Quantum computing in the chemical industry

PRESCOUTER

Quantum computing will disrupt the core of the chemical industry within the next 5 years. Companies need to start preparing their infrastructure for the speedup of quantum computing, which will bring on a revolutionary new way of product development.

Quantum computing (QC) is recognized as a game-changing approach that allows complex computations to be performed more quickly and efficiently than classical computing. For the chemical industry, this means a higher level of precision along with effective and compliant designs when modeling molecules and polymers, among other systems. Therefore, QC will reduce time and costs in researching and developing molecules and chemicals and in the identification of new processes by optimizing the use of resources and increased precision in calculations and modeling.

With the growing market and increasing investment in the quantum computing area, this is an ideal time to adopt this technology. To showcase QC's potential and today's opportunities, this Intelligence Brief profiles six quantum computing startups with chemistry applications that provide software, hardware, or both.

Quantum computing could tackle problems practically impossible for classical computers to solve.

QUANTUM COMPUTERS

Rely on “qubits,” or quantum bits, which can achieve a mixed state (“superposition”) where they are both 0 and 1 simultaneously.

Use quantum mechanics (i.e., atomic or subatomic particle properties such as electrons, neutrinos, and photons). Superposition allows trying all the inputs at once.

Each additional qubit doubles the processing power, so quantum computers are faster than regular computers, factoring huge numbers in a few hours.

vs

CLASSICAL COMPUTERS

Rely on “bits,” which are binary and can hold only a position of 0 or 1.

Operate according to strict rules of logic and can process only one input at a time.

Training machine learning models comes with a high computational cost, which has hindered the development in this field.

To speed up progress in the machine learning fields, researchers have been exploring ways to devise and implement quantum software that enables faster machine learning (e.g. recognizing patterns in data and identifying different objects in an image).

The quantum computing concept was proposed by Richard Feynman (Nobel Prize in Physics) in the early 1980s.

Recent technological developments have taken QC capabilities from the realm of academic exploration to tangible commercial opportunities.

On February 4, 2021, IBM announced its roadmap for building an open quantum software ecosystem with the following targets:

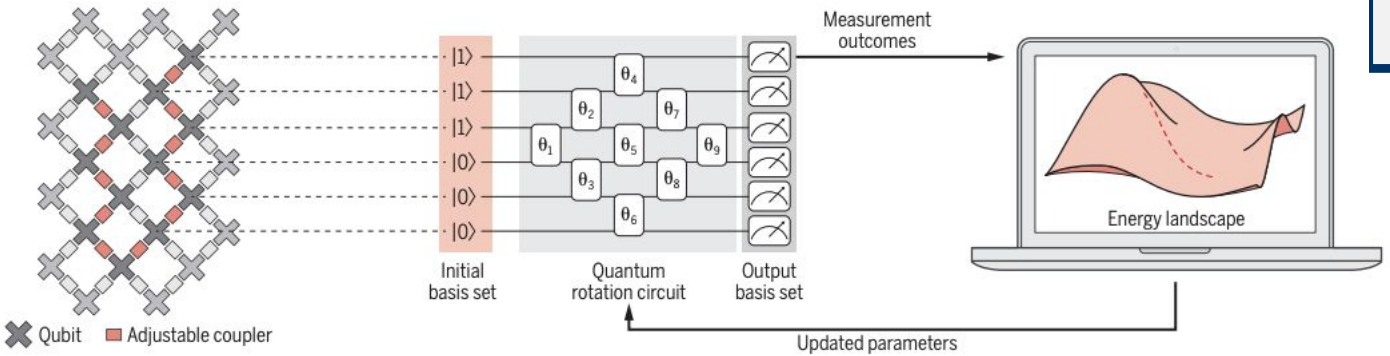
- For 2021: The release of Qiskit runtime, which will lead to a 100x speedup in workloads that exploit iterative circuit execution. This will allow quantum systems to run jobs in just a few hours that, today, can take months.
- By 2022: Run a wider variety of circuits, allowing users to tackle problems previously inaccessible to any quantum processors.
- By 2023: Offer entire families of pre-built runtimes tailored to natural science, optimization, machine learning, and finance domains.
- 2025 and beyond: Development of frictionless quantum computing where the hardware is no longer a concern to users or developers.

D-Wave is world's first commercial supplier of quantum computers. D-Wave uses quantum annealing that can already compete against classical computers and start addressing realistic problems. Glaxosmithkline (GSK) and Volkswagen (VW) are both using D-Wave's technology in drug discovery and traffic optimization, respectively.

The global QC market is expected to grow from USD $472 million in 2021 to USD $1,765 million by 2026, at a CAGR of 30.2%.

In the chemical industry, quantum computing could improve the understanding of systems such as molecular structure and chemical reactions/processes as well as modeling drug interactions.

Although some technical challenges still exist, there are currently companies and examples where QC is being applied to solve a chemical industry problem.



Google Sycamore
The schematic shows the superconducting qubits and the adjustable couplers that connect them.

Quantum circuit
The input states of the wave function are initialized as $|0\rangle$ or $|1\rangle$. Each box with a parameter θ is a rotation gate that is compiled into two two-qubit gates and three single-qubit gates.

Classical calculation
The outcomes are fed into a classical computer that trains the parameters to learn the ground state of the system. The classical parameters that determine the wave function are fed back to the quantum computer, and the calculation is rerun.

Figure. A parameterized quantum circuit, with adequately prepared initial states and with the aid of a classical computer, approximates the wave function of a chemical compound. Source: Stanford University, 2020.

It is estimated that the first quantum computing applications that will be useful for the chemical industry will be available by the early-to-mid 2020s.

