exactly solvable model. *Phys. Rev. Lett.* **2007**, *98*, 150404.
- (340) Rakhmanov, A. L.; Zagorskin, A. M.; Savel’ev, S.; Nori, F. Quantum metamaterials: Electromagnetic waves in a Josephson qubit line. *Phys. Rev. B* **2008**, *77*, 144507.
- (341) Lemeshko, M.; Yao, N. Y.; Gorshkov, A. V.; Weimer, H.; Bennett, S. D.; Momose, T.; Gopalakrishnan, S. Controllable quantum spin glasses with magnetic impurities embedded in quantum solids. *Phys. Rev. B* **2013**, *88*, 014426.
- (342) Zhang, J. F.; Cucchietti, F. M.; Chandrashekhar, C. M.; Laforest, M.; Ryan, C. A.; Ditty, M.; Hubbard, A.; Gamble, J. K.; Laflamme, R. Direct observation of quantum criticality in Ising spin chains. *Phys. Rev. A* **2009**, *79*, 012305.
- (343) Alvarez, G. A.; Suter, D. NMR Quantum Simulation of Localization Effects Induced by Decoherence. *Phys. Rev. Lett.* **2010**, *104*, 230403.
- (344) Bauer, B.; Bravyi, S.; Motta, M.; Chan, G. K. L. Quantum Algorithms for Quantum Chemistry and Quantum Materials Science. *Chem. Rev.* **2020**, *120*, 12685–12717.
- (345) McArdle, S.; Endo, S.; Aspuru-Guzik, A.; Benjamin, S.; Yuan, X. Quantum computational chemistry. *Rev. Mod. Phys.* **2020**, *92*, 015003.
- (346) McCaskey, A. J.; Parks, Z. P.; Jakowski, J.; Moore, S. V.; Morris, T. D.; Humble, T. S.; Pooser, R. C. Quantum chemistry as a benchmark for near-term quantum computers. *Npj Quantum Information* **2019**, *5*, 99.
- (347) Cheng, H. P.; Deumens, E.; Freericks, J. K.; Li, C. L.; Sanders, B. A. Application of Quantum Computing to Biochemical Systems: A Look to the Future. *Frontiers in Chemistry* **2020**, *8*, 587143.
- (348) Saha, S.; Rakshit, A.; Chakraborty, D.; Pal, A.; Deb, B. Optical Feshbach resonances through a molecular dark state: Efficient

- manipulation of p-wave resonances in fermionic Yb-171 atoms. *Phys. Rev. A* **2014**, *90*, 012701.
- (349) Hofer, M.; Riegger, L.; Scazza, F.; Hofrichter, C.; Fernandes, D. R.; Parish, M. M.; Levinsen, J.; Bloch, I.; Folling, S. Observation of an Orbital Interaction-Induced Feshbach Resonance in Yb-173. *Phys. Rev. Lett.* **2015**, *115*, 265302.
- (350) Luhmann, D. S.; Weitenberg, C.; Sengstock, K. Emulating Molecular Orbitals and Electronic Dynamics with Ultracold Atoms. *Physical Review X* **2015**, *5*, 031016.
- (351) Kaufman, A. M.; Lester, B. J.; Foss-Feig, M.; Wall, M. L.; Rey, A. M.; Regal, C. A. Entangling two transportable neutral atoms via local spin exchange. *Nature* **2015**, *527*, 208–211.
- (352) Olson, J.; Cao, Y.; Romero, J.; Johnson, P.; Dallaire-Demers, P.-L.; Sawaya, N.; Narang, P.; Kivlichan, I.; Wasielewski, M.; Aspuru-Guzik, A. NSF Workshop Report: Quantum Information and Computation for Chemistry. *arXiv* **2016**; <https://arxiv.org/ftp/arxiv/papers/1706/1706.05413.pdf> (accessed 2022-01-05).
- (353) Arguello-Luengo, J.; Gonzalez-Tudela, A.; Shi, T.; Zoller, P.; Cirac, J. I. Analogue quantum chemistry simulation. *Nature* **2019**, *574*, 215–218.
