

# Quantum Chemistry

Matthew N. O. Sadiku<sup>1</sup>, Janet O. Sadiku<sup>2</sup>

<sup>1</sup>Roy G. Perry College of Engineering, Prairie View A&M University, Prairie View, TX, USA

<sup>2</sup>Juliana King University, Houston, TX, USA

## ABSTRACT

Quantum chemistry applies quantum mechanics to understand and predict the behavior, structure, and properties of molecules, explaining chemical bonding, reactions, and spectroscopy. Understanding electronic structure and molecular dynamics through the development of computational solutions to the Schrödinger equation is a central goal of quantum chemistry. Quantum chemistry aims to accurately describe various chemical and physical properties of molecules and materials in a very systematic manner. We are entering an exciting new technological era where we can harness the power of individual quantum particles to create a new generation of technology. These quantum technologies will give rise to unparalleled computational capabilities and reshape our notions of security and privacy. The paper examines quantum chemistry and its applications.

**KEYWORDS:** *technology, quantum computing, QC, chemistry, quantum chemistry.*

## INTRODUCTION

Computing has revolutionized science. Advances in classical computing have produced a number of powerful new computing strategies, including parallelization, graphics processing unit computing, and machine learning. Quantum computing has emerged as a candidate to overcome the limits of classical computers. Some of the most exciting potential applications of quantum computers are in the field of chemistry, where more powerful computer simulations could directly lead to significant advancements in areas such as medicine, materials science, energy science, catalysis, and nanotechnology. As a result, chemistry has a prominent position at the forefront of quantum computing developments, leading to quantum chemistry [1].

Quantum chemistry is a powerful tool to study the properties of molecules and their reactions. Recent advances in quantum chemistry methods has made it possible for quantum chemistry calculations to reach accuracies comparable to those obtained in experiments for molecules of moderate sizes. The impact of quantum chemistry has grown with advances in theory, mathematics, and computation, leading to the increase of several orders of magnitude

in the size of systems, which can be described by quantum chemistry.

## QUANTUM COMPUTERS

A quantum computer (QC) behaves according to the laws of quantum mechanics. Thus, quantum computers are different from binary digital electronic computers based on transistors. A major difference between classical and quantum computing lies in the way they encode data. While a digital computer requires that the data be encoded into binary digits (0 or 1), quantum computers use quantum bits, which can be in superpositions of states [2]. In other words, instead of storing information in bits as conventional digital computers do, quantum computers use quantum bits, or qubits, to encode information. (Qubits are the basic units of quantum information.) In addition to ones and zeros, qubits have a third state called “superposition” that allows them to represent a one or a zero at the same time. Figure 1 shows the comparison between the bit and qubit [3]. The computing power of a QC grows exponentially with the number of qubits it uses.

Quantum computers have the potential to perform certain calculations significantly faster than any digital computers. QC consists of a quantum

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processor which operates at a very low temperature (a few tens of mK) and an electronic controller which reads out and controls the quantum processors, as shown in Figure 2 [4]. Several forms of physical media (optical fibers and free space) can be used to deliver quantum information. Figure 3 shows a representation of quantum computing [5].

In quantum system, the computational space increases with the size of the system. This enables exponential parallelism which leads to faster quantum algorithms. Unlike classical computer, QC offers massive parallelism within a single piece of hardware.

A typical quantum computer is shown in Figure 4 [6]. The basic building blocks of quantum computers include quantum gates, quantum memories, quantum CPUs, quantum languages, and quantum languages [7,8]:

- *Quantum Gates:* Quantum computers require quantum gates, which are basically different from classical Boolean gates seen in a conventional computer (AND, XOR and so on). A quantum gate acts on superpositions of different basis states of qubits. The quantum gates perform unitary operations on quantum states and lead to quantum circuits. They are particularly important for quantum error correction and experimental quantum information processing. They can be realized by superconductors, linear optic tools, or quantum dots. Common quantum gates are CNOT and SWAP.
- *Quantum Memories:* Quantum memories store the quantum systems in a quantum register for information processing. Quantum memories are formulated by  $n$  stationary quantum states. Quantum computers are expected to have limited memory.
- *Quantum CPUs:* These use a quantum bus for the communication between the functional elements of a quantum computer. From a computing perspective, quantum CPUs can be approached through quantum adders.
- *Quantum Languages:* These enable us to create an artificial quantum computer to simulate a quantum computing environment. The programming language should follow a functional programming structure, which can compute the process as a whole entity with a proper bounded structure.
- *Quantum Algorithms:* Quantum algorithms are significantly faster than any classical algorithm in solving some problem. Most of the successful quantum algorithms use quantum Fourier transforms in them because they require less

hardware. Popular quantum algorithms include Shor's algorithm (since integer factorization is faster) and Grover's search algorithm.