Potential applications of quantum computing include:

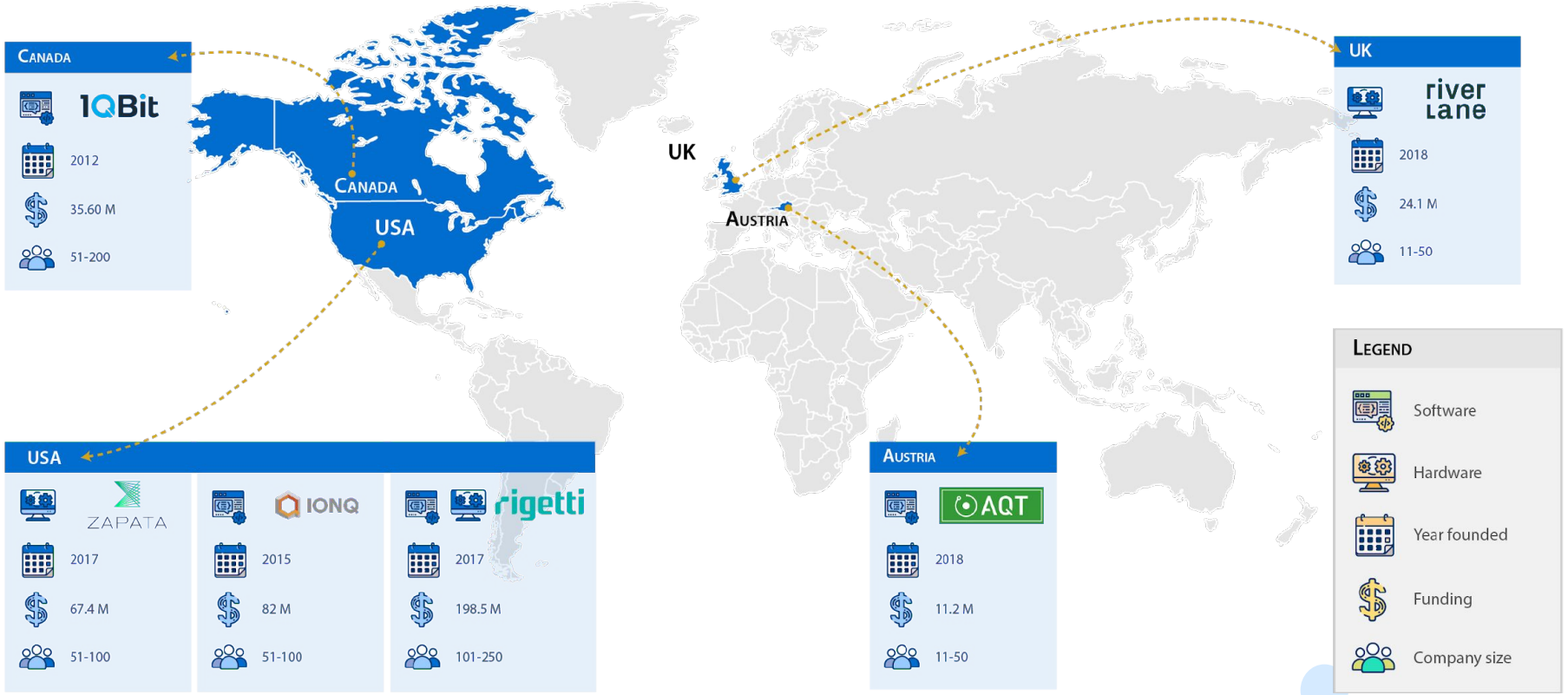
Design of chemicals and products	• Change how new molecules/materials and products are formulated and developed, through the modeling and simulation of quantum-mechanical systems, and the accurate predictions of molecule/product properties. • Improve the effectiveness of R&D departments and reduce lab work.
Production	• Improve yields and reduce byproduct generation through enhanced understanding of reactions and finding new catalysts.
Supply chain	• Optimize supply chains and logistics, reducing costs.
Marketing	• Help to handle business-to-business and business-to-consumer relations.

Source: McKinsey & Company. 2019.

A number of startups are working toward quantum computing applications for the chemical industry. Applications include molecules or materials design, simulation, discovery, and optimization.

	Company	QC applications in Chemistry	Key differentiators	Partners in the chemical or pharmaceutical industries
Software and hardware	Rigetti Computing	Chemistry simulation, materials discovery, and optimization.	Full-stack solutions; Quantum cloud services; Machine learning.	ProteinQure
Software	Zapata Computing Inc.	Process optimization for maximizing yield; simulation and modeling.	Near-term/NISQ-based quantum applications.	BASF We create chemistry
	1QBit	Molecular simulations for the design of new materials.	Hardware-agnostic platforms; Provides a simulation toolkit.	ProteinQure, DOW, Biogen
	Riverlane	Chemistry calculations (ground-state energy) and optimization.	Unify control.	astex pharmaceuticals
Hardware	IonQ	Chemistry and materials simulation; drug discovery.	Full-stack quantum computing products, running at room temperature; Machine learning.	DOW
	AQT	Chemistry calculations and simulations.	Compact processors.	**Not found**

6 QC STARTUPS with chemical applications



Software and Hardware companies

+

rigetti

Rigetti Computing

Website: www.rigetti.com
Contact: Via website
HQ: California, USA
Company size: 101-250
Founded: 2013

Rigetti Computing is a full-stack integrated quantum computing systems company. Their foundations are in quantum processor chips, which are quantum-coherent superconducting microwave devices.

Their quantum cloud services platform enables integration into any public, private or hybrid cloud. Rigetti Computing offers a series of open-source tools through the Forest SDK. These tools include:

- High-level language interfaces
- Devices simulation
- Circuit optimization
- Compilation software for experiment design and algorithm performance

Main (industry) focus

Finance, Insurance, Materials and Chemistry, Pharmaceuticals, Defense, and Energy

Funding

$198.5 million

Key differentiators

Fabrication of quantum computer and superconducting processors; First one-stop shop for quantum computing; Hardware and software

Rigetti Computing

INDUSTRY FOCUS

The value of quantum computing will be reflected in the practical applications. Rigetti hopes to enable a new way of thinking through quantum computing to solve problems across industries. Two main areas of interest:

- Large-scale optimization, where a reduction in fuel consumption will be reflected.
- Materials discovery, by the design and optimization of molecules and synthetic enzymes, and catalysts for food and energy production.

