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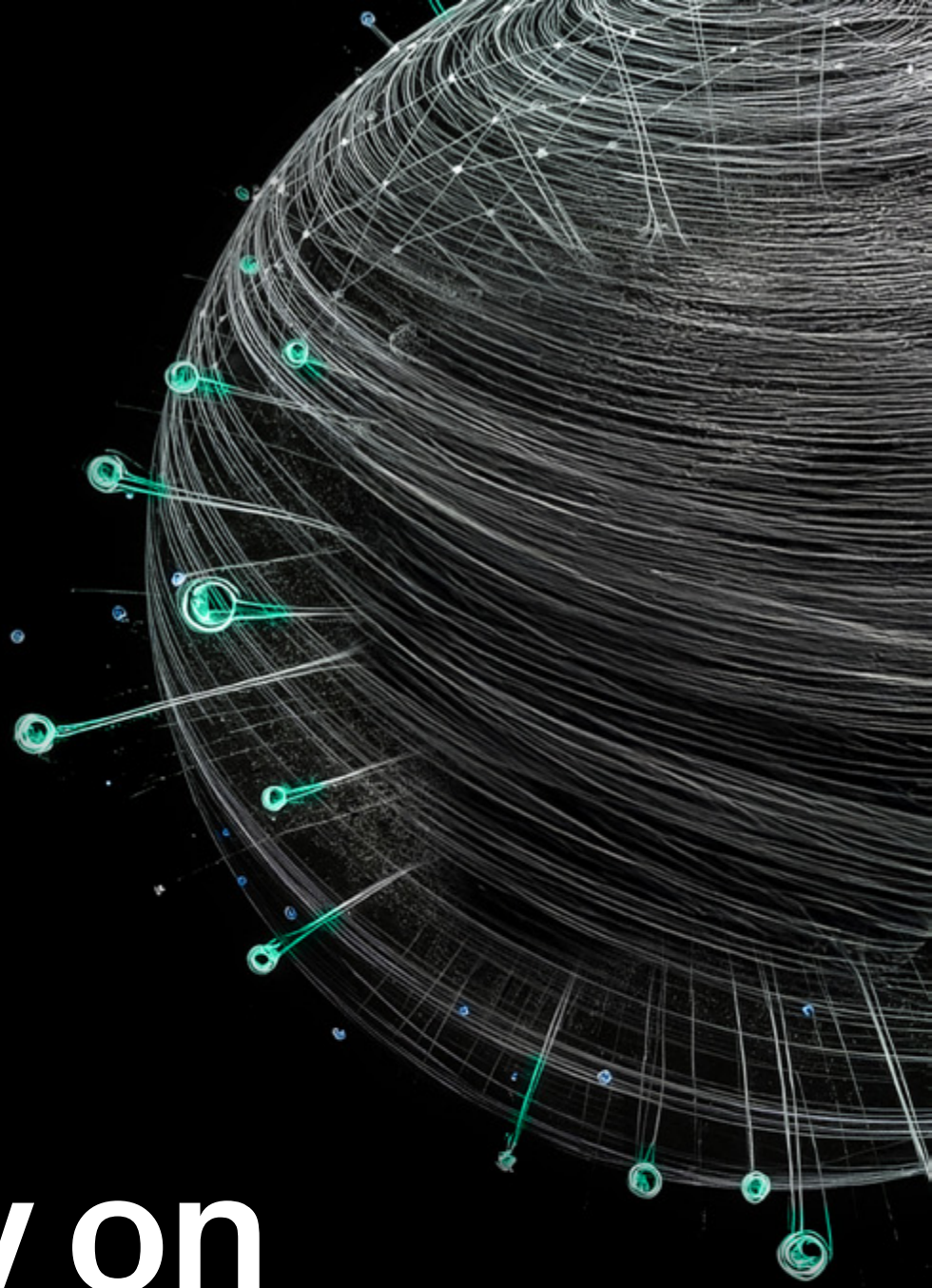

Study on Battery Simulation

Technical Whitepaper

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Summary

The research by IQM presents a hybrid method to simulate complex quantum systems, particularly in battery chemistry. This method combines quantum and classical computing to reduce the required number of qubits while preserving accuracy. Applied to the reductive decomposition of ethylene carbonate in lithium-ion batteries, opening doors to more efficient battery design.