- (354) Wen, J. W.; Kong, X. Y.; Wei, S. J.; Wang, B. X.; Xin, T.; Long, G. L. Experimental realization of quantum algorithms for a linear system inspired by adiabatic quantum computing. *Phys. Rev. A* **2019**, *99*, 012320.
- (355) Somaroo, S.; Tseng, C. H.; Havel, T. F.; Laflamme, R.; Cory, D. G. Quantum simulations on a quantum computer. *Phys. Rev. Lett.* **1999**, *82*, 5381–5384.
- (356) Brown, K. R.; Clark, R. J.; Chuang, I. L. Limitations of quantum simulation examined by simulating a pairing hamiltonian using nuclear magnetic resonance. *Phys. Rev. Lett.* **2006**, *97*, 050504.
- (357) Negrevergne, C.; Somma, R.; Ortiz, G.; Knill, E.; Laflamme, R. Liquid-state NMR simulations of quantum many-body problems. *Phys. Rev. A* **2005**, *71*, 032344.
- (358) Du, J. F.; Xu, N. Y.; Peng, X. H.; Wang, P. F.; Wu, S. F.; Lu, D. W. NMR Implementation of a Molecular Hydrogen Quantum Simulation with Adiabatic State Preparation. *Phys. Rev. Lett.* **2010**, *104*, 030502.
- (359) Lu, D. W.; Xu, N. Y.; Xu, R. X.; Chen, H. W.; Gong, J. B.; Peng, X. H.; Du, J. F. Simulation of Chemical Isomerization Reaction Dynamics on a NMR Quantum Simulator. *Phys. Rev. Lett.* **2011**, *107*, 020501.
- (360) Lu, D. W.; Xu, N. Y.; Xu, B. R.; Li, Z. K.; Chen, H. W.; Peng, X. H.; Xu, R. X.; Du, J. F. Experimental study of quantum simulation for quantum chemistry with a nuclear magnetic resonance simulator. *Philosophical Transactions of the Royal Society a-Mathematical Physical and Engineering Sciences* **2012**, *370*, 4734–4747.
- (361) Zhen, X. L.; Zhang, F. H.; Feng, G. R.; Li, H.; Long, G. L. Optimal experimental dynamical decoupling of both longitudinal and transverse relaxations. *Phys. Rev. A* **2016**, *93*, 022304.
- (362) Ahmed, Z.; Alexeev, Y.; Apollinari, G.; Arvanitaki, A.; Awschalom, D.; Berggren, K. K.; Bibber, K. V.; Bienias, P.; Bodwin, G.; Boshier, M.; Bowring, D.; Braga, D.; Byrum, K.; Cancelo, G.; Carosi, G.; Cecil, T.; Chang, C.; Checchin, M.; Chekanov, S.; Chou, A.; Clerk, A.; Cloet, I.; Crisler, M.; Demarteau, M.; Dharmapalan, R.; Dietrich, M.; Ding, J.; Djuricic, Z.; Doyle, J.; Fast, J.; Fazio, M.; Fierlinger, P.; Finkel, H.; Fox, P.; Gabrielse, G.; Gaponenko, A.; Garcia-Sciveres, M.; Geraci, A.; Guest, J.; Guha, S.; Habib, S.; Harnik, R.; Helmy, A.; Heng, Y.; Henning, J.; Heremans, J.; Ho, P.; Hogan, J.; Hubmayr, J.; Hume, D.; Irwin, K.; Jenks, C.; Karonis, N.; Kettimuthu, R.; Kimball, D.; King, J.; Kovacs, E.; Kriske, R.; Kubik, D.; Kusaka, A.; Lawrie, B.; Lehnert, K.; Lett, P.; Lewis, J.; Lougovski, P.; Lurio, L.; Ma, X.; May, E.; Merkel, P.; Metcalfe, J.; Miceli, A.; Min, M.; Miryala, S.; Mitchell, J.; Mitrovic, V.; Mueller, H.; Nam, S. W.; Nguyen, H.; Nicholson, H.; Nomerotski, A.; Norman, M.; O'Brien, K.; O'Brient, R.; Patel, U.; Penning, B.; Perverzev, S.; Peters, N.; Pooser, R.; Posada, C.; Proudfoot, J.; Rabqa, T.; Rajh, T.; Rescia, S.; Romanenko, A.; Rusack, R.; Schleier-Smith, M.; Schwab, K.; Segal, J.; Shipsey, I.; Shirokoff, E.; Sonnenschein, A.; Taylor, V.; Tschirhart, R.; Tully, C.; Underwood, D.; Vuletic, V.; Wagner, R.; Wang, G.; Weerts, H.; Woollett, N.; Xie, J.; Yefremenko, V.; Zasadzinski, J.; Zhang, J.; Zhang, X.; Zutshi, V. Quantum Sensing for High Energy Physics. *arXiv* **2018**; <https://arxiv.org/abs/1803.11306> (accessed 2022-01-05).