PARTNERSHIP

Rigetti has partnered with ProteinQure, which is a software platform for computational protein drug discovery. ProteinQure, in turn, recently announced a partnership with AstraZeneca to design novel peptide therapeutics.

Figure. Rigetti Computing full stack and Rigetti Quantum Computing Center. Source: (Left) HPC Wire; (Right) Rigetti.

ProteinQure AstraZeneca

Rigetti Computing

CASE STUDY

The 16-qubit Rigetti Aspen processor, along with the 20-qubit IBM Tokyo, were used to simulate alkali metal hydrides (NaH, KH, RbH). The accuracy of the computed ground-state energy served as the primary benchmark metric.

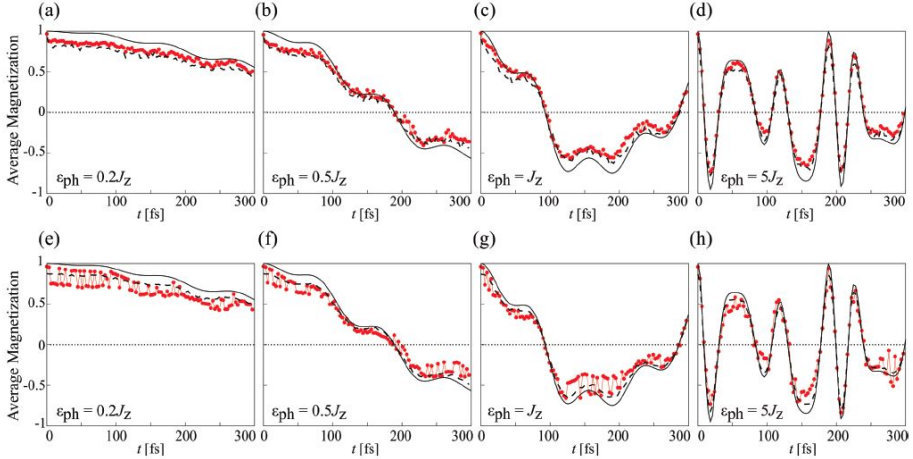


Figure. Simulation results for a 2-qubit system (red dots) on the IBM quantum processor (a)–(d) and the Rigetti Aspen quantum processor (e)–(h) compared to theoretical results from simulated noisy qubits (black, dashed lines) and the wave-function simulator (black, solid lines). The black dotted lines show zero average magnetization [Bassmann et al., 2020].

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Software companies

ZAPATA

1QBit

river Lane

Zapata Computing, Inc.

Website: zapatacomputing.com
Contact: Via website
HQ: Massachusetts, USA
Company size: 51-100
Founded: 2017

Zapata Computing was spun out of Harvard University in 2017. The company develops software and algorithms to be run by quantum computers. They include a comprehensive set of machine learning techniques, classical optimizers, and quantum techniques. The custom quantum workflows and algorithms are focused on commercial and industrial uses.

Zapata offers the Orquestra® platform, which leverages enterprise-grade components at scale, particularly in chemistry, machine learning, and optimization applications.

Main (industry) focus

Finance, Pharmaceuticals, Logistics, Aviation, Materials, Engineering, O&G, and Chemistry

Funding

$64 million

Key differentiators

Algorithms and software development;
Near-term/NISQ-based quantum applications

Zapata Computing, Inc.

INDUSTRY FOCUS

Quantum computation offers new methods for navigating the complexity of the simulation of quantum systems. With the new-found capacity to manipulate quantum states of matter such as superposition and entanglement, quantum computers are positioned to tackle major issues such as determining the electronic structure of molecules with a level of efficiency and accuracy that has remained out of reach of classical computers.

Zapata offers selected quantum use cases for the following chemistry applications:

Optimization

- Process optimization in chemical reaction networks for maximizing yield.

Simulation & Modeling

- Homogeneous and heterogeneous catalysis modeling using electronic structure calculations.
- Singlet-triplet transition energy prediction for organic light-emitting diode (OLED) molecules.
- Quantum-enhanced force-field methods for chemical dynamics simulation.

CASE STUDIES

In the research paper *Quantum chemistry calculations on a trapped-ion quantum simulator* (in collaboration with researchers from Alpine Quantum Technologies, Innsbruck University, Tufts University, the University of Sydney, Harvard, and Google), an algorithm was used to solve a quantum chemistry problem (the calculation of the molecular ground-state energies of H_2 and LiH).

In 2019, chemical company BASF invested in Zapata Computing to scale research and product development in support of quantum readiness across the chemical industry.

Zapata Computing, Inc.