In ambitious attempts to realize practical quantum computers, enormous efforts are still being expended both in designing software (quantum algorithms) and hardware development (physical implementation).

## QUANTUM CHEMISTRY

Quantum chemistry, also called molecular quantum mechanics, is a branch of physical chemistry focused on the application of quantum mechanics to chemical systems, particularly towards the quantum-mechanical calculation of electronic contributions to physical and chemical properties of molecules, materials, and solutions at the atomic level. It is the application of the methods of quantum mechanics to problems of chemical interest, particularly focusing on the organization of electrons in atomic, molecular, and supramolecular systems and their associated properties. In quantum chemistry, key quantum mechanics concepts like quantum states, the uncertainty principle, and wave-particle duality provide insights into the electronic structure and properties of atoms and molecules. Computational chemists use orbitals to describe the location and behavior of electrons in a molecule. Figure 5 shows an electronic structure [9], while Figure 6 shows a molecular spatial representation [10]. Understanding the behavior of matter at the level of molecules—how they bond, react, and change—is crucial for designing better materials, creating new medicines, and solving environmental challenges.

Quantum chemistry provides the fundamental quantum mechanical basis for chemistry, allowing scientists to understand and predict molecular behavior by modeling electrons and their interactions, pushing boundaries in both theoretical understanding and practical applications. It bridges physics and chemistry, revealing why substances behave as they do, crucial for fields from drug design to materials science. It studies how the laws of quantum mechanics can be applied to chemical models and experiments on chemical systems. It encompasses quantum phenomena at all levels, such as the electronic structure of matter. Figure 7 provides an artistic rendering of atomic structure [11].

Quantum chemistry may be applied to the prediction and verification of spectroscopic data as well as other experimental data. Chemists rely heavily on spectroscopy through which information regarding the quantization of energy on a molecular scale can be obtained. Quantum chemistry has a vast variety of different methods, with more accurate methods being generally slower.

Some regard the birth of quantum chemistry as starting with the discovery of the Schrödinger equation and its application to the hydrogen atom. The Schrödinger equation is a mathematical model for particles like electrons that simultaneously behave as waves. It describes the probabilities of where electrons can be found around molecules. It is a fundamental equation in quantum mechanics that describes the electron behavior within atoms and molecules. The first step in solving a quantum chemical problem is usually solving the Schrödinger equation (or Dirac equation in relativistic quantum chemistry) with the electronic molecular Hamiltonian. A further step can consist of solving the Schrödinger equation with the total molecular Hamiltonian in order to study the motion of molecules. This theoretical basis slowly began to be applied to chemical structure, reactivity, and bonding [12].

### APPLICATIONS OF QUANTUM CHEMISTRY

The field of quantum chemistry is so vast that it is impossible to cover all the different areas representing chemical applications. Applications focus on semiconductor materials for natural and artificial photosynthesis. They encompass simulating molecular structures and chemical reactions and advancing drug discovery and design, catalyst design, materials science, and data analytics. Key areas of applications include the following [13,14]:

- *Computational Quantum Chemistry*: This is a rapidly evolving field that is impacting all areas of chemical science through an ever-increasing range of applications at various levels of sophistication. It is rapidly becoming difficult to find forefront articles in top scientific journals without a subsection containing quantum chemical calculations and associated interpretations of the key findings. As the year-to-year gains in speeds of classical computers continue to taper off, computational chemists are increasingly examining quantum computing as a possible route to achieve greater computational performance. In the field of chemistry, quantum algorithm development offers promising propositions for solving classically intractable problems in areas such as electronic structure, chemical quantum dynamics, spectroscopy, and cheminformatics. Chemistry modeling is a natural attribute for quantum computers, although existing methods are impractical to develop near-perfect qubits. A typical result of such modeling is shown in Figure 8 [15].
- *Density Functional Theory (DFT)*: This is the standard method of choice for quantum chemistry because it can provide accurate structures and energies provided that a suitable density functional and basis set are used. DFT has transformed computational studies by approximating electron distributions through functionals—mathematical constructs that predict various energy components as functions of the electron density. Practical investigations of chemicals and materials on any significant scale rely heavily on DFT, which sidesteps this complexity by focusing on electron density rather than on individual electrons.
- *Variational Quantum Eigensolver (VQE)*: This is a hybrid quantum-classical algorithm suited for current, "noisy intermediate-scale quantum" (NISQ) devices. The VQE algorithm is an example of another quantum-classical hybrid algorithm, in which the computation utilizes the strengths of both quantum and classical computing hardware. VQE finds the lowest eigenvalue of Hamiltonians, particularly those in chemical systems. While VQE's application in solving the electronic Schrödinger equation for small molecules has shown success, its scalability is hindered by two main challenges: the complexity of the quantum circuits required and the intricacies involved in the classical optimization process.
- *Experimental Quantum Chemistry*: Experimental quantum chemists rely heavily on spectroscopy – IR spectroscopy, NMR spectroscopy, and scanning probe microscopy – to obtain information about the quantization of energy on a molecular scale. It has great value in supporting and interpreting experimental spectroscopic data. Quantum chemical theories allow us to explain the structure of the periodic table, and quantum chemical calculations allow us to accurately predict the structures of molecules and the spectroscopic behavior of atoms and molecules.
- *Quantum Information Processing*: Quantum information processing technology has attracted attention in recently emerging fields. Among many important and fundamental issues in science, solving the Schrödinger equation (SE) of atoms and molecules is one of the ultimate goals in chemistry, physics, and their related fields. SE is the first principle of non-relativistic quantum mechanics, whose solutions, termed wave functions, can afford any information of electrons within atoms and molecules, predicting their physicochemical properties and chemical reactions.
- *Drug Discovery*: In the future, more and more drugs, materials and catalysts will be designed,



tested, and developed using computer simulations alone. One particular example is catalysis, where elementary rate constants can be modeled using quantum chemical methods.

## BENEFITS

Quantum computing in chemistry holds immense promise, offering the potential to revolutionize our understanding of the structure and dynamics of complex molecular systems, thus accelerating scientific discovery across various fields. Quantum chemistry is a powerful tool to study the ground state of individual atoms and molecules, and the excited and transition states that arise during chemical reactions. Dynamic characteristics of complex chemical reactions can be accurately modeled by a quantum computer. Other benefits include the following [16]:

- *Quantum Networks*: These carry quantum information. We are researching how these networks can create a quantum Internet connecting quantum computers and sensors, as well as how quantum mechanics can unlock new possibilities in communication.
- *Quantum Security Technologies*: Quantum security must be at the forefront of any quantum technology discussion. As quantum computers become more powerful, they will be capable of breaking the most widely used security measures protecting our data and communications. Quantum security technologies will safeguard data and communications from the inevitable threat of quantum computers being used for malicious purposes. Researchers are developing a new generation of encryption to prevent future quantum attacks, as well as researching communications technology that will lock information behind the immutable laws of physics. Quantum technologies have the potential to revolutionize many aspects of the world we live in. They can create unbreakable security for our communications and data. Quantum-safe networks are part of the strategies for future-proof networks to counter emerging quantum security threats.
- *Quantum Sensing*: This will detect natural phenomena that we have never been able to measure before. We are researching both quantum photonic sensors and quantum magnetic-field sensors, which have several potential applications in optical and wireless communications, positioning services, and medicine. Quantum sensors could detect the electrical impulses in the human brain, leading to advances in neuroscience.