- (363) O'Malley, P. J. J.; Babbush, R.; Kivlichan, I. D.; Romero, J.; McClean, J. R.; Barends, R.; Kelly, J.; Roushan, P.; Tranter, A.; Ding, N.; Campbell, B.; Chen, Y.; Chen, Z.; Chiaro, B.; Dunsworth, A.; Fowler, A. G.; Jeffrey, E.; Lucero, E.; Megrant, A.; Mutus, J. Y.; Neeley, M.; Neill, C.; Quintana, C.; Sank, D.; Vainsencher, A.; Wenner, J.; White, T. C.; Coveney, P. V.; Love, P. J.; Neven, H.; Aspuru-Guzik, A.; Martinis, J. M. Scalable Quantum Simulation of Molecular Energies. *Physical Review X* **2016**, *6*, 031007.
- (364) You, J. Q.; Nori, F. Superconducting circuits and quantum information. *Phys. Today* **2005**, *58*, 42–47.
- (365) Grajcar, M.; Van der Ploeg, S. H. W.; Izmalkov, A.; Il'ichev, E.; Meyer, H. G.; Fedorov, A.; Shnirman, A.; Schon, G. Sisyphus cooling and amplification by a superconducting qubit. *Nat. Phys.* **2008**, *4*, 612–616.
- (366) Cloët, I. C.; Dietrich, M. R.; Arrington, J.; A, B.; Bishop, M.; Freese, A.; Gorshkov, A. V.; A, G.; Hafidi, K.; Z, J.; McGuigan, M.; Meurice, Y.; Meziani, Z.-E.; Mueller, P.; Muschik, C.; Osborn, J.; Otten, M.; Petreczky, P.; Polakovic, T.; Poon, A.; Pooser, R.; Roggero, A.; Saffman, M.; VanDevender, B.; Zhang, J.; Zohar, E. Opportunities for Nuclear Physics & Quantum Information Science. *arXiv* **2019**; <https://arxiv.org/pdf/1903.05453.pdf> (accessed 2022-01-05).
- (367) Boghosian, B. M.; Taylor, W. Simulating quantum mechanics on a quantum computer. *Physica D-Nonlinear Phenomena* **1998**, *120*, 30–42.
- (368) Bermudez, A.; Martin-Delgado, M. A.; Solano, E. Exact mapping of the 2 + 1 Dirac oscillator onto the Jaynes-Cummings model: Ion-trap experimental proposal. *Phys. Rev. A* **2007**, *76*, 041801.
- (369) Lamata, L.; Leon, J.; Schatz, T.; Solano, E. Dirac equation and quantum relativistic effects in a single trapped ion. *Phys. Rev. Lett.* **2007**, *98*, 253005.
- (370) Gerritsma, R.; Kirchmair, G.; Zahringer, F.; Solano, E.; Blatt, R.; Roos, C. F. Quantum simulation of the Dirac equation. *Nature* **2010**, *463*, 68–U72.
- (371) Gerritsma, R.; Lanyon, B. P.; Kirchmair, G.; Zahringer, F.; Hempel, C.; Casanova, J.; Garcia-Ripoll, J. J.; Solano, E.; Blatt, R.; Roos, C. F. Quantum Simulation of the Klein Paradox with Trapped Ions. *Phys. Rev. Lett.* **2011**, *106*, 060503.
- (372) Byrnes, T.; Kim, N. Y.; Kusudo, K.; Yamamoto, Y. Quantum simulation of Fermi-Hubbard models in semiconductor quantum-dot arrays. *Phys. Rev. B* **2008**, *78*, 075320.