CASE STUDIES

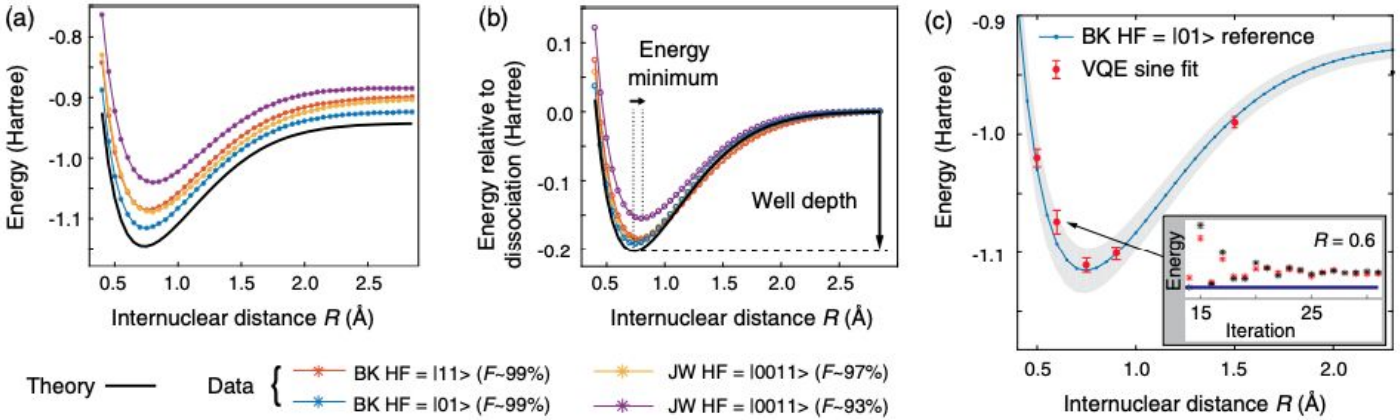

Figure. (a) Potential energy curves of the molecular hydrogen ground state. The black line corresponds to the theoretical value calculated. All other lines are derived from weighted sinusoidal fits to the energy surfaces formed from the experimentally obtained expectation values. The data sets vary the number of qubits, the Hartree-Fock input states, encodings, and gate fidelities. **(b)** Data from panel (a) normalized to the theoretical dissociation energy at large internuclear separations R. The dashed and dotted lines indicate the well depth associated with the binding energy of the molecule and the position of the energy minimum, respectively. **(c)** VQE implementation. The BK HF = |01> parameter-scan fit result is shown as experimental reference with its 1σ confidence band. Points with error bars indicate the five VQE runs performed. The inset shows the last iterations of one particular run that failed to converge to the target value (blue line), with experimental data depicted by red and a noise free circuit simulation shown by black symbols. Source: Hempel et al. 2018.

Zapata Computing, Inc.

CASE STUDY

Quantum workflows. The company claims to have provided a software and hardware interoperable enterprise quantum toolset (Orquestra). Users can build, run, and analyze quantum and quantum-inspired workflows. The company points out that Orquestra is being used with leading hardware interfaces such as IBM, Rigetti Honeywell, and IonQ.

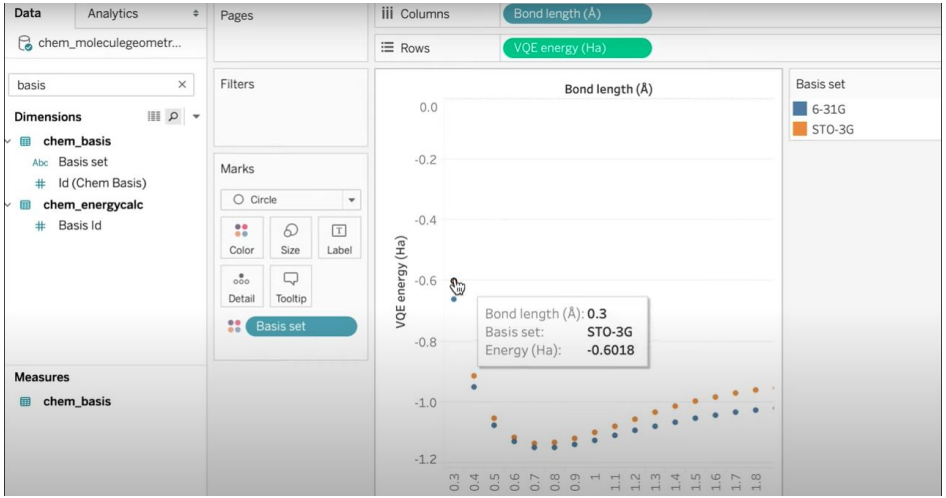

Figure. Image of plotting Orquestra® outputs in Tableau. Source: Zapata Computing..

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1QBit

1QBit

Website: https://1qbit.com
Contact: info@1qbit.com
HQ: Vancouver, Canada
Company size: 21-200
Founded: 2012

Founded in 2012, 1QBit develops applications that aim to solve demanding computational challenges. This allows the scalability of technology by the optimization, simulation, and use of machine learning. Their interdisciplinary technology is able to identify areas within the industry that can benefit from the use of classical and quantum computing architectures. They use their knowledge of quantum and classical processors to build industrial applications on a hardware-agnostic platform.

Main (industry) focus

Computational Finance, Materials Science, Quantum Chemistry, and Life Sciences

Funding

$35.62 million ($45 million CAD)

Key differentiators

Focused on applications, algorithms and APIs; Hardware-agnostic platforms (software).

INDUSTRY FOCUS

The properties of new materials such as catalyst molecules and drug compounds can be anticipated by the simulation of the electronic structure of molecules. Obtaining this information is computationally intensive by classical computing. However, the Quantum-Enabled Molecular ab Initio Simulation Toolkit (QEMIST) makes use of advanced problem decomposition (PD) techniques and quantum computing. QEMIST enables massive parallel simulations by breaking down a computational chemistry task into smaller, independent subproblems. These subproblems can use a combination of interfaces to various classical and quantum solvers to achieve a higher level of accuracy for large-scale, practical molecular simulations.

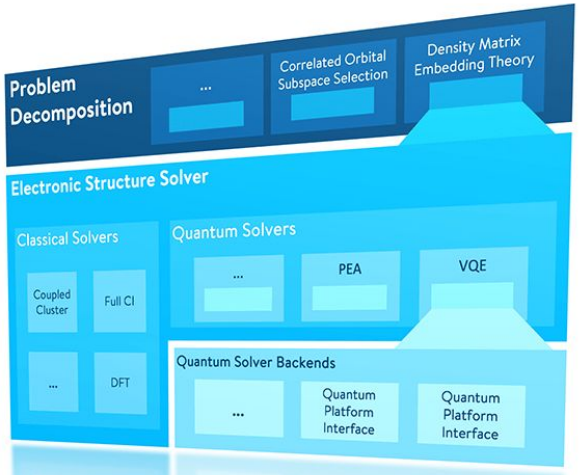

Figure. Quantum-Enabled Molecular ab Initio Simulation Toolkit (QEMIST).