Building Better Car Batteries

Shaping the future of energy storage through quantum computing, and the possibilities look promising.

In the rapidly evolving electric vehicle (EV) market, the race is on to develop cost-efficient, mass-market EVs with longer driving ranges, faster charging capabilities, and durable batteries that meet stringent environmental standards.

In the fast-growing electric vehicle (EV) market, the race is on to create affordable, mass-market EVs with longer ranges, faster charging, and durable batteries that meet high environmental standards.

Currently, one in five cars sold is electric, with the market projected to expand from $500 billion in 2023 to $1.9 trillion by 2032. Despite challenges like supply chain constraints and raw material shortages, EV sales surged in 2023. To address resource concerns, manufacturers are innovating with batteries that have lower cobalt content but higher energy density. These advancements, sometimes backed by billions in R&D, promise benefits for both the environment and the industry's profitability.

While progress has been significant, the challenges are still vast. Now, an exciting scientific endeavor aims to tackle these hurdles by leveraging quantum computing for a transformative breakthrough in battery technology.

In our project, we have developed a new hybrid quantum-classical method and have used it to study the breakdown of ethylene carbonate (EC) in lithium-based batteries. EC is one of the most commonly found solvents for electrolytes used in lithium-ion batteries. While EC is not stable against reductive decomposition by Li, the formation of a solid-electrolyte interface (SEI) alleviates this problem to some extent by passivating the electrode and thereby suppressing the reaction. Understanding the reductive decomposition of EC and the role of the SEI in this process is a key factor in understanding battery safety and performance thus enabling the development of better performing batteries. From simulations we found that our method achieved chemical accuracy using only a small fraction of the original number of required qubits. Consequently, we have shown that future large-scale quantum chemistry calculations can potentially be guided by quantum states prepared on much smaller quantum computers, thus accelerating the path to useful quantum computations.

Read the publication from here: https://arxiv.org/pdf/2408.06160

“Remarkably, our method allows one to compress the truly quantum part of the system down to the size of the available quantum device and then utilize the resulting quantum state to successfully guide a much larger classical calculation ”

– **Fedor Šimkovic,**
Team Lead Fermionic Simulation,
IQM Quantum Computers

The research findings are important for society at large as well. Not all energy storage systems are designed for transportation. Batteries, particularly lithium-based ones, are used in everyday devices like mobile phones, laptops, and power banks. In the near future, they may even power smaller commercial airplanes. Additionally, batteries play a crucial role in energy grid security, helping to adapt to market and weather changes while integrating renewable energy sources.

The rate at which demand for lithium-ion batteries is increasing is staggering. Electric vehicles (EVs) remain the most critical application, accounting for over 90% of the growth in the lithium-ion sector between 2015 and 2023. Additionally, the global battery storage market doubled in 2023. When volumes and scale are this large, even small cost savings in manufacturing or improvements in performance and durability can greatly benefit both the bottom line and the environment.

From classical to quantum

Quantum computing has long been touted as a game-changer for industries that rely on understanding complex chemical interactions, and battery technology is no exception. Traditional computing methods, though powerful, are inherently limited when it comes to simulating and predicting the behavior of atoms and molecules in battery materials due to the growing computational space and the fermionic nature of electrons involved. Classical simulations require immense computing power, yet they still fall short of accurately modeling the intricate interactions within battery chemistries. This is where quantum computing is stepping in, offering a potential solution to these limitations.

