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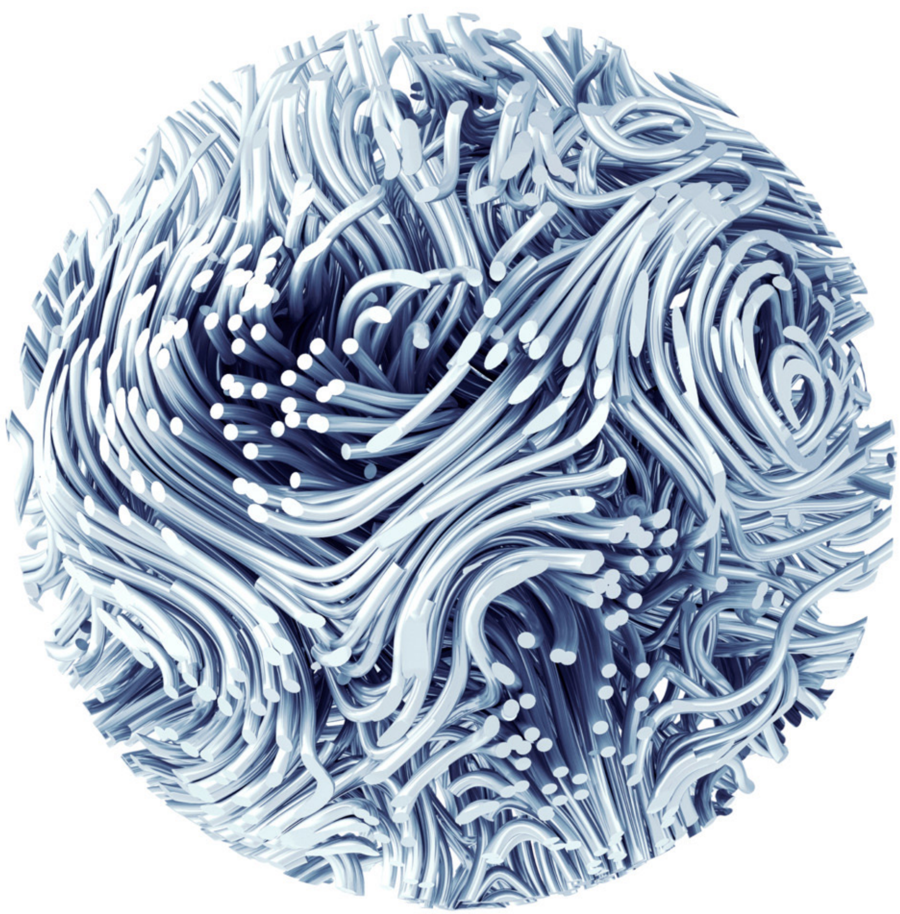
The next big thing? Quantum computing's potential impact on chemicals

The chemical industry is poised to be an early beneficiary of the vastly expanded modeling and computational capabilities of quantum computing. Companies must act now to capture the benefits.

by Florian Budde and Daniel Volz



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Over the past several years, quantum computing has been the subject of a lot of hype. Work underway in the field at tech giants such as IBM and Google has been extensively reported, and this interest has been mirrored by investments in the quantum-computing field by players from a broad array of industries, including the chemical industry. We have been following these developments, and our assessment is that quantum computing could potentially be a game changer for chemical companies.

The chemical industry has been a relatively late adopter of the successive waves of digital innovation and practices moving across business and society. To date, such a stance has not put it at a disadvantage and may in fact have helped it avoid mistakes made by early movers. The chemical industry was a latecomer to enterprise resource planning, but companies did not suffer as the productivity gains from it benefitted all players rather than give any one of them a competitive advantage. The e-commerce wave of the early 2000s proved to be, in effect, largely irrelevant to the industry. Clearly, the implementation of artificial intelligence–based approaches will help the industry to increase productivity significantly across its operations and business activities, but the jury is still out on whether AI will have an impact on the industry beyond that.

Quantum computing, however, may be in a different league. That is because its capabilities could make it possible to significantly improve our understanding of systems governed by quantum mechanics, such as molecular structure and chemical reactions and processes—all at the core of the business of the chemical industry. Players that are able to harness the potential of quantum computing could make better products at lower cost in less time. In this article, we explain what underpins this thesis and how chemical companies should position themselves.