- *Energy Storage Technology*: In a groundbreaking development for energy storage technology, researchers have introduced a novel method for predicting the state of health (SOH) of lithium-ion batteries employing a DSwin-transformer architecture. New materials are designed with desired properties, such as high-efficiency solar cells, improved battery chemistries, and novel superconductors. The reliability of lithium-ion batteries is paramount as they represent the backbone of contemporary electrical energy storage solutions, and any improvement in their management reflects a significant advancement in technology. Figure 9 shows a pack of batteries [17].

## CHALLENGES

Although quantum chemistry has made remarkable advances in bridging quantum mechanics and chemistry, key challenges remain. Technical challenges encompass developing efficient error correction methods to mitigate the effects of noise and errors in quantum hardware, enhancing the reliability and scalability of quantum computing algorithms. Predicting chemical properties using a first principle approach at the atomic scale is a theoretical and computational challenge. Other challenges include the following [1]:

- *Software*: Effective software is crucial to any scientific field. As quantum computing hardware continues to develop, another component that is required in order to make quantum computers useful for chemistry is software. The goal of software is to convert human-inputted instructions into a format that can be carried out on a computer chip. For quantum computers, software is needed to transform human input into physical manipulations of qubits. The goal of quantum computing software for chemistry is to produce a similar type of software that allows any chemist to make use of quantum computers for their own work.
- *Scalability*: The hardware implementation must be scalable, such that the addition of the necessary number of qubits does not affect the overall robustness and accuracy of the quantum computation.
- *Environmental Noise*: One thing all qubit platforms have in common is their sensitivity to environmental noise. Most quantum computers are noise-burdened and costly. While no physical system can be completely isolated from external noise, in classical computing, environmental noise has no significant contribution to the ability to carry out a computation, nor to the accuracy of

the computational results. The advancement of quantum computing in the relatively near future remains limited by challenges associated with the noisy quantum hardware characteristic of the NISQ era.

- **Computational Complexity:** Modeling molecular states with high accuracy is particularly difficult, especially for complex or large systems. Quantum effects become exponentially harder to compute as the number of interacting particles grows. The complexity of simulating a molecular system using Jordan-Wigner encoding is influenced by the structure of the molecule and the nature of electron interactions.

## CONCLUSION

The power of chemistry to prepare new molecules and materials has driven the quest for new approaches to solve problems having global societal impact. Quantum chemistry is the application of quantum mechanics to chemistry, which has existed in some form since the discovery of quantum mechanics itself. It is a division of chemistry that employs quantum mechanics to the study of chemical systems to mathematically describe the fundamental properties of atoms and molecules. Quantum computers will have a big impact on quantum chemistry. The digital computer has paved the way for quantum chemistry to become an essential tool in the modern chemist's toolbox. Quantum chemistry is becoming an indispensable tool in industries that are committed to saving the planet [18]. Quantum chemists envision quantum computers to be transformative tools for chemistry prediction and exploration.

As the field of quantum computing continues to evolve, applications in chemistry are poised to be at the forefront of innovation. As computational power and algorithms continue to improve, quantum chemistry is set to play an increasingly central role in shaping the future of science and technology. More information about quantum chemistry can be obtained from the books in [19-29].

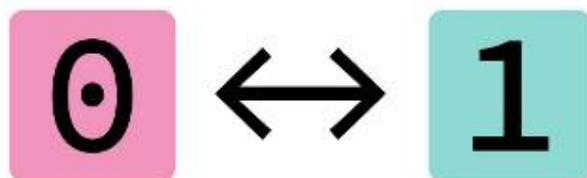
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## TRADITIONAL COMPUTERS

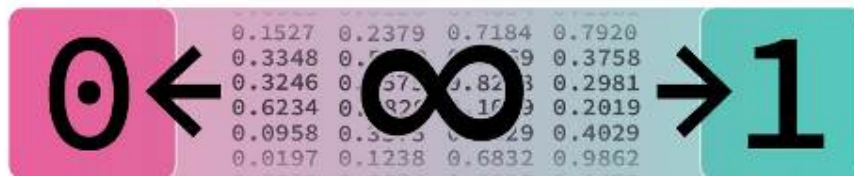
Technology based on 'bits'



Bits have two states: 0 or 1

## QUANTUM COMPUTERS

Technology based on 'qubits'



Qubits have an infinite number of states between 0 and 1

Figure 1 The bit and the qubit [3].



