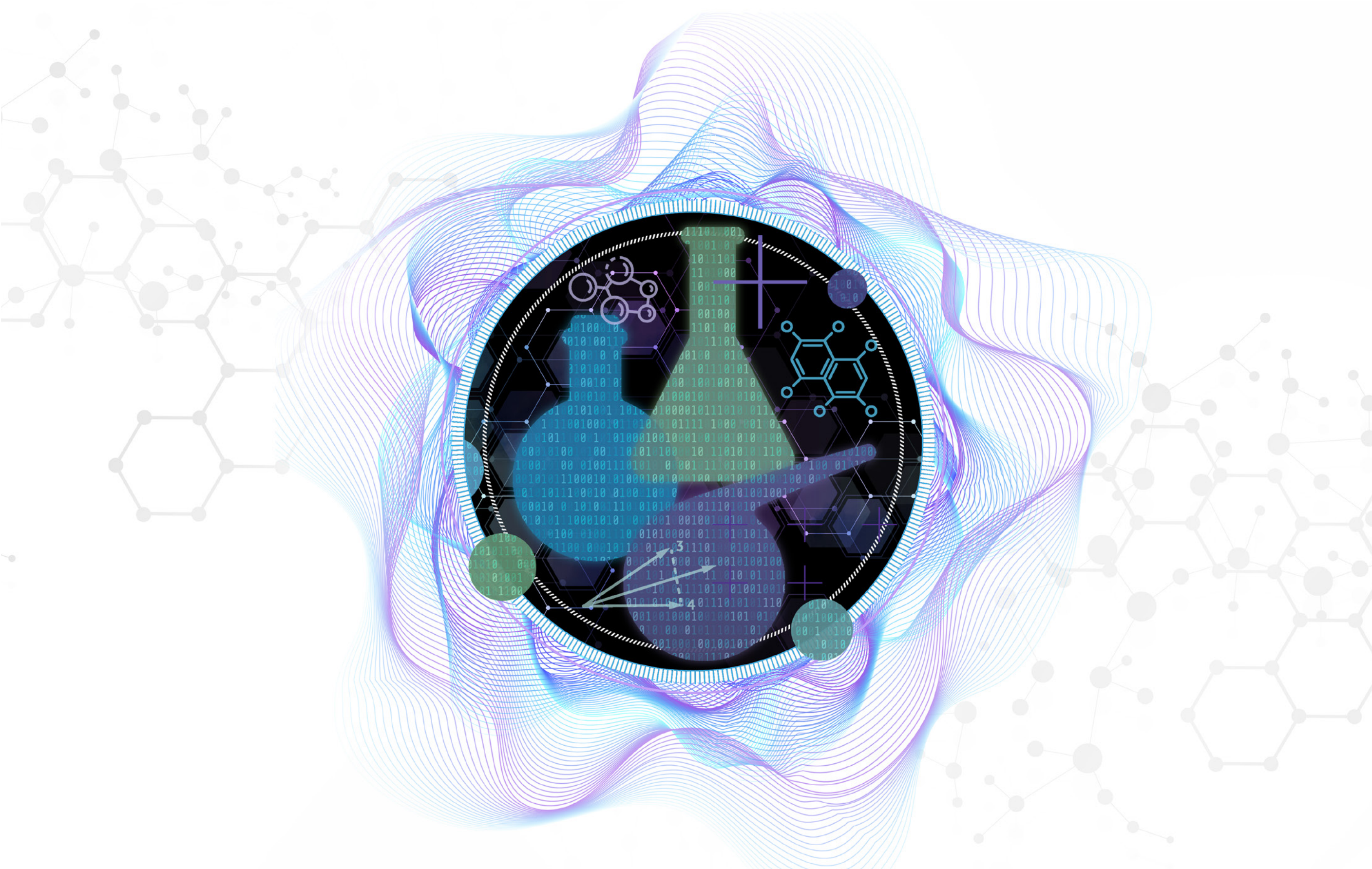

FEATURE

Quantum chemistry

Quantum computing's killer app will turbocharge R&D in multiple industries

Scott Buchholz, Jacob Bock Axelsen, Anh Dung Pham, and Caroline Brown

Unfeasible chemistry and materials science calculations are about to be made possible with quantum computing. Which industries will be the most impacted and how can you prepare?

QUANTUM COMPUTING IS still in its early stages, but it's gaining momentum. It could soon transform health care and life sciences, manufacturing and production, energy, technology, and other industries that leverage quantum chemistry, a discipline that aims to correctly predict the chemical and physical properties and behaviors of molecules and materials.[1] Quantum computing could be a game-changer for any industry that needs to accurately calculate and finely tune molecular properties, predict material behavior, and understand how this behavior will vary with the slightest molecular change.

Although quantum computers exist primarily in labs, their capabilities continue to grow. As researchers work toward large-scale, fault-tolerant quantum processor units, announcements of new milestones, investments, and research partnerships have become commonplace.