What is the opportunity for the chemical industry?

Quantum computing, built on a new approach to computing, uses the laws of quantum mechanics to increase the speed of certain calculations far beyond the capabilities of classical computers (see sidebar, "What are the basics of quantum computing?"). For the chemical industry, the new quantum-computing capabilities open up the possibility of modeling quantum-mechanical systems, such as molecules, polymers, and solids, at a totally different level of precision. It would thus be possible to identify the most effective molecular designs or structures to accomplish specific tasks and achieve required effects—before synthesizing a single molecule in the lab.

Access to this kind of computation resource could dramatically boost the effectiveness of R&D departments and change the way new products are developed, with ramifications across the entire chemical industry (exhibit). Let's look at this in more detail.

Development of new molecules and materials

The design of new small molecules or polymers relies on accurate predictions of molecular properties. While chemical researchers have made a lot of headway with computational-chemistry tools to tackle issues that are ultimately governed by quantum mechanics, today's tools can provide only rough approximations. For example, tools such as density functional theory (DFT) provide approximations of molecular systems and are somewhat effective for research on small molecules but severely limited for areas such as solids, molecules with heavy atoms, or large molecules (such as proteins).

The improved predictive power of quantum computing applied to molecular design work could have important applications in the development of crop-protection chemicals and many other segments of the specialty-chemicals industry, where accurate foresight into the properties of new molecules will speed development. Take the example of new solid-state materials: the design

Exhibit

Quantum computing could lead to early-stage killer applications along the chemical industry's value chain.

Quantum computing's impact potential and tool used during value creation

Step	**1** Design of chemicals[1]	**2** Design of products[2]	**3** Supply chain	**4** Production	**5** Marketing
Impact potential	**Early killer application**	**Early killer application**	Mature quantum computing	**Potential early application**	Mature quantum computing
Quantum tool used	• Quantum simulation • Optimization • Quantum AI[3]	• Quantum simulation • Optimization • Quantum AI[3]	• Optimization	• Quantum simulation • Optimization • Quantum AI[3]	• Optimization
Examples of future applications	• Design molecules and solid materials with required properties, reducing lab work • Use computers to define shape of proteins to make better active ingredients	• Discover more effective formulations by modeling how ingredients affect processes or how complex mixtures behave	• Use quantum computing to optimize supply chains and logistics and to reduce costs	• Improve yields and suppress by-product generation through better understanding of reactions and finding new catalysts • Use quantum algorithms to solve complex optimization problems in heat and mass transport	• Use quantum AI[3] to help handle B2B and B2C customer relations

[1] New molecules.
[2] Formulations and complex assemblies.
[3] Artificial intelligence.

potential opened up by quantum computing could help new-materials development for a number of leading-edge segments, such as battery materials, semiconductors, magnets, and superconductors.

Similarly, with luminescent molecules for OLED[1] displays, it could be possible to model, with a high degree of precision, new molecules that could provide the brightness and hue of the color sought before making them, instead of what is today still largely a trial-and-error process.

New possibilities would also open up in identifying and designing molecular targets that interact best with proteins, tailored to the docking energy of proteins and small substrates. Today's computers are limited in their ability to predict the structure of proteins. Using the power of quantum computing, it may be possible to make progress in this kind of target identification, again with important applications in the development of crop-protection chemicals, biocides, and certain other segments of the specialty-chemicals industry, as well as the pharmaceuticals industry.

Development of new product formulations

Quantum computing could help in the formulation of mixtures by making possible an improved understanding of the complex molecular-level processes involved, as well as by supporting

[1] Organic light-emitting diode.

What are the basics of quantum computing?

Many in the chemical industry, particularly in R&D labs, are used to enlisting quantum mechanics on a daily basis to describe the behavior of molecules and chemical reactions. The concept of quantum computing was proposed by Nobel Prize–winning physicist Richard Feynman as long ago as 1982. Still, the notion of thinking quantum-mechanically for real industrial computing applications remains relatively new.

To understand what makes quantum computers unique requires a brief look at the quantum bit, or qubit, and how it differs from "classical" bits, which serve as the basic unit of information in conventional computing. Qubits exist in a regime that can be described only with the—nonintuitive—laws of quantum mechanics.