- (373) Hauke, P.; Marcos, D.; Dalmonte, M.; Zoller, P. Quantum Simulation of a Lattice Schwinger Model in a Chain of Trapped Ions. *Physical Review X* **2013**, *3*, 041018.
- (374) Semiao, F. L.; Paternostro, M. Quantum circuits for spin and flavor degrees of freedom of quarks forming nucleons. *Quantum Information Processing* **2012**, *11*, 67–75.
- (375) Davoudi, Z.; Hafezi, M.; Monroe, C.; Pagano, G.; Seif, A.; Shaw, A. Towards analog quantum simulations of lattice gauge theories with trapped ions. *Physical Review Research* **2020**, *2*, 023015.
- (376) Nation, P. D.; Blencowe, M. P.; Rimberg, A. J.; Buks, E. Analogue Hawking Radiation in a dc-SQUID Array Transmission Line. *Phys. Rev. Lett.* **2009**, *103*, 078004.
- (377) Gerace, D.; Carusotto, I. Analog Hawking radiation from an acoustic black hole in a flowing polariton superfluid. *Phys. Rev. B* **2012**, *86*, 144505.
- (378) Nation, P. D.; Johansson, J. R.; Blencowe, M. P.; Nori, F. Colloquium: Stimulating uncertainty: Amplifying the quantum vacuum with superconducting circuits. *Rev. Mod. Phys.* **2012**, *84*, 1–24.
- (379) Li, K. R.; Li, Y. N.; Han, M. X.; Lu, S. R.; Zhou, J.; Ruan, D.; Long, G. L.; Wan, Y. D.; Lu, D. W.; Zeng, B.; Laflamme, R. Quantum spacetime on a quantum simulator. *Communications Physics* **2019**, *2*, 122.

- (380) Chiuri, A.; Greganti, C.; Mazzola, L.; Paternostro, M.; Mataloni, P. Linear Optics Simulation of Quantum Non-Markovian Dynamics. *Sci. Rep.* **2012**, *2*, 968.
- (381) National Strategic Overview for Quantum Information Science; <https://www.whitehouse.gov/wp-content/uploads/2018/09/National-Strategic-Overview-for-Quantum-Information-Science.pdf> (accessed 2022-01-05).
- (382) Raymer, M. G.; Monroe, C. The US National Quantum Initiative. *Quantum Science and Technology* **2019**, *4*, 020504.
- (383) Knight, P.; Walmsley, I. UK national quantum technology programme. *Quantum Science and Technology* **2019**, *4*, 040502.
- (384) Harris, M. Europe pledges 1bn euros for applied quantum technology. *Phys. World* **2018**, *31*, 8.
- (385) Riedel, M.; Kovacs, M.; Zoller, P.; Mlynek, J.; Calarco, T. Europe's Quantum Flagship initiative. *Quantum Science and Technology* **2019**, *4*, 020501.
- (386) Zhang, Q.; Xu, F. H.; Li, L.; Liu, N. L.; Pan, J. W. Quantum information research in China. *Quantum Science and Technology* **2019**, *4*, 040503.
- (387) Yin, J.; Cao, Y.; Li, Y. H.; Liao, S. K.; Zhang, L.; Ren, J. G.; Cai, W. Q.; Liu, W. Y.; Li, B.; Dai, H.; Li, G. B.; Lu, Q. M.; Gong, Y. H.; Xu, Y.; Li, S. L.; Li, F. Z.; Yin, Y. Y.; Jiang, Z. Q.; Li, M.; Jia, J. J.; Ren, G.; He, D.; Zhou, Y. L.; Zhang, X. X.; Wang, N.; Chang, X.; Zhu, Z. C.; Liu, N. L.; Chen, Y. A.; Lu, C. Y.; Shu, R.; Peng, C. Z.; Wang, J. Y.; Pan, J. W. Satellite-based entanglement distribution over 1200 kilometers. *Science* **2017**, *356*, 1140–1144.