PARTNERSHIPS & COLLABORATIONS

Microsoft and 1QBit announced a collaboration in May 2019 to disrupt materials innovation with the 1QBit OpenQEMIST Platform and the Microsoft Quantum Development Kit. The implementation of the hybrid algorithm was demonstrated in a hydrogen dissociation experiment.

1QBit also has partnerships with:

- **ProteinQure**, a software platform for computational protein drug discovery
- **Biogen** and **Accenture** to apply quantum computing to accelerate drug design and discovery

Also, in March 2021, the results of the research developed by Dow, 1QBit, and IonQ were published. The study focused on the simulation of properties of materials, in this case, a ring of 10 hydrogen atoms. IonQ, 1QBit, and Dow proposed a new approach to achieve accurate and efficient electronic structure simulation on quantum computers.

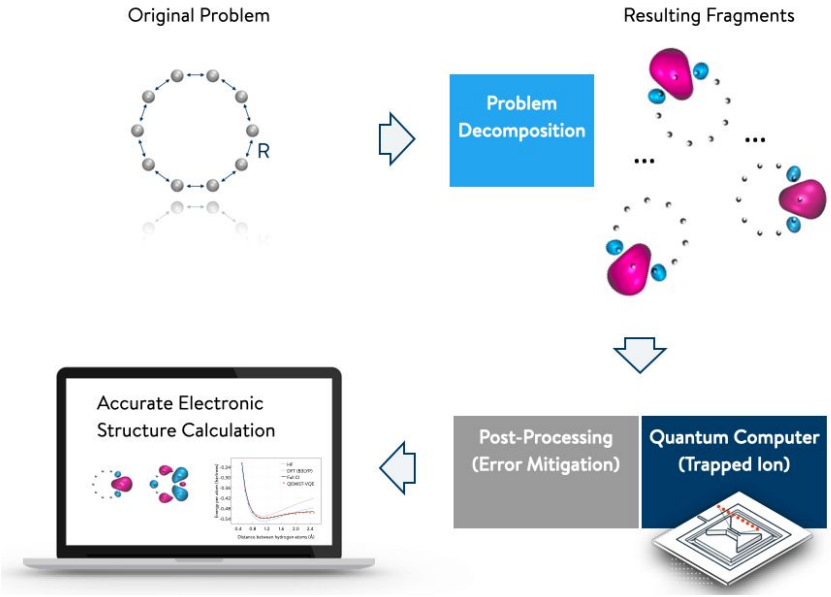

Figure. Problem decomposition method. Source: 1QBit.

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Riverlane

Website: www.riverlane.com
Contact: email

HQ: Cambridge, UK
Company size: 11-50

Founded: 2017

Riverlane was founded in 2017 and backed by the University of Cambridge. Riverlane's vision is to create an operating system that makes quantum software portable across qubit technologies, is scalable to millions of qubits, and teases the highest possible performance out of every qubit, even for applications like error correction that need fast feedback loops. The company has developed an operating system called Deltaflow.OS for quantum computers.

Main (industry) focus

Pharmaceutical, Chemical, Finance, Transport, and Materials

Funding

$24.1 million

Key differentiators

Operating system developer (software); Unify control.

Riverlane

INDUSTRY FOCUS

Riverlane works with the chemical, pharmaceutical, and materials industries to improve algorithms and specify early killer applications of quantum computers. The company offers the Deltaflow operating system. The OS allows access to computing elements such as the CPU, field-programmable gate arrays (FPGAs), and qubits. As a result, users are able to extract more computing power from qubits and at low latency, which is crucial for near-term applications such as quantum chemistry.

Riverlane's application library in Deltaflow.OS is called Anian. It provides quantum chemistry applications and includes patented algorithms such as the accelerated variational quantum eigensolver.

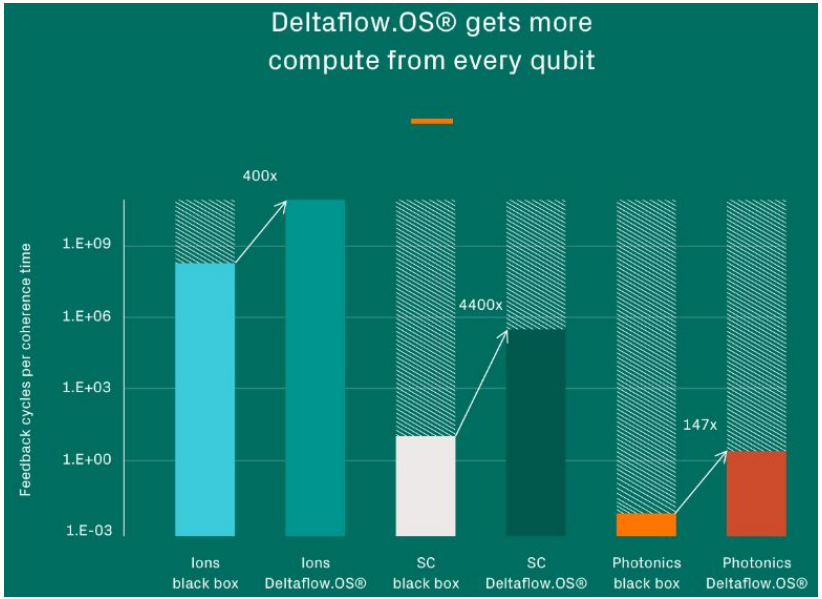

Figure. Deltaflow.OS. Source: Riverlane..

INDUSTRY FOCUS

The Deltaflow project aims to unify the control of two subsystems. The hardware-level language to convert given gates to pulses and the high-level expression language for a user to define their quantum algorithms. This way, a user needs to produce only one program to control the entire quantum computing stack.