Businesses are not sitting idly by as the technology matures. They're working with research organizations to conduct proofs of concept and identify and test promising applications, from solving optimization problems to using artificial intelligence (AI) and machine learning for mathematical modeling. Quantum chemistry is showing early signs of becoming one of quantum computing's killer apps.

Turbocharged research and development

To develop new engineered materials and chemical compounds, researchers typically evaluate thousands of chemical reactions and molecular interactions. Pairing supercomputers with AI and machine learning, scientists can simulate physical and chemical processes. They can also predict and test the properties and behaviors of unknown molecules and materials and find the most promising candidates from a crowded field of initial contenders.[2] For example, they might model the speed of a chemical reaction using a specific molecule at different concentrations or temperatures.

Despite the reliance on an army of high-powered technologies, computational molecular simulation is iterative, time-consuming, and based on meticulous trial-and-error experiments. Even powerful supercomputers can't make exact calculations, and imprecise estimations aren't accurate enough to simulate molecular and atomic interactions, especially in complex molecules. With current methods, it will probably never be feasible to determine the properties of the most complex molecules with high precision.

With quantum computers in their toolkits, scientists will be able to not only conduct more efficient and accurate simulations, but explore molecular and chemical reactions beyond classical computers' current capabilities. Quantum computers will efficiently run algorithms that their classical counterparts can't manage. This will give them an advantage in solving problems that involve multiple, complex interdependencies and correlations (such as predicting molecular structures). For problems that rely on AI and machine learning to identify patterns in data, quantum's advantage will be even greater. Industries that need to simulate or predict the properties and performances of materials and optimize their development processes should be able to dramatically increase the accuracy and speed of research and development (R&D).[3]

At this writing, the world's highest-performing quantum computers don't yet have enough computing power to compete with classical machines.[4] Some applications could require millions of qubits.[5] But there's good news for industries that rely on quantum chemistry: Only about 1,000 logical qubits will probably be needed to simulate materials and molecules, and with the quantum arms race in high gear, the ability to realistically simulate complex molecules is rapidly progressing. Within about five years, as quantum computers become more powerful, their ability to simulate the structures and behaviors of more complex molecules and materials is expected to dramatically improve.[6]

Meanwhile, applications are cropping up in many industries.

Business use cases across multiple industries

From health care and life sciences and manufacturing and industrial production to energy and technology, a diverse group of industries rely on computer simulation and modeling to test and develop new chemical compounds, solid materials, and industrial processes. Three promising applications are health care and life sciences, materials science and discovery, and chemical process simulation and optimization (figure 1).

FIGURE 1

Sample use cases for quantum computational chemistry

Health care and life sciences

Researchers could improve the speed and accuracy of disease diagnosis and treatment, discover new drugs, and develop customized medicines and interventions.

Use cases:
- Drug and pharmaceutical discovery
- Precision medicine
- Disease identification and detection
- Protein folding

Materials science and discovery

Engineers may be able to discover new materials and enhance existing materials to be more durable, efficient, and effective.

Use cases:
- Solar cells
- Clean carbon capture
- High-entropy alloys
- Lossless energy transmissions
- High-speed rail

Chemical process simulation and optimization

Scientists could develop and test new industrial processes that could conserve natural resources, reduce emissions, lower cost, and speed production.

Use cases:
- Ammonia/fertilizer production
- Clean hydrogen production
- Petroleum reservoir production

Source: Deloitte analysis.

Health care and life sciences. The application of quantum computers to health care and life sciences R&D is poised to revolutionize the diagnosis and treatment of diseases. Such a revolution is likely to increase the pace and precision of disease identification and detection, drug and pharmaceutical discovery, genomic analysis, and the development of customized medicines and interventions.

For instance, the need to assess billions of potential drug reactions and side effects on so many individual human systems can stretch the process of bringing a pharmaceutical to market to a decade or more. In early-stage drug discovery and development, pharmaceutical scientists conduct computer-assisted drug discovery. Using tools such as molecular dynamics and density functional theory, they develop computer models and simulations that can predict the impact of millions of macromolecules on diseases and the human body. While such "in-silico" methods are currently neither accurate nor speedy, they're typically safer at this stage than in-vitro methods such as clinical trials.

Quantum computing could change that. It's expected to have an outsized impact on all aspects of the discovery phase. This includes generating scientifically valid evidence pinpointing a disease's biological origins and ensuring that such a biological target can be safely manipulated to achieve therapeutic benefits. Quantum computers could also identify compounds with therapeutically useful, pharmacological, or biological action that could serve as a starting point to improve the strength and precision of the compound. All this could help reduce the time and cost of bringing life-saving drugs to market.