- (388) Ren, J. G.; Xu, P.; Yong, H. L.; Zhang, L.; Liao, S. K.; Yin, J.; Liu, W. Y.; Cai, W. Q.; Yang, M.; Li, L.; Yang, K. X.; Han, X.; Yao, Y. Q.; Li, J.; Wu, H. Y.; Wan, S.; Liu, L.; Liu, D. Q.; Kuang, Y. W.; He, Z. P.; Shang, P.; Guo, C.; Zheng, R. H.; Tian, K.; Zhu, Z. C.; Liu, N. L.; Lu, C. Y.; Shu, R.; Chen, Y. A.; Peng, C. Z.; Wang, J. Y.; Pan, J. W. Ground-to-satellite quantum teleportation. *Nature* **2017**, *549*, 70–73.
- (389) Yamamoto, Y.; Sasaki, M.; Takesue, H. Quantum information science and technology in Japan. *Quantum Science and Technology* **2019**, *4*, 020502.
- (390) Careers and people. *Phys. World* **2018**, *31*, 51–51.
- (391) Government of Canada launches public consultations on National Quantum Strategy; <https://www.canada.ca/en/innovation-science-economic-development/news/2021/07/government-of-canada-launches-public-consultations-on-national-quantum-strategy.html> (accessed 2021-12-21).
- (392) Roberson, T.; Leach, J.; Raman, S. Talking about public good for the second quantum revolution: analysing quantum technology narratives in the context of national strategies. *Quantum Science and Technology* **2021**, *6*, 025001.
- (393) Schiermeier, Q. Russia joins race to make quantum dreams a reality. *Nature* **2020**, *577*, 14.
- (394) Padma, T. V. India bets big on quantum technology. *Nature* **2020**, DOI: [10.1038/d41586-020-00288-x](https://doi.org/10.1038/d41586-020-00288-x).
- (395) Atos and SENAI CIMATEC launch Center of Excellence in Quantum Computing in Brazil; <https://atos.net/wp-content/uploads/2021/05/PR-Atos-and-SENAI-CIMATEC-launch-Center-of-Excellence-in-Quantum-Computing-in-Brazil.pdf> (accessed 2021-12-21).
- (396) Venegas-Gomez, A. Creating a quantum community in Latin America. *Education and Training in Optics & Photonics Conference*; Danner, A. P.-G. A.; Wong, N., Eds.; Optical Society of America: Washington, DC, 2021; p W4A1.
- (397) Quantum leap Africa; <https://quantumleapafrika.org/> (accessed 2022-01-05).
- (398) Forbes, A.; Petruccione, F.; Roux, F. S. Toward a quantum future for South Africa. *AVS Quantum Science* **2021**, *3*, 040501.
- (399) Shim, H. Korea Starts Five-year Development Program for Quantum Computing Technology; <https://k-erc.eu/korea-starts-five-year-development-program-for-quantum-computing-technology/> (accessed 2022-01-05).
- (400) Singh, S. K.; Azzaoui, A. E.; Salim, M. M.; Park, J. H. Quantum Communication Technology for Future ICT – Review. *Journal of Information Processing Systems* **2020**, *16*, 1459–1478.
- (401) Abu Dhabi builds region's first-ever quantum computer; <https://www.khaleejtimes.com/technology/abu-dhabi-builds-regions-first-ever-quantum-computer> (accessed 2022-01-05).
- (402) Israel allocates 60 million to build-first quantum computer; <https://www.bloomberg.com/news/articles/2021-03-03/israel-allocates-60-million-to-build-first-quantum-computer> (accessed 2021-12-21).
- (403) French President Details €1.8b Quantum Plan; <https://www.eetimes.eu/french-president-details-e1-8b-quantum-plan/> (accessed 2021-12-21).
- (404) Normile, D. Flocking to Asia For a Shot at Greatness. *Science* **2012**, *337*, 1162–1166.
- (405) Huang, T.-t. Taiwan aims high with quantum technology investment; <https://www.taiwannews.com.tw/en/news/4071610> (accessed 2021-12-21).
- (406) Ferranti, M. The Netherlands made a huge bet on quantum computing — will it pay off? <https://www.cio.com/article/191607/the-netherlands-made-a-huge-bet-on-quantum-computing-will-it-pay-off.html> (accessed 2021-12-21).
- (407) National quantum initiative supplement to the president's FY 2022 budget; www.quantum.gov/wp-content/uploads/2021/12/NQI-Annual-Report-FY2022.pdf (accessed 2022-01-10).