Hybrid quantum-classical approach is leading the way

In the future, quantum computers are expected to excel in simulating complex chemical systems, offering insights into molecular interactions. Unlike classical computers, which struggle with the enormous computational demands of large-scale simulations, quantum computers will be able to model these systems with much higher accuracy and predictability. This progress will make quantum computing a key tool for scientists exploring complex quantum systems, especially those involving strongly correlated particles. As a result, it will also open new possibilities for discovering entirely new battery chemistries that could completely transform energy storage performance, while also reducing reliance on labor-intensive manual benchwork and cutting down on costs, material use and energy. This synergy between quantum and classical systems holds the potential to accelerate innovation in ways that were previously unimaginable, driving significant progress in chemistry and beyond.

The current generation of quantum computers, known as noisy intermediate-scale quantum (NISQ) devices, still face challenges, including limited qubit numbers and less-than-perfect operations. To overcome these issues, hybrid quantum-classical approaches have been developed. These strategies combine the strengths of both classical and quantum computing, dividing the workload between the two. For example, some methods use classical computers to optimize quantum circuits or employ quantum devices as solvers within larger classical frameworks. For this reason, hybrid approaches that blend classical and quantum computing are currently the most effective way to tackle these challenges.

“Using quantum computers in industry will require bridging the gap between the quality of the machines and the resource demands of the best algorithms. Through this work, we are looking at ways to shrink this gap from the algorithmic perspective and hopefully provide inspiration for others interested in reducing the resource demand of quantum algorithms.”

– **Matthew Kiser,**
Researcher

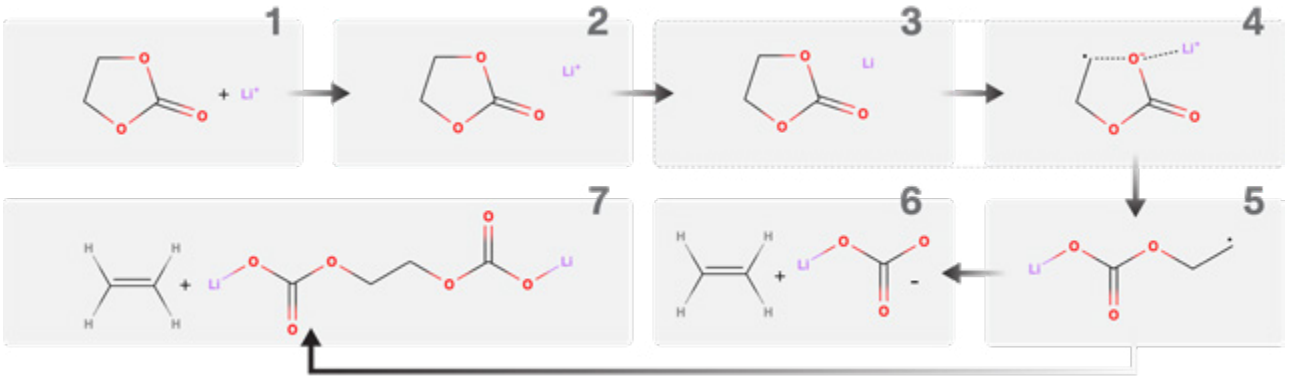


Figure 1: Visual representation of the reductive decomposition of EC in the presence of a lithium ion