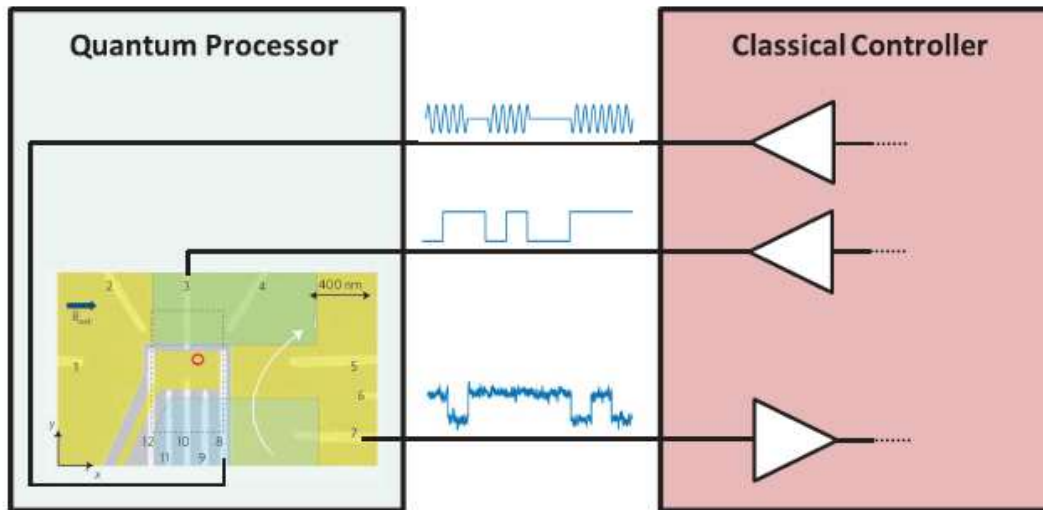


Figure 2 Quantum processor and classical electronic controller [4].

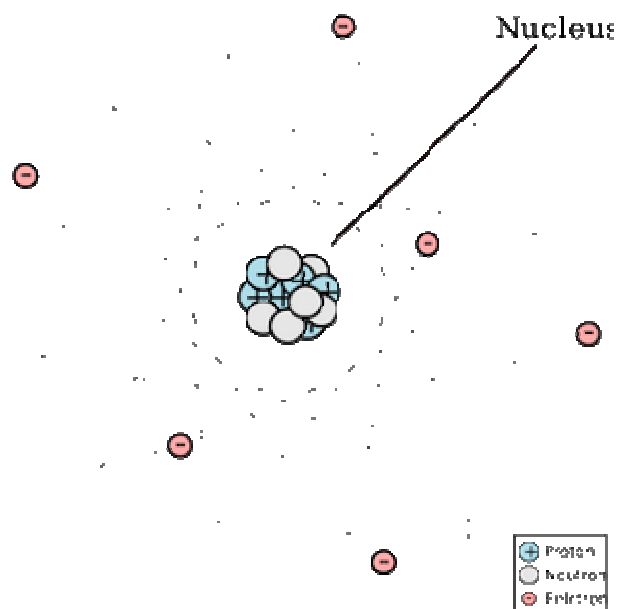


Figure 3 A representation of quantum computing [5].

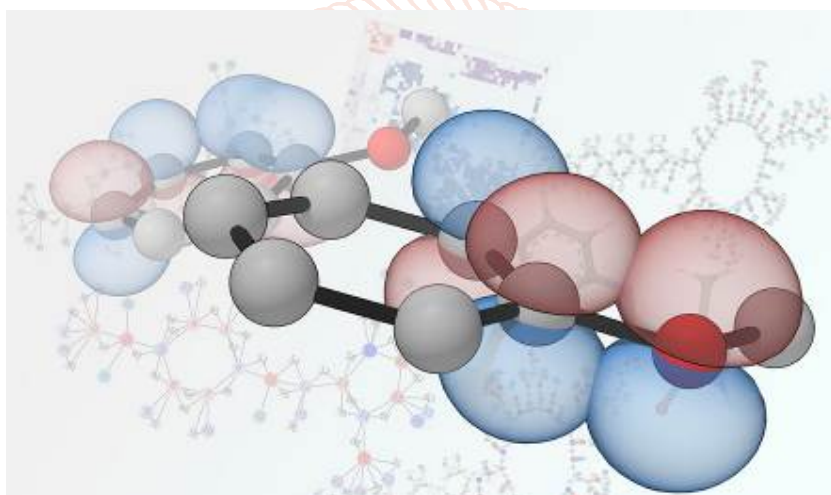


Figure 4 A typical quantum computer [6].