- (408) Kim, Z.; Suri, B.; Zaretsky, V.; Novikov, S.; Osborn, K. D.; Mizel, A.; Wellstood, F. C.; Palmer, B. S. Decoupling a Cooper-Pair Box to Enhance the Lifetime to 0.2 ms. *Phys. Rev. Lett.* **2011**, *106*, 120501.
- (409) Siddiqi, I. Engineering high-coherence superconducting qubits. *Nature Reviews Materials* **2021**, *6*, 875–891.
- (410) Tinkham, M. *Introduction to Superconductivity*, 2nd ed.; McGraw-Hill Book Co.: New York, 1996.
- (411) Zeng, L. J.; Nik, S.; Greibe, T.; Krantz, P.; Wilson, C. M.; Delsing, P.; Olsson, E. Direct observation of the thickness distribution of ultra thin AlO_x barriers in Al/AlO_x/Al Josephson junctions. *J. Phys. D: Appl. Phys.* **2015**, *48*, 395308.
- (412) Tolpygo, S. K.; Bolkhovsky, V.; Weir, T. J.; Wynn, A.; Oates, D. E.; Johnson, L. M.; Gouker, M. A. Advanced Fabrication Processes for Superconducting Very Large-Scale Integrated Circuits. *Ieee Transactions on Applied Superconductivity* **2016**, *26*, 1100110.
- (413) Kreikebaum, J. M.; O'Brien, K. P.; Morvan, A.; Siddiqi, I. Improving wafer-scale Josephson junction resistance variation in superconducting quantum coherent circuits. *Superconductor Science & Technology* **2020**, *33*, 06LT02.
- (414) Doherty, M. W.; Manson, N. B.; Delaney, P.; Jelezko, F.; Wrachtrup, J.; Hollenberg, L. C. L. The nitrogen-vacancy colour centre in diamond. *Physics Reports-Review Section of Physics Letters* **2013**, *528*, 1–45.
- (415) Jelezko, F.; Wrachtrup, J. Single defect centres in diamond: A review. *Physica Status Solidi a-Applications and Materials Science* **2006**, *203*, 3207–3225.
- (416) Rong, X.; Geng, J. P.; Shi, F. Z.; Liu, Y.; Xu, K. B.; Ma, W. C.; Kong, F.; Jiang, Z.; Wu, Y.; Du, J. F. Experimental fault-tolerant universal quantum gates with solid-state spins under ambient conditions. *Nat. Commun.* **2015**, *6*, 8748.
- (417) Wolfowicz, G.; Anderson, C. P.; Diler, B.; Poluektov, O. G.; Heremans, F. J.; Awschalom, D. D. Vanadium spin qubits as telecom quantum emitters in silicon carbide. *Science Advances* **2020**, *6*, No. eaaz1192.
- (418) Kindem, J. M.; Ruskuc, A.; Bartholomew, J. G.; Rochman, J.; Huan, Y. Q.; Faraon, A. Control and single-shot readout of an ion embedded in a nanophotonic cavity. *Nature* **2020**, *580*, 201–204.
- (419) Chen, S. T.; Raha, M.; Phenicie, C. M.; Ourari, S.; Thompson, J. D. Parallel single-shot measurement and coherent control of solid-state spins below the diffraction limit. *Science* **2020**, *370*, 592–595.
- (420) Lu, L.; Joannopoulos, J. D.; Soljacic, M. Topological photonics. *Nat. Photonics* **2014**, *8*, 821–829.
- (421) Ozawa, T.; Price, H. M.; Amo, A.; Goldman, N.; Hafezi, M.; Lu, L.; Rechtsman, M. C.; Schuster, D.; Simon, J.; Zilberberg, O.; Carusotto, I. Topological photonics. *Rev. Mod. Phys.* **2019**, *91*, 015006.

- (422) Hafezi, M.; Demler, E. A.; Lukin, M. D.; Taylor, J. M. Robust optical delay lines with topological protection. *Nat. Phys.* **2011**, *7*, 907–912.
- (423) Wang, Z.; Chong, Y. D.; Joannopoulos, J. D.; Soljacic, M. Observation of unidirectional backscattering-immune topological electromagnetic states. *Nature* **2009**, *461*, 772–U20.