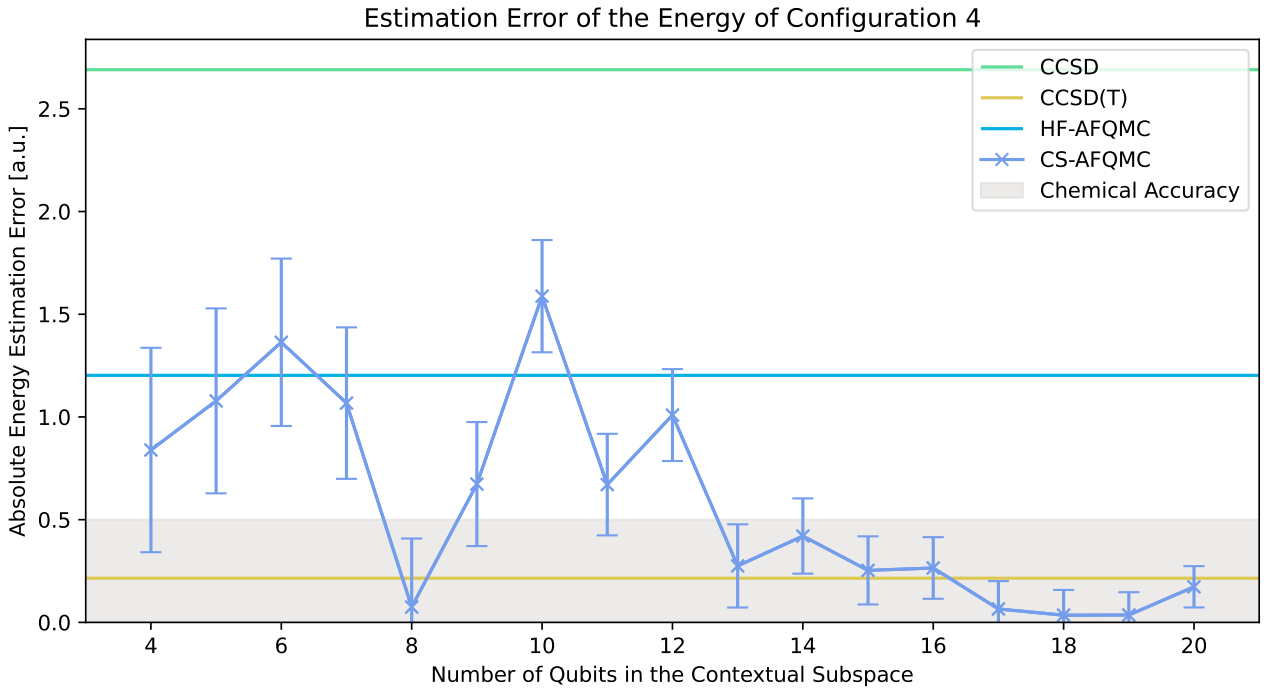


Figure 2: Configuration 4 of Fig. 1. CS-AFQMC converges to the ground-state energy as a function of the number of qubits in the quantum part of the calculation. The algorithm needs 13 qubits to converge within chemical accuracy and 17 qubits to improve upon CCSD(T), a gold-standard classical method. An active space of 32 qubits was used, constructed from a 236 spin-orbital system in the cc-pVDZ basis.

As a starting point, the research teams have chosen Auxiliary-field Quantum Monte Carlo (AFQMC), a classical workhorse in quantum chemistry and condensed matter physics used to compute ground state energies. This algorithm mitigates the infamous fermionic sign problem by guiding Monte Carlo walkers through their overlaps with a trial state that approximates the ground state. A hybrid quantum-classical version of this algorithm, known as QC-AFQMC, has been previously proposed, where the trial state is prepared on a quantum computer. The key advantage is that if a quantum-prepared trial state surpasses the quality of available classical alternatives, the overall hybrid approach improves upon them. The computational task is divided so that the classical and quantum components are utilized to their respective advantages, with no complex communication required between the two.

In the preprint, the teams have demonstrated how quantum trial states prepared in contextual subspaces (CS) can further reduce the required quantum resources needed for guiding much larger AFQMC calculations. The CS method works by splitting the original problem into quantum (contextual) and classical (non-contextual) parts, utilizing artificially defined symmetries to significantly reduce the size of the quantum portion at the cost of some approximation. This method has previously been applied to compute ground state energies of small molecules.

Our approach goes beyond current capabilities by accurately simulating a chemical reaction involving ethylene carbonate molecules and lithium ions using just 13 qubits in a contextual subspace, from a 32-qubit active space. It demonstrates the potential of our technique in hybrid quantum-classical as well as quantum-inspired settings, suggesting it may be able to handle much larger systems than existing methods.