At high level, the Deltaflow programming can be split in the following steps:

1. Programming
2. Simulating
3. Simulating on an emulator
4. Runtime

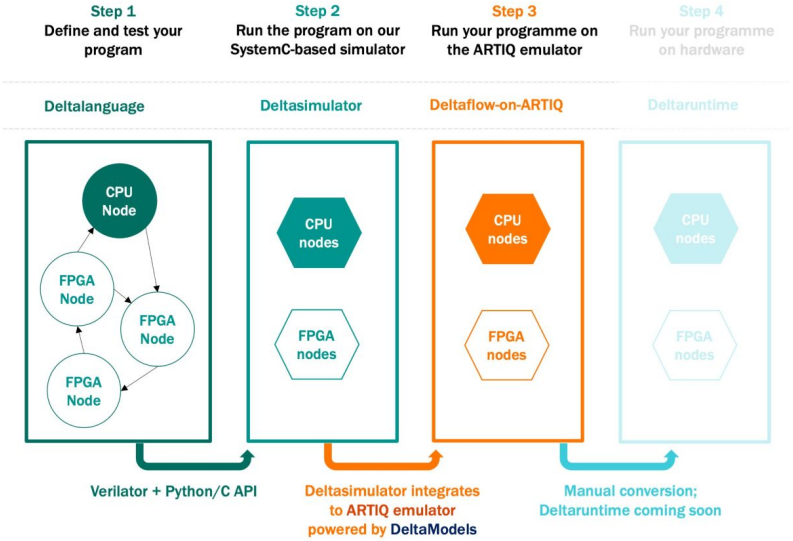

Figure. Deltaflow programming steps. Source: Riverlane.

Riverlane

USE CASE

Computational chemistry calculations are thought to be one of the key potential applications of quantum computers. An important quantity of interest in chemical systems is the ground-state energy. The variational quantum eigensolver (VQE) is an algorithm for finding ground and, with some modification, excited-state energies. It is a hybrid algorithm, making use of both classical and quantum computers. In this way, the required quantum computational resources are kept to a minimum.

In 2020, Riverlane partnered with Astex, a drug discovery and development company, to demonstrate the potential of quantum computing in drug discovery.

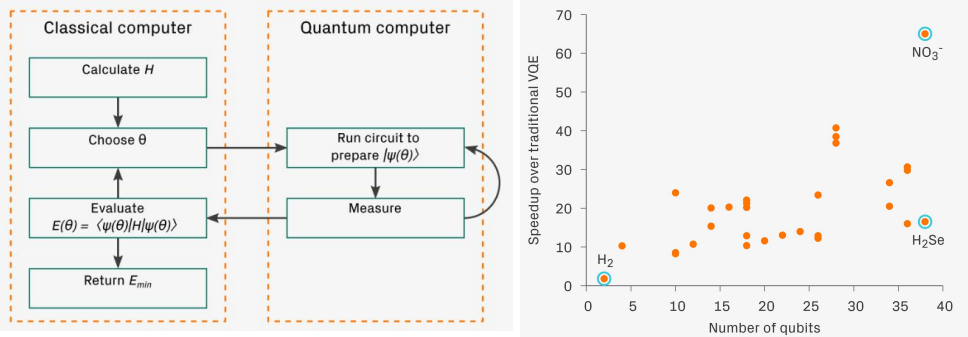

Figure. VQE algorithm highlighting its hybrid nature (left). For different molecular systems, estimates of the average speedup when performing VQE using our SORTED INSERTION method relative to traditional VQE (right). Source: Riverlane.

References:

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Hardware companies

IONQ

AQT

IonQ

Website: https://ionq.com
Contact: info@ionq.com
HQ: Maryland, USA
Company size: 51-100
Founded: 2015

IonQ was founded in 2015 after 25 years of academic research at the University of Maryland and Duke University, with the goal of taking trapped-ion quantum computing out of the lab and into the market. In 2019, IonQ partnered with Microsoft and Amazon Web Services to make quantum computers available via the cloud.

Currently, they are developing full-stack quantum computing products. They transform ytterbium atoms into ytterbium ions and trap them in a 3D space. Then, lasers are used in the operational process, which ranges from the initial preparation to the final readout.

Main (industry) focus

Chemistry and Materials, Climate-Change Action, Logistics and Optimization, Manufacturing, Pharmaceutical and Security Applications

Funding

$82 million

Key differentiator

Hardware developers based on ion trap technology running at room temperature

INDUSTRY FOCUS

Many industries could potentially take advantage of this technology. Some examples are the pharmaceutical industry by improving the formation of drug delivery, the automotive industry by designing better battery materials for electric cars, and the manufacturing industry by optimizing their production lines.

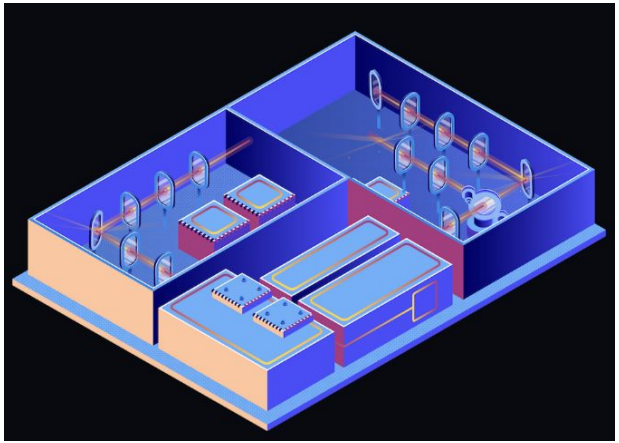

Figure. Trapped-ion quantum computer. Source: IonQ.

RESEARCH AND USE CASES

At the **2017 IEEE International Conference of Rebooting Computing (ICRC)**, IonQ presented the progress on the construction and operation of their quantum computer, showing that their physical platform leads to a highly scalable QC platform based on component technologies that had already been demonstrated in a laboratory setting.

Also, IonQ published a research paper title *Ground-state energy estimation of the water molecule on a trapped-ion quantum computer*. In the paper, researchers described a **co-design framework for solving chemistry problems** on a trapped-ion quantum computer and applied it to estimating the ground-state energy of a water molecule using the VQE method.

In March 2021, the results of the research developed by Dow, 1QBit, and IonQ were published. The study focused on the simulation of properties of materials, in this case, a ring of 10 hydrogen atoms. IonQ, 1QBit and Dow proposed **a new approach to achieve accurate and efficient electronic structure simulation on quantum computers**.