- (424) Kitaev, A. Y. Fault-tolerant quantum computation by anyons. *Annals of Physics* **2003**, *303*, 2–30.
- (425) Fu, L.; Kane, C. L. Superconducting proximity effect and Majorana fermions at the surface of a topological insulator. *Phys. Rev. Lett.* **2008**, *100*, 096407.
- (426) Xu, J. P.; Wang, M. X.; Liu, Z. L.; Ge, J. F.; Yang, X. J.; Liu, C. H.; Xu, Z. A.; Guan, D. D.; Gao, C. L.; Qian, D.; Liu, Y.; Wang, Q. H.; Zhang, F. C.; Xue, Q. K.; Jia, J. F. Experimental Detection of a Majorana Mode in the core of a Magnetic Vortex inside a Topological Insulator-Superconductor $\text{Bi}_2\text{Te}_3/\text{NbSe}_2$ Heterostructure. *Phys. Rev. Lett.* **2015**, *114*, 017001.
- (427) Lian, B.; Sun, X. Q.; Vaezi, A.; Qi, X. L.; Zhang, S. C. Topological quantum computation based on chiral Majorana fermions. *Proc. Natl. Acad. Sci. U.S.A.* **2018**, *115*, 10938–10942.
- (428) Phillips, W. D. Laser cooling and trapping of neutral atoms. *Rev. Mod. Phys.* **1998**, *70*, 721–741.
- (429) Sherson, J. F.; Weitenberg, C.; Endres, M.; Cheneau, M.; Bloch, I.; Kuhr, S. Single-atom-resolved fluorescence imaging of an atomic Mott insulator. *Nature* **2010**, *467*, 68–72.
- (430) Omran, A.; Levine, H.; Keesling, A.; Semeghini, G.; Wang, T. T.; Ebadi, S.; Bernien, H.; Zibrov, A. S.; Pichler, H.; Choi, S.; Cui, J.; Rossignolo, M.; Rembold, P.; Montangero, S.; Calarco, T.; Endres, M.; Greiner, M.; Vuletic, V.; Lukin, M. D. Generation and manipulation of Schrödinger cat states in Rydberg atom arrays. *Science* **2019**, *365*, 570–574.
- (431) Thompson, J. D.; Nicholson, T. L.; Liang, Q. Y.; Cantu, S. H.; Venkatramani, A. V.; Choi, S.; Fedorov, I. A.; Viscor, D.; Pohl, T.; Lukin, M. D.; Vuletic, V. Symmetry-protected collisions between strongly interacting photons. *Nature* **2017**, *542*, 206–209.
- (432) Asenjo-Garcia, A.; Moreno-Cardoner, M.; Albrecht, A.; Kimble, H. J.; Chang, D. E. Exponential Improvement in Photon Storage Fidelities Using Subradiance and “Selective Radiance” in Atomic Arrays. *Physical Review X* **2017**, *7*, 031024.
- (433) Bekenstein, R.; Pikovski, I.; Pichler, H.; Shahmoon, E.; Yelin, S. F.; Lukin, M. D. Quantum metasurfaces with atom arrays. *Nat. Phys.* **2020**, *16*, 676–681.
- (434) Olekhno, N. A.; Kretov, E. I.; Stepanenko, A. A.; Ivanova, P. A.; Yaroshenko, V. V.; Puhtina, E. M.; Filonov, D. S.; Cappello, B.; Matekovits, L.; Gorlach, M. A. Topological edge states of interacting photon pairs emulated in a topoelectrical circuit. *Nat. Commun.* **2020**, *11*, 1436.
- (435) Wei, H. R.; Long, G. L. Hybrid quantum gates between flying photon and diamond nitrogen-vacancy centers assisted by optical microcavities. *Sci. Rep.* **2015**, *5*, 12918.
- (436) Vernooy, D. W.; Furusawa, A.; Georgiades, N. P.; Ilchenko, V. S.; Kimble, H. J. Cavity QED with high-Q whispering gallery modes. *Phys. Rev. A* **1998**, *57*, R2293–R2296.