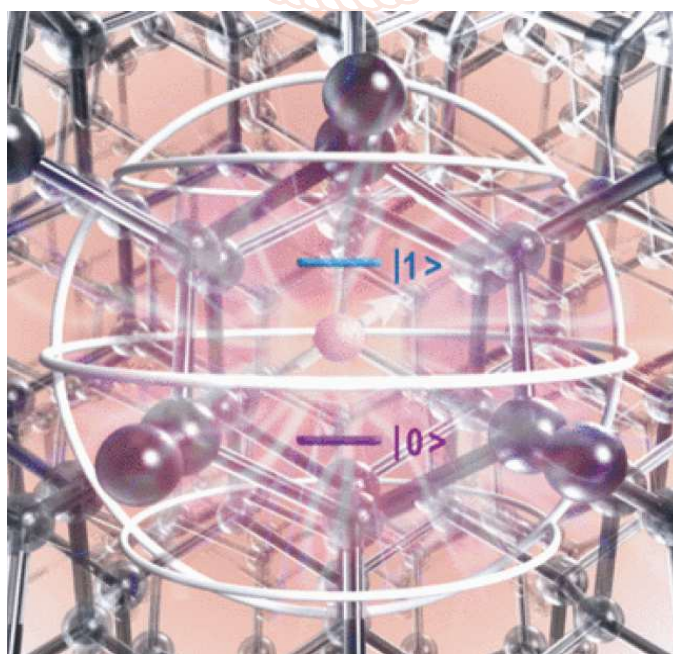
### Atom (carbon-12)



**Figure 5** An electronic structure [9].

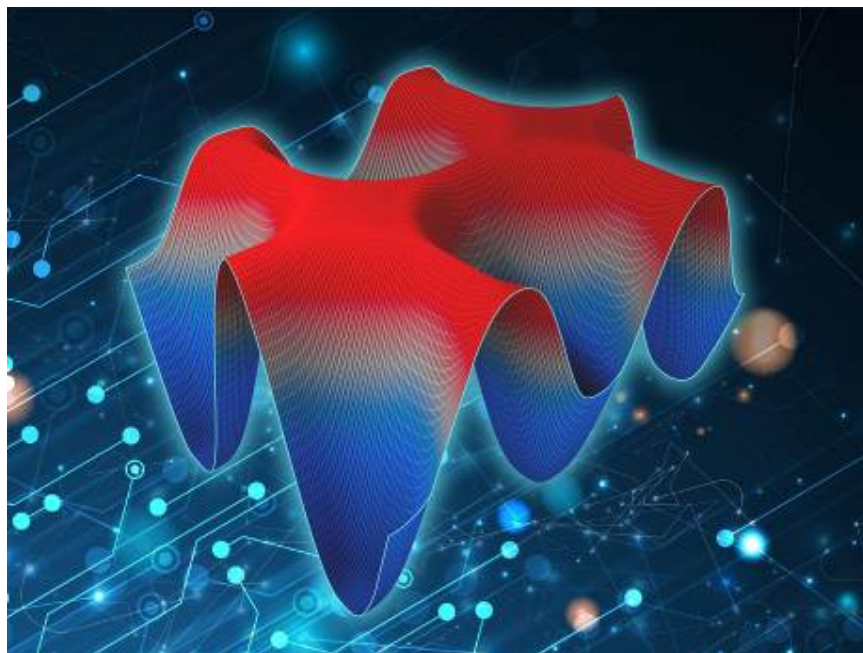


**Figure 6** A molecular spatial representation [10].



**Figure 7** An artistic rendering of atomic structure [11].





**Figure 8 A typical result of chemistry modeling [15].**



**Figure 9 A pack of batteries [17].**