Another potential use case for quantum computers is precision medicine—the design of individualized interventions and treatments. Existing standardized therapies and treatment protocols don't take into account individual genetic and biological factors, behaviors, socioeconomic considerations, or environmental factors that can boost or diminish treatment impact. For example, consider that 31% of patients can't safely metabolize Tamoxifen, a common cancer treatment,[7] or that there are more than 7,000 known rare diseases—affecting more than 30 million people in the United States alone—and that most of them are incurable or have very expensive treatments.[8]

By helping shed light on the correlations and dependencies of various contributing factors, quantum-enhanced machine learning could advance medical research. With it, researchers could predict the efficacy of drugs and treatments, design individual treatment plans that could improve patient outcomes, and even forecast the risk of future diseases to allow for earlier or preventative treatments.

Materials science and discovery. Materials designers use complex calculations to predict the mechanical, optical, and physical properties of ceramics, glasses, polymers, metal alloys, and composite materials. Quantum computers could help design engineers create better materials by giving them more precise control over molecular reactions.

For instance, to develop the most efficient solar cells, energy researchers seek to understand the interaction of sunlight with thousands of combinations of silicon- and polymer-based materials, organometallic compounds, and inorganic substances. More accurate predictions of how materials interact with light could help create more efficient solar panels and LED devices.

Likewise, energy companies are working to test, develop, and scale carbon capture technologies that use less energy to strip carbon dioxide (CO_2) from power plant emissions. Current carbon capture methods, which rely on water to absorb CO_2, are costly, inefficient, and polluting, and scientists have recently developed absorbent solids that can be used for more effective carbon capture.[9] Quantum computing could help build on these innovations, leading to the discovery of highly porous solid materials for capturing CO_2.

Chemical process simulation and optimization. Quantum computing could help scientists develop and test new industrial processes that could help conserve natural resources, reduce emissions, lower costs, and speed production.

For example, large-scale production of ammonia-based fertilizers relies on the Haber-Bosch process, a 100-year-old, energy-intensive method of nitrogen fixation that consumes between 3% and 5% of the world's annual natural gas production.

Producing fertilizers using the Haber-Bosch process alone accounts for 1% to 2% of the world's annual energy supply and is responsible for 2% to 3% of global CO_2 emissions.[10] Similarly, the production of hydrogen for use in hydrogen fuel cells relies on industrial methods for splitting water molecules into hydrogen and oxygen. But these existing methods are energy-intensive, rely on expensive and rare metals, and create waste carbon, which limits the use of hydrogen as a clean, green source of energy.[11]

Quantum computers could streamline both processes by enabling scientists to discover new catalyst materials that would reduce energy requirements for ammonia production and water-splitting. This would result in technological breakthroughs for producing fertilizers and hydrogen fuel cells.

Get prepared for quantum computing

Given the current rate of advancement and the fact that only 1,000 or so qubits may be needed to simulate molecules, chemical reactions, and materials, quantum computers will be able to meaningfully tackle computational chemistry problems sooner rather than later. Organizations that use computational chemistry or traditional materials discovery to conduct experimental studies and predict the structure of molecules may have a good business case for taking a proactive approach to quantum computing. As next steps, consider the following:

- **Understand industry impact.** Learn about quantum computing's potential repercussions in your industry. What complex problems could quantum help you solve? Be aware of important technology developments and pay attention to how others in your field are investing in and experimenting with quantum technologies.

- **Prioritize computational chemistry use cases.** Given that quantum computers may be useful for computational chemistry before they're useful for other applications, start exploring use cases today. Prioritize those that can deliver high value and can be addressed by quantum computers.

- **Investigate the quantum ecosystem.** A growing number of technology vendors, startups, and independent and academic research labs are working to commercialize capabilities to simplify quantum-based computational chemistry use cases. Through research and collaboration with internal and external quantum experts, explore and understand how your organization could leverage the quantum ecosystem and its resources.

- **Develop a strategy.** Bring together existing talent with the appropriate skills and knowledge to develop a quantum strategy. Even if the strategy is to take no immediate action, determine a trigger event—for example, an announcement from a competitor or the achievement of a certain technological milestone—that will serve as a prompt for further quantum investments and exploration.

- **Monitor technology and industry developments.** Decide who on your team will lead the quantum charge when it's time to engage, and make sure they stay up to date on quantum developments and research. They can help you refine your strategy as events warrant. Keep in mind your stated trigger event and don't let it pass by without taking the appropriate action.

Like many other emerging technologies, quantum computing is expected to bring many advantages to early movers. By strategically beginning to explore quantum computing's opportunities today, organizations that leverage quantum chemistry can get a head start on their competitors.

Endnotes

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Quantum technologies, and their heady promise, are in the news. With the promise of breakthrough innovations in drug development, financial modeling, climate change, traffic optimization, machine learning, batteries, and more, is now the time to invest? By the same token, how much concern is warranted about quantum computing's future ability to break today's encryption standards? As business and technology leaders strive to make thoughtful choices for today and tomorrow, what needs to be done to get ready for a quantum-enabled future? What future risks need to be considered—and potentially mitigated—starting today? Contact the authors for more information or read more about our quantum computing services on Deloitte.com.

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