- (437) Nielsen, M. A. Cluster-state quantum computation. *Reports on Mathematical Physics* **2006**, *57*, 147–161.
- (438) Lu, C. Y.; Zhou, X. Q.; Guhne, O.; Gao, W. B.; Zhang, J.; Yuan, Z. S.; Goebel, A.; Yang, T.; Pan, J. W. Experimental entanglement of six photons in graph states. *Nat. Phys.* **2007**, *3*, 91–95.
- (439) Yokoyama, S.; Ukai, R.; Armstrong, S. C.; Sornphiphatphong, C.; Kaji, T.; Suzuki, S.; Yoshikawa, J.; Yonezawa, H.; Menicucci, N. C.; Furusawa, A. Ultra-large-scale continuous-variable cluster states multiplexed in the time domain. *Nat. Photonics* **2013**, *7*, 982–986.
- (440) Raussendorf, R.; Browne, D. E.; Briegel, H. J. Measurement-based quantum computation on cluster states. *Phys. Rev. A* **2003**, *68*, 022312.
- (441) Asavanant, W.; Shiozawa, Y.; Yokoyama, S.; Charoensombutamon, B.; Emura, H.; Alexander, R. N.; Takeda, S.; Yoshikawa, J.; Menicucci, N. C.; Yonezawa, H.; Furusawa, A. Generation of time-domain-multiplexed two-dimensional cluster state. *Science* **2019**, *366*, 373–376.
- (442) Quantum Computing Technology Update Across the Energy; <https://www.epri.com/research/products/00000003002019627> (accessed 2021-12-21).
- (443) Giani, A. Quantum computing opportunities in renewable energy. *Nature Computational Science* **2021**, *1*, 90–91.
- (444) Giani, A.; Eldredge, Z. Quantum Computing Opportunities in Renewable Energy. *SN Computer Science* **2021**, *2*, 393.
- (445) Ho, A.; McClean, J.; Ong, S. P. The Promise and Challenges of Quantum Computing for Energy Storage. *Joule* **2018**, *2*, 810–813.
- (446) Jones, J. S. Going atomic scale with quantum computing in the power sector; <https://www.smart-energy.com/industry-sectors/digitalisation/going-atomic-scale-with-quantum-computing-in-the-power-sector/> (accessed 2021-12-21).
- (447) Herhold, A. Quantum computing research at ExxonMobil. Q2B 2020; <https://www.youtube.com/watch?v=OrBR7aUSL40> (accessed 2121-12-21).
- (448) Brasington, L. A Quantum Leap for Energy and Power; <https://www.cleantech.com/a-quantum-leap-for-energy-and-power/> (accessed 2021-12-21).
- (449) Alqarqaz, Q. How Microsoft Could Redefine the Power Industry with Quantum Computing; <https://spectrum.ieee.org/how-microsoft-could-redefine-the-power-industry-with-quantum-computing> (accessed 2021-12-21).
- (450) Ajagekar, A.; You, F. Q. Quantum computing for energy systems optimization: Challenges and opportunities. *Energy* **2019**, *179*, 76–89.
- (451) Khodaei, A. How quantum computing is poised to support sustainable power grids; <https://www.greenbiz.com/article/how-quantum-computing-poised-support-sustainable-power-grids> (accessed 2021-12-21).
- (452) McMillin, P.; Fontana, C. Introducing Quantum Computing into the World of Energy and Utilities; <https://centricconsulting.com/blog/introducing-quantum-computing-into-the-world-of-energy-and-utilities/> (accessed 2021-12-21).
- (453) Parney, B.; Garcia, J.; Womack, D. Exploring quantum use cases for chemicals and petroleum. *IBM* **2019**; <https://www.ibm.com/thought-leadership/institute-business-value/report/quantum-chemical-petroleum#> (accessed 2021-12-21).
- (454) BP and IBM Quantum Network to Advance Use of Quantum Computing in Energy; <https://energyindustryreview.com/tech/bp-and-ibm-quantum-network-to-advance-use-of-quantum-computing-in-energy/> (accessed 2021-12-21).
- (455) Lessard, R. Quantum Computing Applications for the Energy Industry; <https://www.software.slb.com/blog/quantum-computing-applications-for-the-energy-industry> (accessed 2021-12-21).