A conventional computer is built on transistor-based classical bits that are operated by voltages and can be in only one of two states: 0 or 1. A quantum computer instead uses quantum physics–based systems, such as superconducting loops or ions hovering in magnetic fields (so-called ion traps), which are operated by lasers or microwave irradiation. Because of the laws of quantum mechanics, such systems can be held in a special physical state, superposition, as a result of an effect called entanglement. This allows isolated qubits to form larger systems, in which each qubit exists in multiple states—0 and 1—simultaneously.

The implications of these effects for a quantum computer are dramatic. Qubits can process a much larger amount of information with a relatively small number of qubits compared with conventional computers. On top of this, calculations with qubits are not done one step at a time but in a probabilistic manner, giving them the potential to solve certain types of problems much faster—in certain cases, orders of magnitude faster. All of this allows quantum computers to do computations that are not technically feasible with conventional computing. A much-quoted example is the factorization of very large prime numbers, which has important potential ramifications in cryptography: using a classical algorithm with current supercomputers would require a time period on the order of the age of the universe, but the problem could be addressed by a sufficiently large quantum computer in a few hours.

Qubits use the characteristics of quantum-mechanical systems to solve complex equations in a probabilistic manner, and a computation solved with a quantum algorithm has only a certain probability of being correct. The combination of greater speed with probabilistic solutions means quantum-computing capabilities fit well with a certain subset of computing needs and applications, including optimization, simulation, and AI. It also means quantum computers are likely to coexist alongside conventional high-performance computers that are better positioned to solve nonprobabilistic problems, with the two fused as hybrid systems for tackling a range of applications.

the optimization of such mixtures to make more effective products for the whole range of applications that chemicals support.

Developing a new cleaning-product formulation, for example, is today based on the triangulation of the experience of a technician, essentially trial-and-error experiments, and theoretical models (in part based on conventional computations, though the models employed are often crude simplifications of reality). Quantum computing could help this process with optimization calculations to understand exactly how, for example, detergent molecules interact with a wine stain on a fiber and to identify the best active ingredients and formulations to remove it. A team using a quantum computer and the appropriate algorithm could reduce the required calculation time to seconds.

Quantum computing could also help development work in the related area of complex assemblies, such as composites, effect pigments, and opto-electronic devices for displays. These require hybrid approaches combining simulations, optimization, and artificial intelligence to identify the best materials to be used (in terms of thicknesses, concentrations, and structure)—all of which maps directly onto quantum computing's promise. Some chemical companies are already working in this area, using existing computing methods to develop OLED architectures for use in TVs and smartphone displays. Harnessing quantum-computing capabilities here has the potential to accelerate the research process substantially.

Optimizing production operations

In addition, simulations based on quantum computing could be used to better understand reaction mechanisms, to design improved catalysts, and to optimize process conditions. Probabilistic quantum computing–based AI could also be used to find nonintuitive data correlations that would help in fine-tuning process conditions in order to decrease by-product generation and to optimize yields.

Why is the chemical industry well placed?

First-generation quantum computers—annealers and gate-type designs—are already being commercialized by companies such as IBM and D-Wave, but we are still in the early days of this technology. The largest systems today are still below 100 quantum bits (qubits), and further work is needed on key performance aspects, such as reliability and error correction, but advances are regularly being announced. Over the past five years, the number of physical qubits in gate-based systems has roughly doubled each year. The driver behind the progress is a neck-and-neck race among a field of players ranging from major corporations to around 100 start-up companies, which are all striving to build the first quantum computer and sets of algorithms powerful enough to tackle industry-relevant problems.

The principal reason chemical companies could be early adopters this time is that the level of performance needed from a quantum computer to undertake computations that could benefit chemical companies is a moderate one. A report recently coauthored by BASF and the Karlsruhe Institute of Technology extrapolated the number of logical qubits needed to simulate chemical processes such as the seminal Haber-Bosch ammonia process to roughly 1,000 qubits.[2] In contrast, extrapolations for a typical RSA encryption application (such as the factorization of a 1,024-bit prime number) suggest a resource requirement of about 1.5 million qubits.[3]

Why is it that even moderately powered quantum computers could benefit chemical companies but not other industries with demanding computing needs? The reason is that chemistry and the chemical industry by their nature are dealing with molecular manipulations governed by the laws of quantum mechanics. Even the most basic problems associated with manipulating these molecules could gain from approaches using quantum computing. As a result, there's a lower threshold to find a quantum-computing tool that can be useful in the chemical context.