More performance, yet environmentally friendly

Despite the current state of quantum hardware which still struggles with large-scale industrial applications, breakthroughs may be on the horizon.

As our collaboration demonstrates, we have developed a method that significantly reduces the resource demands of quantum systems. This innovation may allow even modest-sized quantum computers to simulate critical battery reactions, bringing us closer to the development of advanced battery materials.

From our lab to simulations...

Over the years, the process of developing new battery technologies has evolved from physical lab experiments to computer simulations, significantly reducing the time and cost associated with innovation. Now, with the emergence of quantum computing, we are at the edge of another major shift.

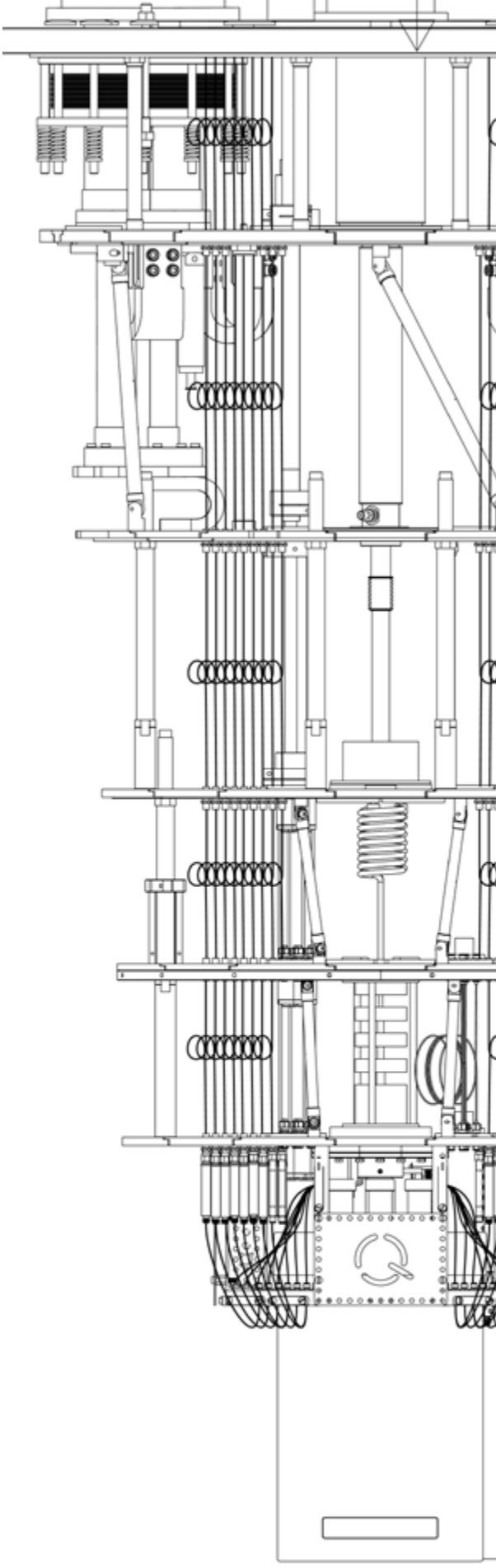
... and into the world

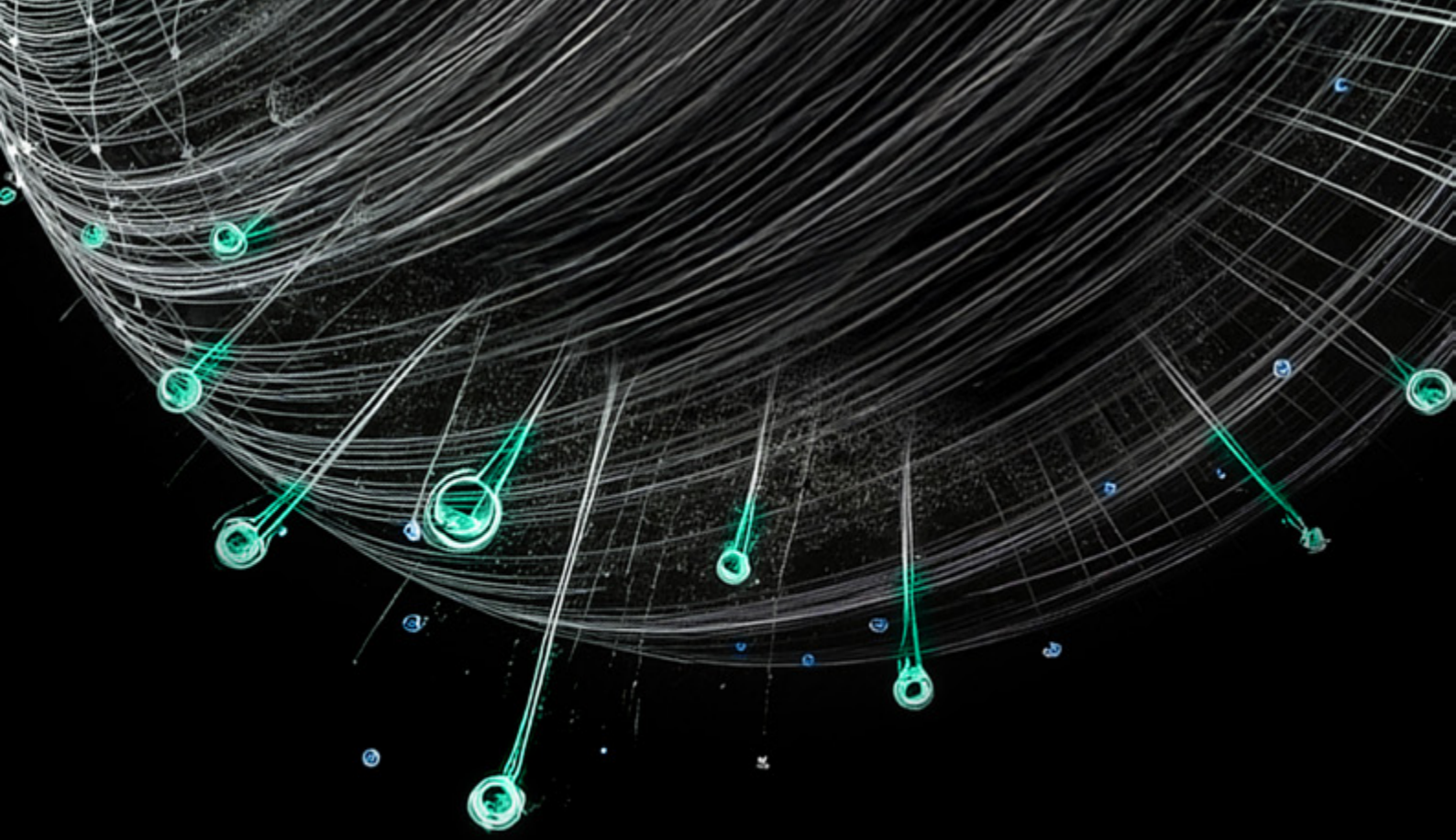
In conclusion, the scientific project represents a significant step forward in the quest for better electric car batteries. As quantum computing progresses, the vision of more efficient, longer lasting, and eco-friendly batteries could soon be reality, reshaping the future of electric mobility for generations to come. This progress promises to revolutionize transportation, while also laying the foundation for a more sustainable and prosperous future for everyone.

About IQM

We build and deliver quantum computers for the world

At IQM, we are pioneers in quantum computing, founded in 2018 with a vision to create impactful quantum solutions for humanity's future. Our diverse, international team is dedicated to establishing Europe as a leader in quantum technology. We focus on sustainable practices and collaborate with research institutions, universities, and enterprises to advance the capabilities of quantum computers. Our mission is to develop innovative solutions that prioritize human welfare and drive transformation across various industries.





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