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AQT | Alpine Quantum Technologies

Website: https://www.aqt.eu
Contact: info@aqt.eu
HQ: Innsbruck, Austria
Company size: 11-50
Founded: 2018

AQT (Alpine Quantum Technologies) is an Austrian startup founded in 2018. The main goal of the company is to construct a commercial quantum computer using ion trap technology. Additionally, dedicated laser pulses are used to manipulate each qubit, enabling general-purpose quantum computing.

The trapped-ion approach is scalable and applicable across a wide range of industry verticals, such as material design, finance, and pharmaceuticals.

Main (industry) focus

General Purpose (Physics, Chemistry, Materials, Finance, Pharmaceuticals, etc.)

Funding

$11.2 million

Key differentiators

Development of compact processors by ion trap technology and large-scale quantum computers (hardware)

AQT | Alpine Quantum Technologies

INDUSTRY FOCUS

AQT is developing general-purpose quantum information processors for applications in factoring, high-energy physics, and quantum chemistry simulations, among others. AQT claims that its ion trap technologies offer a clear roadmap to large-scale quantum computers ranging from scalable ion-trap processors to photonic networks connecting quantum computers.

Some of the AQT's achievements are:

- Realization of a scalable Shor's algorithm (Shor's algorithm for factoring integers is one example in which a quantum computer outperforms the most efficient known classical algorithms).
- Topologically encoded quantum error correction.
- Quantum chemistry calculations using a digital quantum simulator based on trapped ions.
- 14-qubit entanglement creation and coherence.

Figure. Rack-mounted ion-trap quantum processor Source: AQT.

AQT | Alpine Quantum Technologies

CASE STUDY

For the study *Quantum Chemistry Calculations on a Trapped-Ion Quantum Simulator*, researchers performed an experimental implementation of an algorithm to solve a quantum chemistry problem by implementing the VQE algorithm to calculate the molecular ground-state energies of H_2 and LiH molecules. There was an indication of the potential for adaptive implementation focused on reaching a high chemical accuracy.

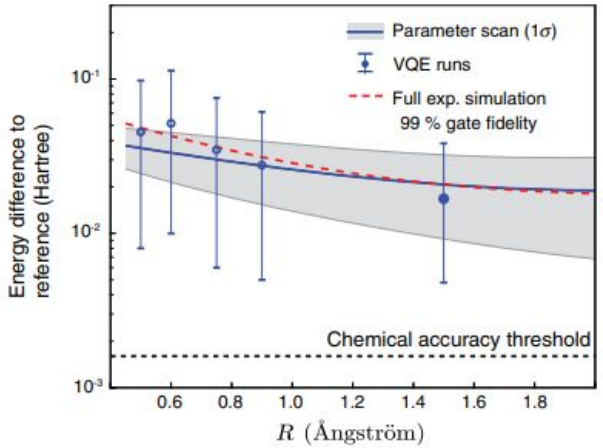

Figure. Energy errors of the reconstructed H2 potential energy surface and the influence of decoherence. Differences are given with respect to the full configuration interaction (FCI) calculation performed in the chosen molecular basis. The red line corresponds to a full simulation of the quantum circuit, including multiple decoherence channels and the experimentally determined gate fidelity. Source: Hempel et al., 2018.

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Expert Interview

Yudong Cao, PhD

CTO & Founder, Zapata Computing

ZAPATA

Yudong Cao has a background in Mechanical Engineering and Computer Science. He obtained his PhD in Computer Science from Purdue University in 2016, and after graduation, he joined the Aspuru-Guzik group at Harvard University. The main focus of Yudong's work at Harvard was on developing and deploying algorithms for noisy intermediate-scale quantum devices. This work has served as the foundation for the applications and solutions Zapata can offer their enterprise clients today. Yudong continues to work on developing quantum and quantum-inspired algorithms for near-term applications.

What kind of immediate and future applications will chemical companies have for quantum computing?

In the past two decades, significant advances have been made in developing algorithms and physical hardware for quantum computing, heralding a revolution in the simulation of quantum systems. Practical challenges in simulating quantum systems on classical computers have been widely recognized in the quantum physics and quantum chemistry communities over the past century. Although many approximation methods have been introduced, the complexity of quantum mechanics remains hard to appease. The advent of quantum computation brings new pathways to navigate this challenging, complex landscape. By manipulating quantum states of matter and taking advantage of unique features such as superposition and entanglement, quantum computers promise to efficiently deliver accurate results for many important problems in quantum chemistry, such as analyzing the electronic structure of molecules.

Chemistry is one of the areas in which quantum computing promises to have the greatest impact. Today, quantum-enhanced optimization or machine learning is promising for use cases such as protein folding optimization or novel molecule generation. However, for drug and materials discovery, many use cases are quite far off in the future (10+ years) because of the number of qubits required to solve those problems. Examples include agrochemical development, lithium battery modeling, solar cell modeling, and drug design.

Chemistry is one of the areas in which quantum computing promises to have the greatest impact.

What would you currently estimate is the size of the QC market for chemical applications?

There is no easy way to calculate this and it's difficult to estimate. We've seen reports approaching $100M for total QC spend in 2025, and assume approx. $20-25M in software spend. Current spend is likely in the low double digit millions.

Is there a particular space where QC could deliver the most value for companies in the chemical space?

It's difficult to say. Compared with machine learning and optimization, simulation and modeling of quantum systems have a generally stronger scientific case for exponential algorithmic advantage over existing classical methods. On the other hand, the relatively incremental and heuristic algorithmic improvement due to quantum-enhance machine learning and optimization is amplified by the business value that these use cases generate.

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What kind of problems is quantum computing ready to tackle in the chemical industry?