Experts from industry and academia estimate that the first quantum-computing applications that promise to be useful for the chemical industry will require between roughly 1,000 and 10,000 qubits and may be here by the early-to-mid 2020s. This means that the chemical industry is likely to be able to do useful quantum computations much sooner than the other industries where quantum computing is expected to play an important role.

In addition, the entry barrier is low for the chemical industry because using quantum computers will fit well with the industry's current research approach. Quantum computing with new and more accurate algorithms will be able to complement DFT and other tools. Most important, it will not be necessary to make fundamental changes in the ways research is done. Next, this lower threshold for providing value to chemical companies is already

[2] Michael Kühn et al, "Accuracy and resource estimations for quantum chemistry on a near-term quantum computer," *arXiv:1812.06814 [quant-ph]*, 2018.

[3] Muhammad Ahsan et al, "Designing a million-qubit quantum computer using resource performance simulator," *Association of Computing Machinery Journal on Emerging Technologies in Computing Systems*, Volume 12, Issue 4, 2015.

Being open to collaboration will help chemical companies to hit the ground running to pilot-test the first quantum-computing use cases, and will help them to build up the right amount of internal capabilities.

encouraging quantum-computer and algorithm developers to target the chemical industry. That could spark a virtuous circle of demand and take-up of quantum computing by the industry.

It is not yet clear which quantum-computing player will win the race to build the first quantum computer able to address industry-related challenges and how exactly it will make qubits that work. More than a dozen concepts are being evaluated, and there is no clear consensus on how best to make a quantum computer with one million qubits. However, once the performance level that enables quantum computers to help in business applications has been attained, it should be possible to link up with chemical companies quickly. This is because all the serious players plan to bring quantum computing to end users via cloud services, which should enable a rapid uptake by chemical-industry users.

What steps should chemical players take?

A dozen or more chemical players have publicly launched quantum-computing activities, and many more are no doubt evaluating quantum computing. Drawing on our knowledge about what drives digital excellence in chemicals, we recommend that business leaders consider three steps to engage with quantum computing.

First, businesses need to clearly understand the specific opportunities that quantum computing could bring them. To find, assess, and implement use cases is going to require not only "translators" capable of turning company-specific requirements into clear specifications that quantum suppliers can deliver but also domain experts with intimate knowledge of a chemical company's business and processes and the ability to point out potential applications for the new technology.

Second, to succeed in quantum computing requires a make–partner–buy strategy. In the past three years, an ecosystem of more than 100 players ranging from large digital corporations to start-up companies has emerged. These players are eager to co-develop solutions for relevant use cases together with the end users who own them. The limited number of acquisition candidates means chemical companies will need to consider investments in, or partnering with, less mature start-ups—that is, ones still developing a working product. Being open to collaboration will help chemical companies to hit the ground running to pilot-test the first use cases and, at the same time, will help them to build up the right amount of internal capabilities. Chemical companies are unlikely to invest in their own hardware in the next few years, but they should consider how to secure access to a quantum cloud provider.

Third, dedicated departments need to be built up in-house to deliver the potential. At quantum computing's current level of technology readiness, this is likely to require establishing centralized groups with the mission to identify, test, and scale up first application use cases throughout the organization. These groups will also have to attract quantum-computing talent, which is going to be a crucial issue in the future. Many chemical companies are already struggling to attract recruits with capabilities in digital technologies such as AI, and quantum computing is going to require even more specialized skills.

Quantum computing has the potential to enable chemical companies to make better products at lower cost in less time. For this reason, it deserves a careful appraisal and monitoring of its progress by chemical-industry management teams. As they should be aware, there's no shortage of appetite in chemical-company R&D labs to apply quantum-computing approaches to explore beyond the limits of what is currently possible with molecular modeling. There may also be a broader learning here: while the chemical industry has not been disrupted yet by digital advances that have taken other parts of the business world by storm, it needs to look for opportunities that could truly deliver new types of competitive advantage. All the pointers indicate that the pace of innovation is only likely to accelerate, and quantum computing is a case in point.

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