The nearest term opportunities are in **optimization and machine learning**. Examples across the value chain (not just R&D) include:

- GANs to generate novel chemicals
- Process optimization in chemical reaction networks for maximizing yield
- Manufacturing optimization
- Logistic network optimization
- Advertising/marketing optimization

Farther out problems include **simulation & modeling problems** such as:

- Homogeneous and heterogeneous catalysis modeling using electronic structure calculations
- Singlet-triplet transition energy prediction for OLED molecules
- Quantum-enhanced force-field methods for chemical dynamics simulation

Do you think there are technological and economic challenges that need to be addressed to integrate QC into the chemical industry processes?

Technological challenges: It is one thing to develop quantum algorithms in a R&D environment where benchmarks are carried out on a curated set of problem instances, and an entirely different issue if one would like to deploy an end-to-end quantum solution in a production environment. In the latter case, one needs to grapple with the often heterogeneous legacy enterprise IT systems, along with other issues related to operating systems, networking, database, regulation, and so on. This operationalization problem should not be overlooked if we were to integrate QC into industry processes.

Economic challenges: One key challenge is the "build or buy" decision-making. Some of the forward-looking enterprises in the chemistry space are actively investing resources to build an internal team of quantum computing specialists, while others partner with companies such as Zapata for developing their quantum computing programs. The barrier of entry for doing value-generating work in QC remains high, and any company contemplating entering this space will need to think carefully about the "build or buy" issue.

How are you integrating quantum technologies with the classical computing tools to achieve your goals in the chemical industry?

We address the quantum-classical integration issue from two perspectives: science and engineering.

From the science perspective, we want to transform a computational problem such as electronic structure calculation in a way such that the parts of the problem that can be efficiently addressed classically are delegated to classical computing resources, while the quantum computers are only exposed to parts of the problem that capture its inherent complexity. In the case of electronic structure calculation, this “inherently complex” part is the ability to generate and consistently measure strongly correlated electronic wavefunctions.

From the engineering perspective, we adopt the latest cloud technologies such as containerization and workflow management to make sure that the various parts of our quantum solution built using a diverse collection of tools and quantum programming frameworks can be interoperable, modular, and extensible

What considerations should a chemical company keep in mind before starting to work with QC?

In the next several years, we will see quantum-enabled solutions delivered as production systems. Then, when increasingly capable quantum devices come online, having deployment architectures in place that can utilize these machines will be critical.

The road to quantum advantage requires the right use case, algorithm, and access to quantum hardware; but moreover, what is key to succeed is having proper, supportive infrastructure and performant classical-quantum approach. A quantum computing solution, delivered in production, only creates business value when it works with the complex, fragmented architectures of data and compute in massive organizations.

Companies interested in pursuing quantum advantages should figure out how to implement/deploy a quantum solution within the organization's complex, fragmented architectures of data and compute – they cannot afford to solely focus on use case exploration while they wait for the quantum devices to mature.

That means companies interested in pursuing quantum advantages should figure out how to implement/deploy a quantum solution within the organization's complex, fragmented architectures of data and compute – they cannot afford to solely focus on use case exploration while they wait for the quantum devices to mature.

And again – we advise pursuing nearer-term use cases in ML and optimization to create business impact sooner and get to production. Then customers will be positioned to swap in hardware as it matures. For an effective partnership, we would bring quantum expertise but want to collaborate with domain experts, end users, and devops who will implement solutions.

How are quantum computing projects in chemistry generally financed?

For quantum chemical calculations using purely classical methods, there is already a mature commercial software ecosystem with players such as Schrodinger. Significant funding may be directed to software licensing. For quantum chemical calculations using quantum devices, **this is still rather nascent and the funding is concentrated on NRE projects**. There are some libraries such as OpenFermion and other proprietary tools built by companies targeting specific use cases. Software licensing remains rare if any at this point. But we expect that to change in the coming years.

> **Initiative typically sits with the partner (on the software or hardware site) that has a customer with a problem to solve.**

How do you establish links between the QC startups to discuss collaborations?

Hard to say, this can be different each time. **We are currently partnered with almost all quantum hardware providers** – from pureplay hardware providers like IonQ and Honeywell to hybrid players like IBM and cloud providers like AWS. Initiative typically sits with the partner (on the software or hardware site) that has a customer with a problem to solve. For example, we have customers who have a solution that we are benchmarking across quantum hardware backends (including classical simulators) on our platform, Orquestra. This unlocks progress for industry and our entire ecosystem.

About the Authors

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Marija is the Technical Director for PreScouter's Chemical, Materials, and Packaging verticals. She has worked across topics such as product and process improvement and development and sustainability throughout the chemicals, materials, and packaging industry. Marija completed her Master's degree in Chemical Engineering from Belgrade University and her PhD in Organometallic Chemistry and Catalysis at the Swiss Federal Institute of Technology (ETH Zurich). Prior to her PhD, Marija worked in the chemical industry on the synthesis of new textile dyes.

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Potential Next Steps

- ✔ PreScouter can look for more companies and researchers developing QC solutions based on your technical and business parameters
- ✔ PreScouter can conduct anonymous interviews with companies and researchers
- ✔ PreScouter can organize direct consultations between you and Subject Matter Experts (SMEs) in the space

SOME POSSIBILITIES THAT PRESCOUTER CAN OFFER FOR CONTINUATION OF OUR RELATIONSHIP

About PreScouter

PRESCOUTER PROVIDES CUSTOMIZED RESEARCH AND ANALYSIS

PreScouter helps clients gain competitive advantage by providing customized global research. We act as an extension to your in-house research and business data teams in order to provide you with a holistic view of trends, technologies, and markets.

Our model leverages a network of 3,000+ advanced degree researchers at tier 1 institutions across the globe to tap into information from small businesses, national labs, markets, universities, patents, startups, and entrepreneurs.

CLIENTS RELY ON US FOR:

Innovation Discovery: PreScouter provides clients with a constant flow of high-value opportunities and ideas by keeping you up to date on new and emerging technologies and businesses.

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Customized Insights: PreScouter finds and makes sense of technology and market information in order to help you make informed decisions.

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